Supporting Information

Manganese catalyzed chemo-selective synthesis of acyl cyclopentenes: a combined experimental and computational investigation

Koushik Sarkar,[a] Prativa Behera,[b] Lisa Roy,[b,*] and Biplab Maji [a,*]

[a] Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India

[b] Institute of Chemical Technology Mumbai – IOC Odisha Campus Bhubaneswar, Bhubaneswar 751013, India

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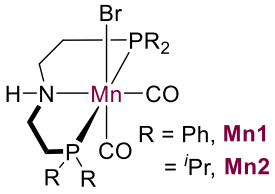
1. General information

All the reactions were conducted under an inert atmosphere. Oven-dried glassware is used. Solvents were dried under the standard protocol. All the solvents were degassed and stored over activated molecular sieves (4 Å). The chemicals were purchased from Avra Synthesis, Sigma-Aldrich, TCI India, Alfa Aeser, and BLD Pharma without further purification unless otherwise mentioned. Ligands and metal complexes were prepared according to the previously published procedures.

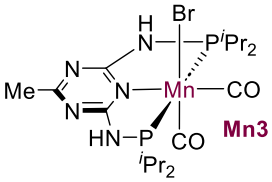
^{1}H, ^{13}C, NMR spectra were collected using BRUKER (^{1}H: 500 MHz, ^{13}C: 126 MHz) and JEOL (^{1}H: 400 MHz, ^{13}C: 101 MHz) instrument. NMR data was taken in the ppm unit and referenced against the solvent residual peaks. Coupling constants (J) are reported in Hertz (Hz). Coupling patterns are indicated as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), td (triplet of doublet), or m (multiplet). We also checked reaction optimization using Thermo-fisher scientific GCMS with Column DB5MS (30 m × 0.25 mm × 0.5 mm). Mass spectral analyses were done in Bruker micrOTOF-Q II Spectrometer. For thin-layer chromatography (TLC) analysis, Merck precoated TLC plates (silica gel 60 F254/ 0.25 mm) were used. Visualization was accomplished by UV light (254 nm). All the kinetics study has been done using gas chromatography using an appropriate internal standard.

2. Catalyst preparation

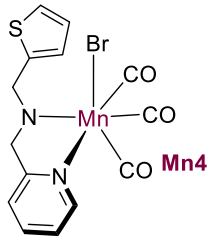
All the catalysts **Mn1-Mn4** were prepared according to the previous reports.[1-5]



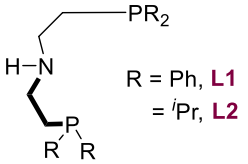
R = Ph, **Mn1**
= ^{i}Pr, **Mn2**



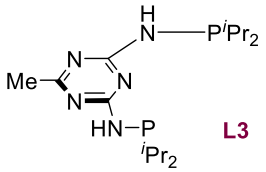
Mn3



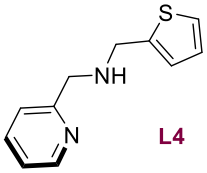
Mn4



R = Ph, **L1**
= ^{i}Pr, **L2**



L3



L4

Mn1: In a 20 mL Schlenk tube ^{Ph}MACHO (**L1**, 0.1 mmol) was taken in 3 mL toluene under Argon atmosphere, followed by the addition of $Mn(CO)_5Br$ (0.11 mmol). The reaction was stirred for 24 h at 110 °C. The reaction mixture was then cooled to ambient temperature, evaporated under a vacuum, washed with hexane, and dried once more under a vacuum. A yellowish-colored solid catalyst was prepared with a yield of 92%.

Mn2: In a 20 mL Schlenk tube $^{i\text{-}Pr}$MACHO (**L2**, 0.1 mmol) was taken in 3 mL toluene under Argon atmosphere, followed by the addition of Mn $(CO)_5Br$ (0.11 mmol). The reaction mixture was stirred for 24 h at 110 °C. The reaction mixture was then cooled to ambient temperature, evaporated under a vacuum, washed with hexane, and dried once more under a vacuum. A yellowish color solid catalyst was prepared with a yield of 90%.

Mn3: In a 20 mL Schlenk tube (**L3**, 0.1 mmol) was taken in 3 mL toluene under Argon atmosphere, followed by the addition of Mn $(CO)_5Br$ (0.11 mmol). The reaction was stirred for 24 h at 110 °C. After that, the reaction mixture was cooled to room temperature, followed by evaporation under vacuum, then washed with hexane, and again dried under vacuum. A yellowish color solid catalyst was prepared with a yield of 98%

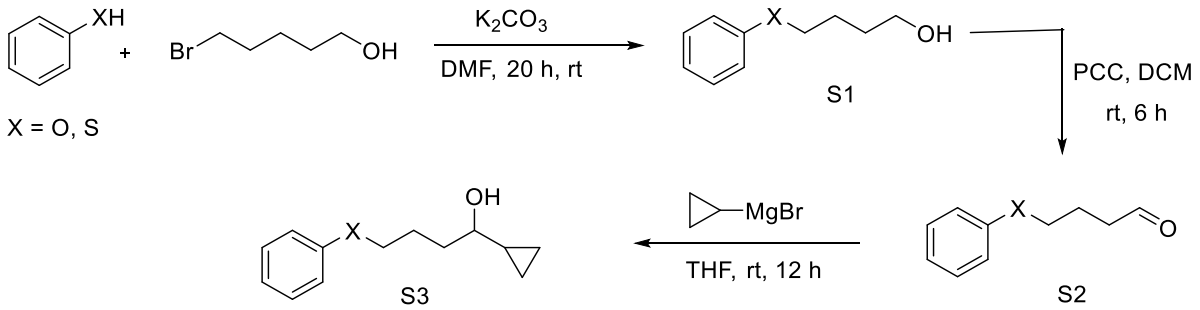
Mn4: In a 20 mL Schlenk tube (**L4**, 0.1 mmol) was taken in 3 mL THF under Argon atmosphere, followed by the addition of Mn $(CO)_5Br$ (1.1 equiv.) reaction was stirred for 3 h at 80 °C. After that, the reaction mixture was cooled to room temperature, followed by evaporation under vacuum, and then washed with hexane. An orange-colored solid catalyst was prepared with a yield of 98%.

3. Synthesis of starting materials

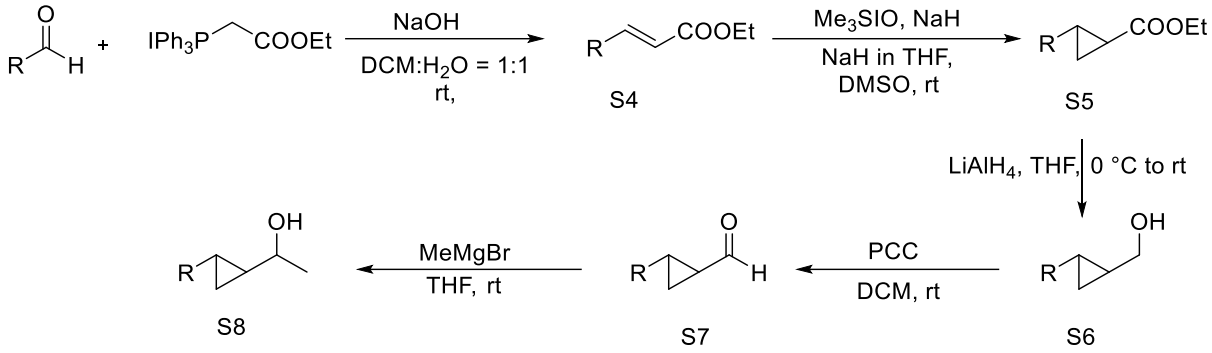
General Procedure A (GPA): In a 25 ml oven-dried Schlenk tube, magnesium turnings (6 mmol, dried), and iodine (20 mol%) were poured into 7 mL THF/Et_2O followed by dropwise addition of aryl halide (3 mmol). The mixture was refluxed for 1 h. Into the prepared Grignard reagent, aldehyde (3 mmol in 3 mL THF) was added dropwise at 0 °C and then stirred at room temperature for 3 h. 7 mL of NH_4Cl solution was used to quench the reaction mixture and washed with THF/Et_2O (10 x 2 mL). Dried with Na_2SO_4, evaporated in a vacuum, and purified by column chromatography using Hexane and AcOEt to obtain the product.

General Procedure B (GPB): In a 25 ml oven-dried Schlenk tube, magnesium turnings (6 mmol, dried) and iodine (20 mol%) were poured into 7 mL THF/Et_2O followed by dropwise addition of alkyl halide (3 mmol). The mixture was refluxed for 3 h. Into the prepared Grignard reagent, aldehyde (3 mmol in 3 mL THF) was added dropwise at 0 °C and then stirred at room temperature for 3 h. 7 mL of NH_4Cl solution was used to quench the reaction mixture and washed with THF/Et_2O (10 x 2 mL). Dried with Na_2SO_4, evaporated in a vacuum, and purified by column chromatography using Hexane and Et_2O to obtain the product.

General Procedure C (GPC). In a 50 mL round bottom flask, phenol or thiophenol (5 mmol) was stirred for 30 min in a 10 mL DMF containing K_2CO_3 (2 equiv.) solution at room temperature. In the reaction mixture 5-bromopentanol (4 mmol) was added drop wisely, and the mixture was stirred for 20 h at room temperature. After purification of the reaction mixture, we obtained **S1**, which is further oxidized using PCC (1 equiv.). in DCM (20 mL) for 6 h at room temperature, then purified the mixture to obtain **S2**. Cyclopropylmagnesiumbromide (1.5 equiv.) was added slowly into the solution 5 mL THF containing **S2** at room temperature. The reaction mixture was stirred for 12 h. The reaction mixture was quenched by aqueous NH_4Cl (10 mL) and washed with Ether (10 mL). The organic part was concentrated under vacuum and purified by column chromatography using 10% EtOAc in Hexane to obtain **S3**.

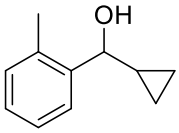


General procedure D (GPD). In a 100 mL round bottom flask, Witting salt (1 equiv.) was added to NaOH (2 equiv.) containing 30 mL of DCM and 20 mL of H_2O mixture at room temperature. After 15 min stirring, aldehyde (10 mmol) was added, and the reaction was kept for 12 h. The organic part was separated, dried in a vacuum, and the obtained crude olefin **S4** was used without further purification. A THF (0.6 M) solution of NaH (1.05 equiv.) and Me_3SIO (1.15 equiv.) was stirred for 1 h at room temperature. A DMSO (1 M) solution of the olefin **S4** was added dropwise. The total reaction mixture was then stirred for 16 h at 55 °C. The reaction mixture was quenched with water (100 mL) and washed with Ether (20 mL). The compound was purified by column chromatography to obtain **S5**. The reduction of **S5** with $LiAlH_4$ (1.5 equiv.) in 10 mL THF for 12 h at room temperature yields the alcohol **S6**. The oxidation of **S6** was carried out with PCC (1.5 equiv.) in 20 mL DCM for 6 h at room temperature. The reaction mixture was filtered and purified by flash column chromatography to obtain **S7**. Freshly prepared **S7** was treated with MeMgBr (1.5 equiv.) in 10 mL THF solution at room temperature, and the mixture was stirred for 6 h. Quenched the reaction mixture with aqueous NH_4Cl (10 mL) and washed with 20 mL (10 mL x 2 times) ether. The organic part was purified by column chromatography using 10% EtOAc in hexane to obtain **S8**.

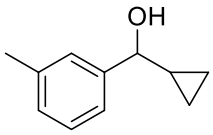


3.1 Characterization data of the starting materials

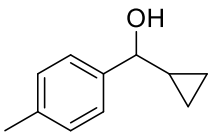
Cyclopropyl(o-tolyl)methanol:[6] Synthesized according to **GPA**. A colorless liquid was separated through column chromatography using 10% EtOAc in hexane as the eluent. Yield = 85% (4.2 mmol, 688 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.25 – 7.14 (m, 3H), 4.44 (d, *J* = 7.6 Hz, 1H), 2.38 (s, 3H), 2.00 (s, 1H), 1.32 (qt, *J* = 8.0, 5.1 Hz, 1H), 0.66 – 0.59 (m, 1H), 0.55 – 0.48 (m, 1H), 0.42 – 0.31 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.5, 135.4, 130.5, 127.5, 126.2, 126.1, 74.1, 19.5, 17.7, 3.4, 2.2.



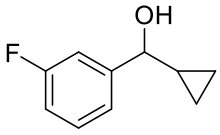
Cyclopropyl(m-tolyl)methanol:[6] Synthesized according to **GPA**. A colorless liquid was separated through column chromatography using 10% EtOAc in hexane as the eluent. Yield = 80% (2.4 mmol, 389.0 mg) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 – 7.22 (m, 3H), 7.14 (d, *J* = 7.3 Hz, 1H), 4.00 (d, *J* = 8.4 Hz, 1H), 2.40 (s, 3H), 2.01 (s, 1H), 1.25 (dq, *J* = 11.3, 4.1 Hz, 1H), 0.72 – 0.63 (m, 1H), 0.58 (tt, *J* = 8.7, 4.9 Hz, 1H), 0.50 (dq, *J* = 9.8, 4.9 Hz, 1H), 0.40 (dq, *J* = 9.8, 4.9 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 143.9, 138.0, 128.3, 126.8, 123.2, 78.6, 21.6, 19.2, 3.7, 2.9.



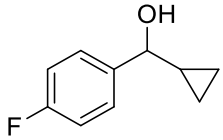
Cyclopropyl(p-tolyl)methanol:[6] Synthesized according to **GPA**. A colorless liquid compound was obtained with yield = 92% (2.74 mmol, 476 mg). The compound was separated through column chromatography using 10% EtOAc in hexane.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 3.98 (d, *J* = 8.3 Hz, 1H), 2.37 (s, 3H), 1.25-1.18 (m, 1H), 0.66-0.61 (m, 1H), 0.57-0.52 (m, 1H), 0.49-0.44 (m, 1H), 0.39 – 0.33 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.1, 141.0, 137.2, 129.1, 126.1, 78.5, 21.2, 19.2, 3.7, 2.9.



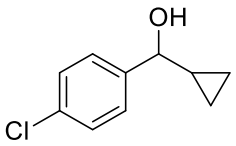
Cyclopropyl(3-fluorophenyl)methanol: Synthesized according to **GPA**. A colorless liquid compound was obtained with yield = 65% (1.95 mmol, 323.7 mg). The compound was separated through column chromatography using 10% EtOAc in hexane. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.37 – 7.25 (m, 1H), 7.23 – 7.10 (m, 2H), 6.99 (td, *J* = 8.3, 2.5 Hz, 1H), 4.02 (d, *J* = 8.4 Hz, 1H), 2.20 (s, 1H), 1.25 – 1.10 (m, 1H), 0.70 – 0.53 (m, 2H), 0.53 – 0.33 (m, 2H). **^{13}C NMR** (126 MHz, CDCl3) δ 162.3 (J = 245.7 Hz), 139.7 (J = 2.52 Hz), 127.8 (*J* = 8.8 Hz), 115.25 (*J* = 20.16 Hz), 78.00, 19.4, 3.7, 3.0.



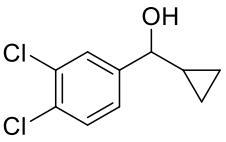
Cyclopropyl(4-fluorophenyl)methanol:[6] Synthesized according to **GPA**. A light yellowish color liquid was obtained with yield = 65% (1.95 mmol, 323.7 mg). The compound was separated through column chromatography using 10% EtOAc in hexane. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 8.3, 5.4 Hz, 2H), 7.03 (t, *J* = 8.5 Hz, 2H), 3.99 (d, *J* = 8.4 Hz, 1H), 2.04 (d, *J* = 2.7 Hz, 1H), 1.21-1.16 (m, 1H), 0.66-0.61 (m, 1H), 0.59-0.54 (m, 1H), 0.48-0.44(m, 1H), 0.38-0.33 (m, 1H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.3 (d, *J* = 245.4 Hz), 139.7 (d, *J* = 3.0 Hz), 127.8 (d, *J* = 8.2 Hz), 115.2 (d, *J* = 21.3 Hz).



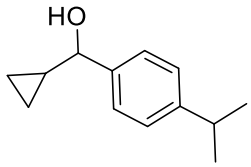
(4-chlorophenyl)(cyclopropyl)methanol:[6] Synthesized according to **GPA.** A light yellowish color was obtained with yield = 60% (1.8 mmol, 327 mg). The compound was purified through column chromatography using 10% EtOAc in hexane.**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 – 7.29 (m, 4H), 3.97 (d, *J* = 8.4 Hz, 1H), 1.21 – 1.11 (m, 1H), 0.66 – 0.52 (m, 2H), 0.54-0.47 (m, 1H), 0.27-0.19 (m, 1H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.4, 133.2, 128.6, 127.5, 77.9, 19.4, 3.7, 3.0



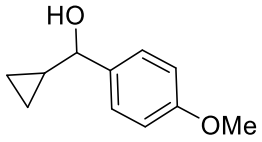
Cyclopropyl(3,4-dichlorophenyl)methanol:[6] Synthesized according to **GPA.** Light yellowish color was obtained with yield = 55% (1.65 mmol, 358 mg). The compound was purified through column chromatography using 10% EtOAc in hexane. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 (s, 1H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.24 (s, 1H), 3.96 (d, *J* = 8.5 Hz, 1H), 2.07 (t, *J* = 3.1 Hz, 1H), 1.17-1.09 (m, 1H), 0.64-0.59 (m, 2H), 0.49 – 0.34 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.2, 132.5, 131.4, 130.4, 128.1, 125.5, 19.5, 3.7, 3.2



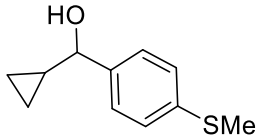
Cyclopropyl(4-isopropylphenyl) methanol: Synthesized according to **GPA.** A colorless liquid was obtained with yield = 85% (2.55 mmol, 484 mg). The compound was purified through column chromatography using 10% EtOAc in Hexane. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 10 Hz, 2H), 7.23 (d, J = 5 Hz, 2H), 3.99 (d, *J* = 8.3 Hz, 1H), 2.94-2.89 (m, 1H), 1.26 (d, *J* = 7.0 Hz, 6H), 0.67-0.61 (m, 1H), 0.58-0.53 (m, 1H), 0.51 – 0.44 (m, 1H), 0.40 – 0.34 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.4, 126.6, 126.2, 78.6, 34.0, 24.1, 19.1, 3.7, 3.0. **HRMS (ESI-TOF) m/z**: $[M+Na]^+$ Calcd for $[C_{13}H_{18}O]$: 213.1286, found 213.1268.



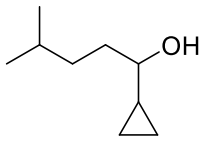
Cyclopropyl(4-(methylthio)phenyl)methanol:[6] Synthesized according to **GPA.** White solid compound was separated through column chromatography using 10% EtOAc in hexane as an eluent. Yield = 65% (1.95 mmol, 378 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 4.00 (d, *J* = 8.3 Hz, 1H), 2.50 (s, 3H), 1.25-1.18 (m, 1H), 0.68 – 0.62 (m, 1H), 0.60 – 0.54 (m, 1H), 0.50-0.45 (m, 1H), 0.40-0.35 (m, 1H). **13C NMR** (126 MHz, $CDCl_3$) δ 159.0, 136.1, 128.1, 127.3, 116.1, 114.8, 113.7, 113.2, 78.2, 55.3, 19.0, 3.6, 2.7.



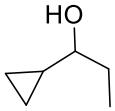
Cyclopropyl(4-(methylthio)phenyl)methanol: Synthesized according to **GPA.** A white solid was separated through column chromatography using 10% EtOAc in hexane as an eluent. Yield = 65% (1.95 mmol, 378 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 4.00 (d, *J* = 8.3 Hz, 1H), 2.50 (s, 3H), 1.25-1.18 (m, 1H), 0.68 – 0.62 (m, 1H), 0.60 – 0.54 (m, 1H), 0.50-0.45 (m, 1H), 0.40-0.35 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.9, 137.6, 127.7, 127.6, 126.9, 126.7, 78.3, 19.3, 16.1, 3.7, 2.9. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{11}H_{15}OS]$: 195.0844, found 195.0834.



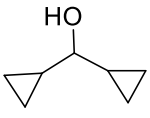
1-cyclopropyl-4-methylpentan-1-o: Synthesized according to **GPB.** A colorless oily liquid was obtained with yield = 80% (2.4 mmol, 340.8 mg) yield. This compound was isolated through column chromatography using 10% Et_2O in hexane as an eluent. Careful evaporation is required during vacuum. **^{1}H NMR** (400 MHz, CDCL3) δ 2.86 – 2.79 (m, 1H), 1.62-1.58 (m, 4H), 1-34-1.23 (m, 2H), 0.90 (dd, *J* = 6.7, 2.5 Hz, 6H), 0.55 – 0.45 (m, 2H), 0.29 – 0.18 (m, 2H). **^{13}C NMR** (101 MHz, CDCl3) δ 35.2, 34.98, 28.30, 22.81, 22.67, 18.17, 2.95, 2.54. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_9H_{19}O]$: 143.1436, found 143.1436.



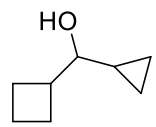
1-cyclopropylpropan-1-ol:[7] Synthesized according to **GPB.** A colorless oily liquid was obtained. This compound was isolated through column chromatography using 10% Et_2O in hexane as an eluent. Careful evaporation is required during vacuum. Yield = 60% (1.8 mmol, 180 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.74-2.70 (m, 1H), 2.10 (s, 1H), 1.63 – 1.46 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H), 0.83-0.78 (m, 1H), 0.46-0.37 (m, 2H), 0.24 – 0.10 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 78.1, 30.1, 17.5, 10.1, 2.7, 2.3.



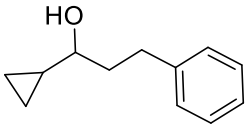
Dicyclopropylmethanol:[7] Synthesized according to **GPB.** A colorless oily liquid was obtained. This compound was isolated through column chromatography using 10% Et_2O in hexane as an eluent. Careful evaporation is required during vacuum. Yield = 60% (1.8 mmol, 202 mg).**^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.41 (t, *J* = 8.0 Hz, 1H), 1.79 (s, 1H), 1.02-0.96 (m, 2H), 0.50-0.44 (m, 4H), 0.30 – 0.23 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 80.0, 17.0, 2.2, 2.1.



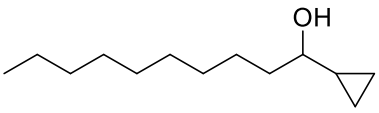
Cyclobutyl(cyclopropyl)methanol:[7]Synthesized according to **GPB.** A colorless oily liquid was obtained. This compound was isolated through column chromatography using 10% Et_2O in hexane as an eluent. Careful evaporation is required during vacuum. Yield = 64% (3.2 mmol, 403 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.84 – 2.79 (m, 1H), 2.55 – 2.44 (m, 1H), 2.04 – 1.77 (m, 6H), 1.59 (s, 1H), 0.83 – 0.74 (m, 1H), 0.51 – 0.38 (m, 2H), 0.29 – 0.20 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 80.0, 41.6, 24.7, 24.6, 18.4, 15.6, 2.6, 1.5.



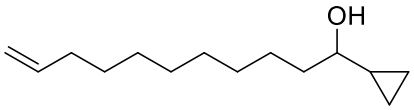
1-cyclopropyl-5-(phenylthio)pentan-1-ol:[7] Synthesized according to **GPB.** A colorless liquid was separated through column chromatography using Et_2O and hexane. Yield = 55% (2.75 mmol, 484 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 2H), 7.24 – 7.15 (m, 3H), 2.92 – 2.68 (m, 3H), 1.97 – 1.89 (m, 2H), 1.67 – 1.62 (m, 1H), 0.99 – 0.90 (m, 1H), 0.57-0.46 (m, 2H), 0.30 – 0.17 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 151.6, 135.9, 128.4, 125.6, 34.4, 30.5, 24.7, 21.3.



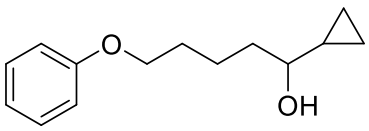
1-cyclopropyldecan-1-ol: Synthesized according to **GPB.** A colorless liquid was obtained with yield = 65% (1.95 mmol, 386 mg). The compound was separated through column chromatography using 10% Et_2O in hexane. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.88-2.82 (m, 1H), 1.62 – 1.52 (m, 4H), 1.27 (d, *J* = 6.3 Hz, 14H), 0.88 (t, *J* = 6.7 Hz, 4H), 0.54-0.47 (m, 2H), 0.28-0.19 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 37.4, 32.0, 29.9, 29.8, 29.5, 25.9, 22.8, 18.2, 14.2, 2.9, 2.5.



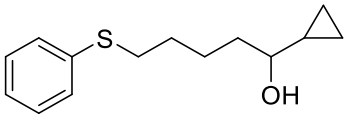
1-cyclopropylundec-10-en-1-ol: Synthesized according to **GPB.** A colorless liquid was obtained with yield = 66% (1.8 mmol, 787 mg). The compound was separated through column chromatography using 10% EtOAc in hexane. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.85-5.77 (m, 1H), 4.98 (d, *J* = 17.1 Hz, 1H), 4.92 (d, *J* = 10.1 Hz, 1H), 2.85 (q, *J* = 6.9 Hz, 1H), 2.03 (q, *J* = 7.2 Hz, 2H), 1.61-1.53 (m, 3H), 1.37 (t, *J* = 6.7 Hz, 3H), 1.29 (s, 8H), 0.91-0.85 (m, 1H), 0.54-0.45 (m, 2H), 0.35 – 0.12 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 139.4, 114.2, 37.4, 33.9, 29.9, 29.7, 29.6, 29.3, 29.1, 25.9, 18.2, 2.9, 2.5. **HRMS (ESI-TOF) m/z**: $[M+Na]^+$ Calcd for $[C_{13}H_{18}O]$: 213.1286, found 213.1268.



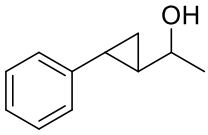
1-cyclopropyl-5-phenoxypentan-1-ol: Synthesized according to **GPC.** The compound was isolated as a colorless liquid through column chromatography using 10% EtOAc in hexane with yield = 54% (1.62 mmol, 356.4 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 2H), 6.96 – 6.87 (m, 3H), 3.98 (t, *J* = 6.5 Hz, 2H), 2.89 (dt, *J* = 8.4, 5.8 Hz, 1H), 1.84-1.80 (m, 2H), 1.70 – 1.59 (m, 4H), 0.94-0.89 (m, 1H), 0.59 – 0.44 (m, 2H), 0.32 – 0.19 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.2, 129.5, 120.6, 114.6, 67.9, 37.0, 29.5, 22.5, 18.1, 2.9, 2.6.



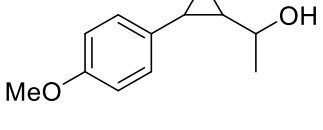
1-cyclopropyl-5-(phenylthio)pentan-1-ol: Synthesized according to **GPC.** The compound was isolated as a colorless liquid through column chromatography using 10% EtOAc in hexane with yield = 62% (1.86 mmol, 439.6 mg)**. ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 6.9 Hz, 2H), 7.31 – 7.28 (m, 2H), 7.22 – 7.14 (m, 1H), 2.96 (td, *J* = 7.3, 2.7 Hz, 2H), 2.87 (s, 1H), 1.70 (d, *J* = 8.5 Hz, 2H), 1.62 (d, *J* = 9.8 Hz, 3H), 1.50 (s, 1H), 0.90 (dt, *J* = 8.6, 4.4 Hz, 1H), 0.55-0.49 (m, 2H), 0.36 – 0.11 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 129.2, 129.0, 125.9, 36.8, 33.8, 29.5, 25.1, 18.2, 2.9, 2.6. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $[C_{14}H_{20}OS]$: 259.1133, found 259.1148.



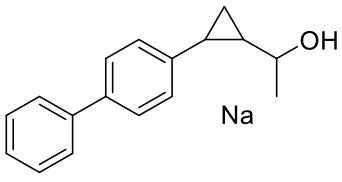
1-((2S)-2-phenylcyclopropyl)ethan-1-ol:[8] Synthesized according to **GPD**. The compound was separated using 10% Et_2O in hexane obtained as a colorless liquid with yield = 55% (1.1 mmol, 178.3 mg). dr = 1:1. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.4 Hz, 2H), 7.23 – 7.18 (m, 1H), 7.12 – 7.07 (m, 2H), 2.54-2.50 (m, 1H), 2.31 (s, 3H), 2.23-2.20 (m, 1H), 1.69-1.60 (m, 1H), 1.60 (s, 1H), 1.40-1.36 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.8, 128.5, 126.1 126.0, 125.8, 125.7, 71.9, 31.0, 29.2, 22.5, 21.5,13.43 .



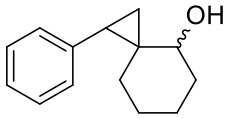
1-(2-(4-methoxyphenyl)cyclopropyl)ethan-1-ol:[6] Synthesized according to **GPD**. The compound was separated using 10% Et_2O in hexane obtained as a colorless liquid with yield = 62%(1.24 mmol, 238.4 mg). dr = 1:1. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.05 – 6.97 (m, 2H), 6.81 (dd, *J* = 8.8, 2.5 Hz, 2H), 3.77 (d, *J* = 1.4 Hz, 3H), 3.35 (q, *J* = 6.8 Hz, 1H), 1.76 (dd, *J* = 9.1, 4.7 Hz, 1H), 1.70 (d, *J* = 12.4 Hz, 1H), 1.32 (dd, *J* = 11.7, 6.2 Hz, 3H), 1.19 (dddd, *J* = 10.6, 8.1, 5.0, 2.7 Hz, 1H), 0.93 (dt, *J* = 8.7, 5.2 Hz, 1H), 0.86 (ddd, *J* = 14.2, 8.5, 5.9 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.9, 157.9, 134.7, 134.5, 127.2, 127.1, 113.9, 72.0, 55.4, 30.4, 30.4, 22.9, 22.5, 20.7, 20.2, 13.4, 12.9. **HRMS (ESI-TOF) m/z**: $[M+Na]^+$ Calcd for $[C_{12}H_{17}O_2Na]$: 215.1048, found 215.1054.



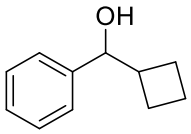
1-(2-([1,1'-biphenyl]-4-yl)cyclopropyl)ethan-1-ol: Synthesized according to **GPD**. The compound was purified through column chromatography using 10% EtOAc in hexane as eluent. The compound was isolated with 85% (0.85 mmol, 196.4 mg). dr = 1:1. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.59 – 7.54 (m, 2H), 7.50 (dd, *J* = 8.2, 1.6 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.30 (m, 1H), 7.15 (dd, *J* = 8.0, 5.8 Hz, 2H), 3.42 (q, *J* = 6.1 Hz, 1H), 2.01 – 1.82 (m, 1H), 1.36 (dd, *J* = 8.3, 6.2 Hz, 3H), 1.08 – 0.92 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.9, 141.6, 141.0, 141.0, 138.7, 128.7, 127.11, 127.09, 127.05, 127.03, 126.9, 126.3, 126.2, 71.75, 71.72, 31.0, 30.9, 22.8, 22.5, 21.1, 20.5, 13.9, 13.5. **HRMS (ESI-TOF) m/z:** $[M+Na]^+$ Calcd for $[C_{17}H_{18}ONa]$ 261.1255, found 261.1255.



1-phenylspiro[2.5]octan-4-ol:[9, 10a] Compound was purified through column chromatography using 10% EtOAc in hexane yield 60%. dr = 1:0.6. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 (t, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 2.1 Hz, 1H), 7.26 – 7.25 (m, 1H), 7.22 (s, 1H), 7.19 (t, *J* = 7.7 Hz, 6H), 3.45 – 3.40 (m, 1H), 3.40 – 3.36 (m, 1H), 2.18-2.11(m, 2H), 2.03-1.98 (m, 1H), 1.87-1.80 (m, 2H), 1.80 – 1.74 (m, 1H), 1.73 – 1.60 (m, 7H), 1.51 – 1.39 (m, 4H), 1.34 – 1.22 (m, 4H), 1.16 (m, 1H), 0.96-0.90 (m, 3H), 0.87-0.82 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 139.0, 129.1, 129.1, 129.0, 128.2, 128.0, 127.9, 125.8, 125.8, 74.5, 36.7, 33.0, 30.8, 30.7, 27.3, 24.6, 24.3, 23.3, 21.9.



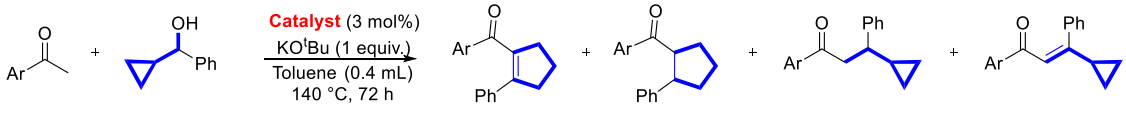
cyclobutyl(phenyl)methanol:[10b] Synthesized according to **GPA**. A colorless liquid was separated through column chromatography using 10% EtOAc in hexane as the eluent. Yield = 90% (4.5 mmol, 729 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.44-7.41 (m, 2H), 7.39 – 7.33 (m, 2H), 7.32 – 7.27 (m, 1H), 4.01 (d, *J* = 8.3 Hz, 1H), 1.27-1.18 (m,1H), 0.68-0.61 (m, 1H), 0.60 – 0.51 (m, 1H), 0.51-0.45 (m, 1H), 0.43 – 0.33 (m, 1H).



4. Detailed reaction optimization and characterization data for the products in Tables 2,3

4.1 Reaction procedure: In a 15 ml reaction tube, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken and kept in a vacuum for 5 min. After flashing with Ar, toluene (0.4 mL) was added, followed by the stepwise addition of cyclopropane-derived alcohol (**2a**, 0.2 mmol) and pentamethylacetophenone (**1a**, 0.1 mmol). The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred (250 rpm) for 72 h. After that, the reaction was quenched by adding 2-3 drops of water. It was then passed through a small Na_2SO_4 pad and evaporated under a vacuum. A small portion of the crude was analyzed via gas chromatography using mesitylene as an internal standard to obtain the selectivity. Purification via column chromatography using AcOEt/hexane mixture as an eluent yield **3a**.

4.2 Screening of catalyst for table 1[a]

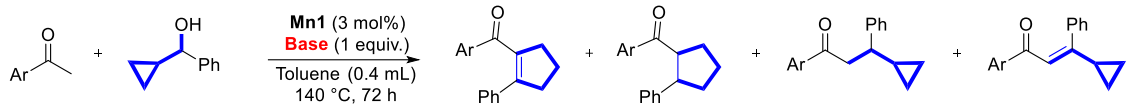


1a **2a** **3a** **4a** **5a** **6a**

Entry	Catalyst variation (3 mol%)	recovery of 1a	recovery of 2a	recovery of 16a (ketone from 2a)	Yield of			
					3a	4a	5a	6a
1	**Mn1**	2%	85%	11%	90%	n.d	5%	2%
2	**Mn2**	5%	59%	10%	51%	2%	3%	n.d
3	**Mn3**	8%	25%	35%	51%	4%	2%	n.d
4.	**Mn4**	6%	86%	n.d	72	22%	n.d	n.d
5	without **Mn1**	>99%	190%	10%	n.d	n.d	n.d	n.d

[a]Reaction condition: (0.1 mmol) of Pentamethylacetophenone (**1a**), 1-phenyl-1-cyclopropane-methanol (**2a**, 2 equiv.), **Catalyst** (3 mol%), K^{t}OBu (1 equiv.), 140 °C, 72 h., Toluene (0.4 mL). All the Yields were determined using GCMS, as mesitylene was used as the internal standard. n.d. = not determined (the amount is too small to be integrated reliably).

4.3 Screening of Base for table 1[a]

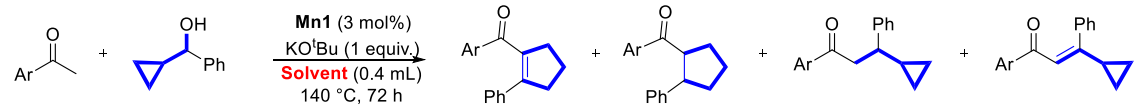


1a **2a** **3a** **4a** **5a** **6a**

Entry	Base variation (1.0 equiv.)	recovery of 1a	recovery of 2a	recovery of 17a (ketone from 2a)	Yield of			
					3a	4a	5a	6a
1	KOH	55%	n.d	165%	34%	n.d	2%	n.d
2	KO^{t}Bu	2%	85%	11%	90%	n.d	5%	2%
3	NaO^{t}Bu	44%	n.d	145%	45%	n.d	n.d	n.d
4	LiO^{t}Bu	40%	n.d	144%	20%	n.d	3%	n.d
5	Cs_2CO_3	85%	n.d	186%	n.d	n.d	n.d	n.d

[a]Reaction condition: (0.1 mmol) of Pentamethylacetophenone (**1a**), 1-phenyl-1-cyclopropane-methanol (**2a**, 2 equiv.), **Mn1** (3 mol%), Base (1 equiv.), 140 °C, 72 h., Toluene (0.4 mL). All the Yields were determined using GCMS, as mesitylene was used as the internal standard. n.d. = not determined (the amount is too small to be integrated reliably).

4.4 Screening of solvents for table 1[a]

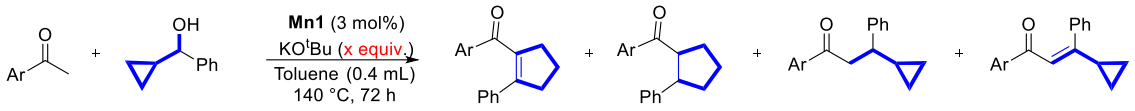


1a **2a** **3a** **4a** **5a** **6a**

Entry	Solvent (0.4 mL)	recovery of 1a	recovery of 2a	recovery of 17a (ketone from 2a)	Yield of			
					3a	4a	5a	6a
1	^{t}AmOH	50%	n.d	150%	4%	n.d	n.d	n.d
2	p-Xylene	1%	43%	15%	65%	3%	n.d	n.d
3	hexane	3%	n.d	75%	87%	4%	n.d	n.d
4	THF	28%	n.d	96%	24%	xx	n.d	4%
5	1,4-dioxane	4%	n.d	11%	34%	4%	n.d	n.d
6	toluene	2%	85%	11%	90%	n.d	5%	2%

[a]Reaction condition: (0.1 mmol) of Pentamethylacetophenone (**1a**), 1-phenyl-1-cyclopropane-methanol (**2a**, 2 equiv.), **Mn1** (3 mol%), K^{t}OBu (1 equiv.), 140 °C, 72h., Solvent (0.4 mL). All the Yields were determined using GCMS, as mesitylene was used as the internal standard. n.d. = not determined (the amount is too small to be integrated reliably).

4.5 Screening of concentration of KO^{t}Bu for table 1[a]

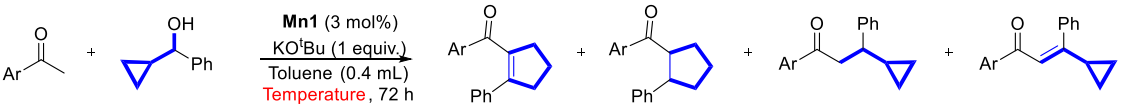


1a 2a 3a 4a 5a 6a

Entry	[KO^{t}Bu] variation (x equiv.)	recovery of 1a	recovery of 2a	recovery of 17a (ketone from 2a)	Yield of 3a	Yield of 4a	Yield of 5a	Yield of 6a
1	0.2 equiv KO^{t}Bu	25%	n.d	66%	n.d	n.d	n.d	n.d
2	1.0 equiv. KO^{t}Bu	2%	85%	11%	90%	n.d	5%	2%
3	1.5 equiv KO^{t}Bu	0%	n.d	18%	36%	6%	n.d	n.d
4	w/o KO^{t}Bu	>99%	180%	20%	n.d	n.d	n.d	n.d

[a]Reaction condition: (0.1 mmol) of Pentamethylacetophenone (**1a**), 1-phenyl-1-cyclopropane-methanol (**2a**, 2 equiv.), **Mn1** (3 mol%), K^{t}OBu (x equiv.), 140 °C, 72h., Toluene (0.4 mL). All the Yields were determined using GCMS, as mesitylene was used as the internal standard. n.d. = not determined (the amount is too small to be integrated reliably).

4.6 Screening of temperature for table 1[a]

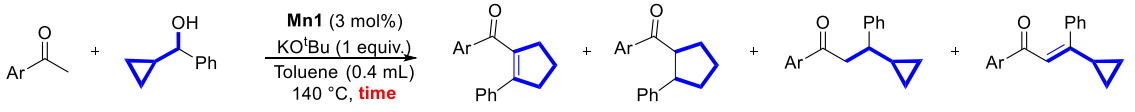


1a 2a 3a 4a 5a 6a

Entry	Temperature	recovery of 1a	recovery of 2a	recovery of 17a (ketone from 2a)	Yield of 3a	Yield of 4a	Yield of 5a	Yield of 6a
1	110 °C	70%	90%	70%	20%	n.d	2%	15%
2	120 °C	50%	50%	110%	35%	n.d	2%	5%
3	130 °C	4%	n.d	15%	58%	2%	n.d	n.d
4	140 °C	2%	85%	11%	90%	n.d	5%	2%
5	150 °C	0%	n.d	7%	66%	3%	n.d	n.d

[a]Reaction condition: (0.1 mmol) of Pentamethylacetophenone (**1a**), 1-phenyl-1-cyclopropane-methanol (**2a**, 2 equiv.), **Mn1** (3 mol%), K^{t}OBu (1 equiv.), temperature, 72h., Toluene (0.4 mL). All the Yields were determined using GCMS, as mesitylene was used as the internal standard. n.d. = not determined (the amount is too small to be integrated reliably).

4.7 Screening of time for table 1[a]



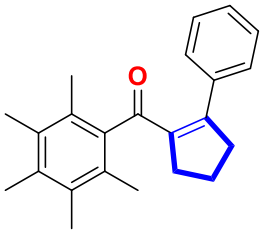
1a 2a 3a 4a 5a 6a

Entry	time (h) variation	recovery of 1a	recovery of 2a	recovery of 17a (ketone from 2a)	Yield of 3a	Yield of 4a	Yield of 5a	Yield of 6a
1	24 h	85%	20%	180%	5%	n.d	n.d	6%
2	36 h	40%	10%	95%	43%	2%	n.d	5%
3	48 h	30%	10%	110%	53%	n.d	2%	10%
4	60 h	5%	n.d	80%	60%	n.d	3%	7%

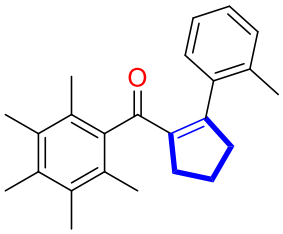
[a]Reaction condition: (0.1 mmol) of Pentamethylacetophenone (**1a**), 1-phenyl-1-cyclopropane-methanol (**2a**, 2 equiv.), **Mn1** (3 mol%), K^{t}OBu (1 equiv.), temperature, 72h., Toluene (0.4 mL). All the Yields were determined using GCMS, as mesitylene was used as the internal standard. n.d. = not determined (the amount is too small to be integrated reliably).

4.8 Characterization data of cyclopentene products

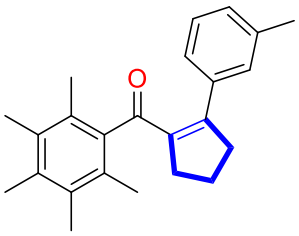
(2,3,4,5,6-pentamethylphenyl)(2-phenylcyclopent-1-en-1-yl)methanone(3a): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless liquid was isolated, which under vacuum became solid. X-ray and melting point is given below (see section 4.4). Yield = 75% (24 mg, 0.075 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.98 – 6.87 (m, 3H), 6.77 (dd, *J* = 6.9, 1.9 Hz, 2H), 2.97 – 2.82 (m, 4H), 1.99 (m, *J* = 6.7 Hz, 5H), 1.93 (s, *J* = 4.3 Hz, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.4, 157.1, 139.8, 139.7, 137.2, 134.8, 132.3, 128.4, 126.7, 126.5, 126.2, 43.2, 34.1, 21.5, 17.6, 16.4, 15.7. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{23}H_{28}O]$: 319.2062, found 319.2058.



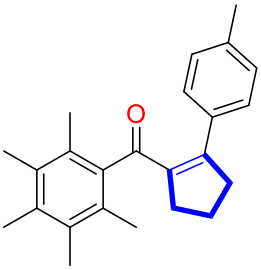
(2,3,4,5,6-pentamethylphenyl)(2-(o-tolyl)cyclopent-1-en-1-yl)methanone (3b): The compound was purified by column chromatography using EtOAc / hexane (2:98) and a floppy solid was obtained. Yield = 51% (17 mg, 0.051 mmol) white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.73 (d, *J* = 7.9 Hz, 2H), 6.68 (d, *J* = 8.0 Hz, 2H), 2.90 (t, *J* = 7.6 Hz, 2H), 2.84 (t, *J* = 7.6 Hz, 2H), 2.19 (s, 3H), 2.04 (s, 3H), 1.98 (d, *J* = 7.9 Hz, 2H), 1.94 (d, *J* = 6.2 Hz, 12H). **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{24}H_{30}O]$: 333.2218, found 333.2225.



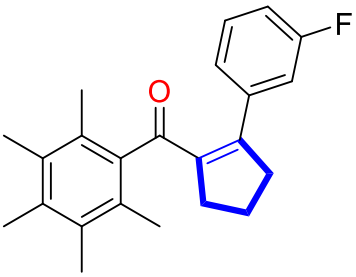
(2,3,4,5,6-pentamethylphenyl)(2-(m-tolyl)cyclopent-1-en-1-yl)methanone (3c): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a floppy solid was obtained. Yield = 55% (0.055 mmol, 18.2 mg) (white solid). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.86 (t, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 6.64 (d, *J* = 7.5 Hz, 1H), 6.45 (s, 1H), 2.96 (t, *J* = 7.8 Hz, 2H), 2.88 – 2.81 (m, 2H), 2.05 (s, 3H), 2.02 (s, 3H), 2.01 – 1.96 (m, 2H), 1.94 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.4, 157.5, 139.9, 139.7, 137.2, 136.4, 134.6, 132.2, 128.4, 127.2, 127.0, 126.6, 123.1, 43.3, 34.0, 21.5, 21.1, 17.7, 16.4, 15.7. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{24}H_{30}O]$: 333.2218, found 333.2231.



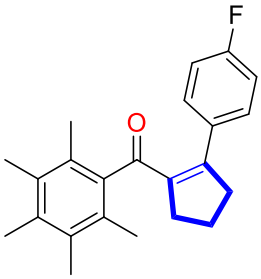
(2,3,4,5,6-pentamethylphenyl)(2-(p-tolyl)cyclopent-1-en-1-yl)methanone (3d): The compound was purified by column chromatography using EtOAc / hexane (2:98). Yield = 60% (20 mg, 0.060 mmol) white solid. **^{1}H NMR** (400 MHz, $CDCL_3$) δ 6.90 – 6.82 (m, 2H), 6.71 (t, *J* = 8.5 Hz, 1H), 6.55 (d, *J* = 7.3 Hz, 1H), 2.97 – 2.90 (m, 2H), 2.74 (s, 2H), 2.06 (s, 3H), 2.01 (d, *J* = 2.4 Hz, 5H), 1.93 (s, 12H). **^{13}C NMR** (101 MHz, $CDCL_3$) δ 200.4, 157.4, 139.4, 136.6, 134.8, 134.2, 132.2, 128.4, 127.3, 126.1, 43.0, 34.1, 21.5, 21.2, 17.6, 16.5, 15.7. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{24}H_{30}O]$: 333.2218, found 333.2225.



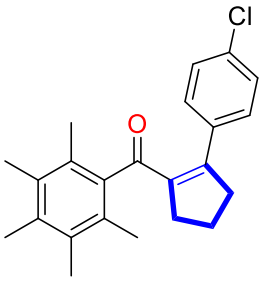
(2-(3-fluorophenyl)cyclopent-1-en-1-yl) (2,3,4,5,6-pentamethylphenyl)methanone (3e): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a light yellowish liquid was isolated. Yield = 50% (16.8 mg, 0.05 mmol). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.92 (td, *J* = 7.9, 5.9 Hz, 1H), 6.64 (td, *J* = 8.5, 2.6 Hz, 1H), 6.59 (dd, *J* = 7.6, 1.4 Hz, 1H), 6.36 (dt, *J* = 9.8, 2.0 Hz, 1H), 2.99-2.92 (m, 2H), 2.85-2.81 (m, 2H), 2.02 (s, 3H), 2.01 – 1.97 (m, 2H), 1.94 (d, *J* = 3.5 Hz, 12H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.0, 161.8 (d, *J* = 245.2 Hz), 139.6, 139.4 (d, *J* = 8.2 Hz), 135.1, 132.5, 128.5, 128.1 (d, *J* = 8.4 Hz), 121.8 (d, *J* = 2.9 Hz), 113.3 (dd, *J* = 29.8, 21.7 Hz), 43.2, 34.1, 21.5, 17.6, 16.4, 15.7. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -114.80 – -114.88 (m). **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{23}H_{27}OF]$: 337.1968, found 337.1954.



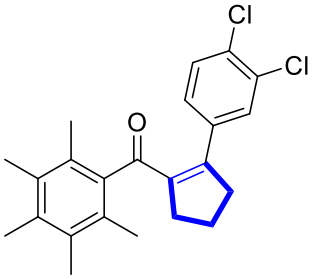
2-(4-fluorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone(3f): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless liquid was isolated. Yield = 45% (15.2 mg, 0.045 mmol). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.98 – 6.88 (m, 3H), 6.79 – 6.75 (m, 2H), 2.96 – 2.90 (m, 2H), 2.89 – 2.83 (m, 2H), 2.03 – 1.97 (m, 5H), 1.93 (d, *J* = 5.7 Hz, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.4, 157.1, 139.8, 139.7, 137.2, 134.8, 132.2, 128.4, 126.6, 126.5, 126.2, 43.2, 34.2, 21.5, 17.6, 16.4, 15.7. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -114.75 – -114.80 (m). **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{23}H_{27}OF]$: 337.1968, found 337.1984.



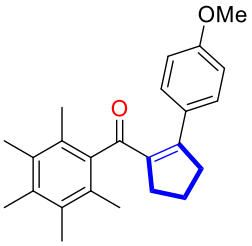
(2-(4-chlorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone (3g): The compound was purified by column chromatography using EtOAc / hexane (1:99), and a colorless liquid was isolated. Yield = 45% (0.045 mmol, 15.9 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.88 (d, *J* = 8.5 Hz, 2H), 6.67 (d, *J* = 8.1 Hz, 2H), 2.94-2.90 (m, 2H), 2.87 – 2.78 (m, 2H), 2.08 (s, 3H), 1.99 (d, *J* = 7.4 Hz, 2H), 1.97 (s, 6H), 1.92 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.0, 155.6, 140.5, 139.6, 135.6, 132.7, 132.5, 128.4, 127.4, 126.8, 42.9, 34.0, 21.4, 17.6, 16.5, 15.7. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{23}H_{26}OCl]$: 353.1672, found 353.1700**.**



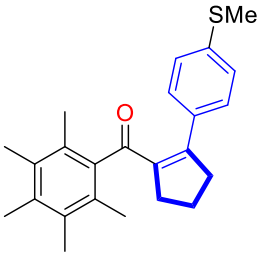
2-(3,4-dichlorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone (3h): The compound was purified by column chromatography using EtOAc / hexane 3:97), and a colorless liquid was isolated. Yield = 55% (0.055 mmol, 21 mg) .**^{13}C NMR** (126 MHz, $CDCl_3$) δ 198.0, 156.6, 140.6, 132.9, 132.1, 132.0, 130.8, 130.5, 128.0, 127.9, 125.3, 124.0, 114.7, 83.1, 17.9, 16.7, 11.5, 11.5, 3.7, 2.6. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{23}H_{27}OCl_2]$: 387.1282, found 387.1296.



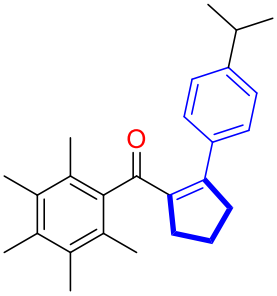
(2-(4-methoxyphenyl)cyclopent-1-en-1-yl)(2,3,4,5,6 pentamethylphenyl)methanone(3i): The **c**ompound was purified using column chromatography using EtOAc / Hexane (5:95). Yield = 50% (17.5 mg, 0.045 mmol). **^{1}H NMR** (400 MHz, CDCL3) δ 6.80 (d, *J* = 9.0 Hz, 2H), 6.48 (d, *J* = 8.6 Hz, 2H), 3.70 (s, 3H), 2.90-2.82 (m, 4H), 2.05 (s, 3H), 1.96 (d, *J* = 10.4 Hz, 14H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.2, 158.0, 139.2, 138.2, 133.7, 131.4, 128.6, 127.5, 126.9, 111.3, 54.3, 41.8, 33.4, 20.6, 16.5, 15.5, 14.8. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{24}H_{30}O_2]$: 349.2168, found 349.2115.



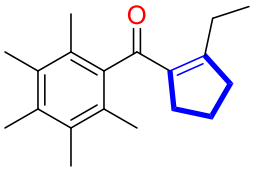
(2-(4-(methylthio)phenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone(3j): The compound was purified by column chromatography using EtOAc / hexane (5:95) was isolated. Yield = 60% (0.06 mmol, 21.8 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.80 (d, *J* = 8.4 Hz, 2H), 6.71 (d, *J* = 8.5 Hz, 2H), 2.91 (t, *J* = 7.6 Hz, 2H), 2.84 (t, *J* = 7.7 Hz, 2H), 2.39 (s, 3H), 2.07 (s, 3H), 1.97 (s, 8H), 1.93 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.2, 156.5, 139.8, 139.77, 137.2, 135.0, 133.9, 132.3, 128.4, 126.7, 124.7, 42.8, 34.1, 21.4, 17.6, 16.5, 15.84, 15.7. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for [$C_{24}H_{30}OS$]: 365.1939, found 365.1945.



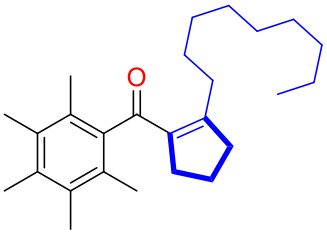
2-(4-isopropylphenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone (3k): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless liquid was isolated. Yield = 56% (0.056 mmol, 20.2 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.85 – 6.65 (m, 4H), 2.97 – 2.92 (m, 2H), 2.90 – 2.83 (m, 2H), 2.74-2.69 (m, 1H), 2.02 (s, 3H), 1.99 (d, *J* = 8.2 Hz, 2H), 1.95 (s, 12H), 1.14 (dt, *J* = 6.9, 1.4 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.4, 157.5, 147.6, 139.9, 139.4, 134.5, 134.3, 132.2, 128.5, 126.3, 124.7, 43.2, 34.1, 33.8, 24.0, 21.5, 17.7, 16.6, 15.7. **HRMS(ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{26}H_{34}O]$: 361.2531.



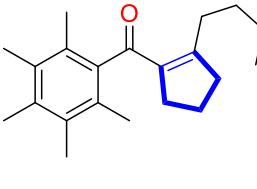
(2-ethylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone(3l): The compound was purified by column chromatography using Et_2O / hexane (1:99), and a colorless liquid was isolated. Yield = 88% (24 mg, 0.088 mmol). **^{1}H NMR** (400 MHz, CDCL3) δ 2.68 – 2.54 (m, 4H), 2.23 (s, 3H), 2.17 (s, 6H), 2.11 (d, *J* = 5.5 Hz, 2H), 2.06 (s, 6H), 1.81 (p, *J* = 7.6 Hz, 2H), 0.86 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.7, 162.0, 140.9, 136.8, 135.0, 132.9, 128.1, 38.7, 33.9, 23.1, 21.3, 17.2, 16.8, 16.1, 12.3. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{19}H_{28}O]$: 271.2062, found 271.2071.



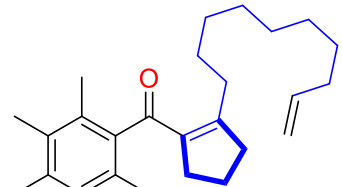
(2-nonylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone (3m): The compound was purified by column chromatography using Et_2O / hexane (1:99), and a colorless liquid was isolated. Yield = 52% (0.052 mmol,19.2 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.67 (t, *J* = 7.9 Hz, 2H), 2.55 (t, *J* = 7.8 Hz, 2H), 2.23 (s, 3H), 2.17 (s, 6H), 2.05 (s, 6H), 1.95 (q, *J* = 8.9 Hz, 2H), 1.81 (q, *J* = 7.6 Hz, 2H), 1.28 – 1.18 (m, 8H), 1.06 (p, *J* = 7.0 Hz, 2H), 0.97 (t, *J* = 7.5 Hz, 2H), 0.89 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.6, 161.1, 140.9, 137.4, 134.9, 132.9, 128.2, 39.4, 33.8, 32.0, 30.0, 29.8, 29.4, 28.2, 22.8, 21.3, 17.3, 16.8, 16.1, 14.2, 9.0, 7.7. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{26}H_{42}O]$: 369.3157, found 369.3174.



(2-isopentylcyclopent-1-en-1-yl) (2,3,4,5,6-pentamethylphenyl)methanone (3n): The compound was purified by column chromatography using Et_2O / hexane (1:99), and a colorless liquid was isolated. Yield = 77% (24 mg, 0.077 mmol). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.69 (t, *J* = 7.7 Hz, 2H), 2.55 (t, *J* = 7.7 Hz, 2H), 2.29 – 2.11 (m, 11H), 2.05 (s, 6H), 1.80 (p, *J* = 7.3 Hz, 2H), 1.20 (dt, *J* = 13.4, 6.4 Hz, 1H), 1.06 (dt, *J* = 11.8, 6.2 Hz, 2H), 0.64 (d, *J* = 6.7 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.6, 161.2, 140.9, 137.4, 135.0, 133.0, 128.1, 39.6, 37.0, 33.7, 28.6, 28.1, 22.2, 21.3, 17.3, 16.7, 16.0. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{22}H_{34}O]$: 313.2531, found 313.2539

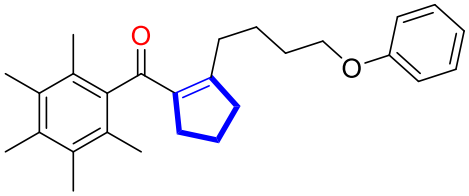


(2-(dec-9-en-1-yl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone(3o): The compound was purified by column chromatography using Et_2O / hexane (1:99), and a colorless liquid was isolated with a mixture with 1-cyclopropylundec-10-en-1-one (**2o**). (overall yield 27 mg). A yield of **3o** = 45% was determined from NMR. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.87 – 5.76 (m, 1H), 5.03 – 4.90 (m, 2H), 2.67 (t, *J* = 7.6 Hz, 2H), 2.55 (t, *J* = 7.7 Hz, 2H), 2.23 (d, *J* = 3.6 Hz, 4H), 2.18 (d, *J* = 10.1 Hz, 9H), 2.13 (s, 2H), 2.05 (s, 8H), 1.96 (s, 2H), 1.84 – 1.77 (m, 2H), 1.35 (q, *J* = 7.4 Hz, 2H), 1.28 – 1.15 (m, 9H), 1.07 (t, *J* = 7.8 Hz, 2H), 1.01 – 0.94 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 210.2, 200.6, 161.1, 140.9, 139.3, 137.4, 135.0, 133.2, 132.9, 128.2, 127.1, 114.30, 39.42, 33.94, 33.77, 33.25, 30.05, 30.02, 29.84, 29.63, 29.38, 29.2, 29.1, 28.2, 21.3, 17.33, 17.26, 17.20, 16.8, 16.10, 16.07. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{27}H_{42}O]$: 381.3157, found 381.3128.

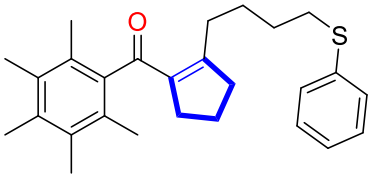


(2,3,4,5,6-pentamethylphenyl)(2-(3-phenylpropyl)cyclopent-1-en-1-yl)methanone(**3p**): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless liquid was isolated. Yield = 61% (22 mg, 0.061 mmol). **^{1}H NMR** (400 MHz, CDCl3) δ 7.16 (dq, *J* = 14.0, 7.5 Hz, 3H), 6.83 (d, *J* = 7.2 Hz, 2H), 2.70 (t, *J* = 7.7 Hz, 2H), 2.60 (t, *J* = 7.7 Hz, 2H), 2.49 (dd, *J* = 10.3, 6.4 Hz, 2H), 2.30 (q, *J* = 8.9 Hz, 2H), 2.25 (s, 3H), 2.17 (s, 6H), 2.05 (s, 6H), 1.82 (q, *J* = 7.7 Hz, 2H). **^{13}C NMR** (101 MHz, CDCL3) δ 200.5, 159.5, 141.6, 140.9, 138.1, 135.3, 133.2, 128.4, 128.2, 126.0, 39.7, 34.3, 33.8, 32.3, 29.8, 21.3, 17.4, 16.8, 16.1. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{25}H_{32}O]$: 347.2375, found 347.2354

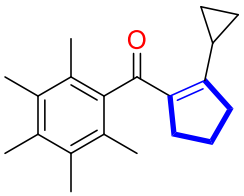
(2,3,4,5,6-pentamethylphenyl)(2-(4-phenoxybutyl)cyclopent-1-en-1-yl)methanone (3q): The compound was purified by column chromatography using EtOAc / hexane (2:98), and white solid was isolated. Overall yield 90% with 50:50 of **3q**:1-cyclopropyl-5-phenoxypentan-1-one (**2q**). Yield of **3q** = 45%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 4H), 6.99 – 6.86 (m, 6H), 4.00 (t, *J* = 3.6 Hz, 2H), 3.82 (t, *J* = 6.2 Hz, 2H), 2.74 – 2.65 (m, 4H), 2.61 (t, *J* = 7.8 Hz, 2H), 2.26 (d, *J* = 2.7 Hz, 3H), 2.20 (s, 6H), 2.17 – 2.12 (m, 2H), 2.10 (s, 6H), 1.99-1.95 (m, 1H), 1.86-1.82 (m, 6H), 1.58 – 1.42 (m, 5H), 1.07-1.02 (p, *J* = 3.8 Hz, 2H), 0.91-0.87 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 210.9, 200.6, 160.3, 159.1, 140.8, 135.1, 133.0, 129.6, 129.5, 128.1, 120.7, 120.7, 114.6, 114.6, 67.5, 67.5, 43.1, 39.3, 33.8, 29.7, 29.5, 28.9, 24.7, 21.3, 20.7, 20.5, 17.3, 17.3, 16.8, 16.8, 16.1, 16.1, 10.8. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{27}H_{35}O_2]$: 391.2637, found 391.2629.



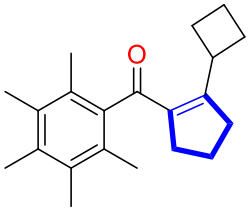
(2,3,4,5,6-pentamethylphenyl)(2-(4-(phenylthio)butyl)cyclopent-1-en-1-yl)methanone (**3r**): The compound was purified by column chromatography using EtOAc / hexane (2:98), and white solid was isolated. Yield = 58%.(0.058 mmol, 23.5 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 4H), 7.21-7.17 (m, 1H), 2.74 – 2.70 (m, 2H), 2.67 (t, *J* = 7.4 Hz, 2H), 2.56 (t, *J* = 7.6 Hz, 2H), 2.22 (s, 3H), 2.17 (s, 6H), 2.06 (s, 8H), 1.82 (t, *J* = 7.4 Hz, 2H), 1.39 (s, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.6, 160.02, 140.83, 136.84, 135.17, 133.03, 129.04, 128.99, 128.14, 125.91, 39.24, 33.80, 33.20, 29.38, 29.33, 27.16, 21.30, 17.34, 16.80, 16.09. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for [$C_{27}H_{35}OS$] 407.2409 found 407.2423.



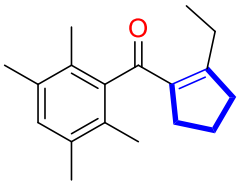
(2-cyclopropylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone (3s): The compound was purified by column chromatography using Et_2O / hexane (1:99), and a colorless liquid was isolated. Yield =40% (0.04 mmol, 11.3 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.62 (t, *J* = 7.4 Hz, 2H), 2.20 (d, *J* = 5.3 Hz, 6H), 2.17 (s, 6H), 2.09 (s, 6H), 1.75 (p, *J* = 7.6 Hz, 2H), 0.64 (t, *J* = 7.5 Hz, 4H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.6, 162.3, 141.2, 134.8, 132.9, 128.2, 34.2, 34.1, 21.2, 17.2, 16.8, 16.1, 12.0, 7.6. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{20}H_{28}O]$: 283.2062, found 283.2069.



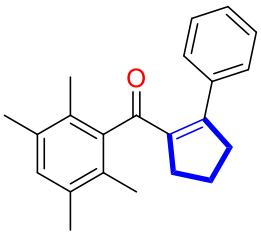
(2-cyclobutylcyclopent-1-en-1-yl) (2,3,4,5,6-pentamethylphenyl)methanone (3t): The compound was purified by column chromatography using Et_2O / hexane (1:99), and a colorless liquid was isolated. Yield = 50% (15 mg, 0.05 mmol). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.75 – 2.69 (m, 2H), 2.63 – 2.57 (m, 2H), 2.24 (s, 3H), 2.19 (d, *J* = 5.2 Hz, 1H), 2.18 (s, 6H), 2.02 (s, 6H), 1.93 (qd, *J* = 9.1, 2.4 Hz, 2H), 1.88 – 1.77 (m, 4H), 1.76 – 1.67 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.5, 162.4, 141.0, 136.5, 135.0, 132.9, 128.1, 36.0, 35.0, 34.2, 27.4, 21.4, 18.8, 17.2, 16.8, 16.1. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{21}H_{30}O]$: 297.2218, found 297.2232.



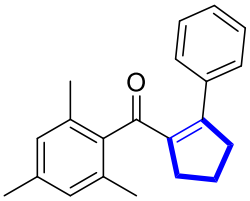
(2-ethylcyclopent-1-en-1-yl)(2,3,5,6-tetramethylphenyl)methanone (3v): The compound was purified by column chromatography using Et_2O / hexane (1:99), and a colorless liquid was isolated. Yield = 74% (0.074 mmol, 18.9 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.93 (s, 1H), 2.68 – 2.61 (m, 2H), 2.57 (t, *J* = 7.7 Hz, 2H), 2.19 (s, 6H), 2.09 – 2.03 (m, 2H), 2.01 (s, 6H), 1.81 (p, *J* = 7.6 Hz, 2H), 0.84 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.3, 162.4, 143.1, 136.7, 134.3, 131.4, 128.7, 38.8, 33.8, 23.3, 21.3, 19.6, 16.0, 12.3. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{18}H_{26}O]$: 257.1907, found 257.1919.



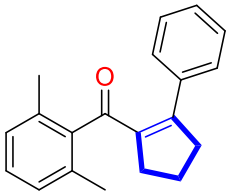
(2-phenylcyclopent-1-en-1-yl)(2,3,5,6-tetramethylphenyl)methanone (3w): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a solid was separated. Yield = 73% (0.073 mmol, 22.2 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.99 – 6.93 (m, 3H), 6.83 – 6.79 (m, 2H), 6.58 (s, 1H), 2.96-2.92 (m, 2H), 2.89-2.86 (m, 2H), 2.01 – 1.98 (m, 2H), 1.97 (s, 6H), 1.91 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.2, 157.2, 141.9, 139.4, 137.1, 133.7, 131.3, 129.0, 127.2, 126.9, 126.2, 43.2, 34.2, 21.5, 19.3, 16.4. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{22}H_{26}O]$: 305.1905, found 305.1902.



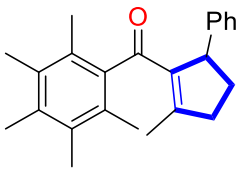
mesityl(2-phenylcyclopent-1-en-1-yl)methanone(3x): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless solid was isolated. Yield = 62% (0.062 mmol,18.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.01 (dt, *J* = 14.8, 7.2 Hz, 3H), 6.92 (d, *J* = 6.6 Hz, 2H), 6.47 (s, 2H), 2.90 (td, *J* = 8.7, 4.6 Hz, 4H), 2.07 (d, *J* = 16.6 Hz, 10H), 2.00 (p, *J* = 7.8 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.4, 156.0, 139.3, 138.7, 138.0, 136.9, 133.8, 128.1, 127.3, 127.2, 126.7, 42.6, 34.6, 21.8, 21.0, 19.6. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for [$C_{21}H_{25}O$]: 291.1749, found 291.1745.



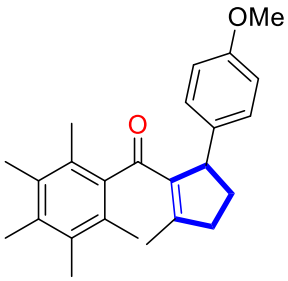
2,6-dimethylphenyl)(2-phenylcyclopent-1-en-1-yl)methanone (3y): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless solid was isolated. Yield= 65%.(0.065 mmol, 17.9 mg).**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.04 – 6.98 (m, 3H), 6.92 (dd, *J* = 7.9, 1.7 Hz, 2H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.66 (d, *J* = 7.6 Hz, 2H), 2.96 – 2. 87 (m, 4H), 2.10 (s, 6H), 2.04-1.98 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.1, 156.6, 141.4, 138.9, 136.8, 133.7, 128.3, 127.4, 127.3, 126.6, 42.8, 34.4, 21.7, 19.6. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for [$C_{20}H_{23}O$]: 277.1592, found 277.1596



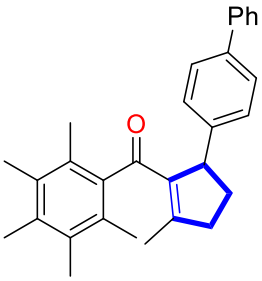
5-methyl-2-phenylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone (8a): Yield = 52% (0.052 mmol, 35 mg). The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless solid was isolated. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.18 (t, *J* = 7.4 Hz, 2H), 7.15 – 7.10 (m, 1H), 7.02 (d, *J* = 7.3 Hz, 2H), 4.17 (d, *J* = 9.4 Hz, 1H), 2.91 – 2.81 (m, 1H), 2.59 – 2.51 (m, 1H), 2.40 – 2.31 (m, 1H), 2.21 (s, 3H), 2.19 – 1.99 (m, 6H), 1.94 – 1.69 (m, 9H), 1.62 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.7, 157.5, 146.0, 140.9, 140.2, 135.0, 132.8, 128.2, 127.5, 126.0, 77.4, 77.2, 76.9, 52.4, 41.1, 31.8, 29.8, 16.8, 16.3, 16.0. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{24}H_{30}O]$: 333.2231, found 333.3318.



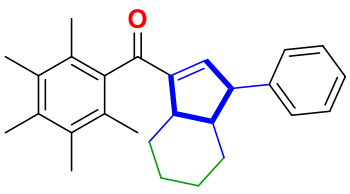
(5-(4-methoxyphenyl)-2-methylcyclopent-1-en-1-yl)(2,3,4,5,6)pentamethylphenyl)methanone (8b): The compound was purified by column chromatography using EtOAc / hexane (5:95), and a colorless solid was isolated. Yield = 58%. (0.058 mmol, 21 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.92 (d, *J* = 8.1 Hz, 2H), 6.72 (d, *J* = 8.2 Hz, 2H), 4.12 (s, 1H), 3.77 (s, 3H), 2.83 (dt, *J* = 17.9, 8.6 Hz, 1H), 2.57 – 2.47 (m, 1H), 2.33 (dq, *J* = 12.9, 9.2 Hz, 1H), 2.19 (d, *J* = 10.0 Hz, 4H), 2.16 – 2.04 (m, 6H), 1.93 – 1.68 (m, 9H**). ^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.8, 157.9, 157.1, 141.1, 140.3, 138.3, 134.9, 128.4, 113.5, 55.4, 51.5, 41.0, 31.9, 16.9, 16.8, 16.3, 16.0. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{25}H_{30}O_2]$: 363.2324, found 363.2337.



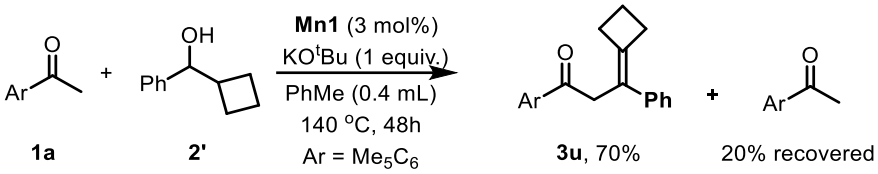
(5-([1,1'-biphenyl]-4-yl)-2-methylcyclopent-1-en-1-yl)(2,3,4,5,6)-pentamethylphenyl)methanone (8c): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a white solid was isolated. Yield = .40% (0.040 mmol, 16.3 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.59 – 7.54 (m, 2H), 7.46 – 7.38 (m, 4H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 7.7 Hz, 2H), 4.20 (s, 1H), 2.92-2.85 (m, 1H), 2.62 – 2.53 (m, 1H), 2.43-3.35 (m,1H), 2.21 (s, 9H), 1.98 – 1.71 (m, 9H), 0.90 – 0.85 (m, 1H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.8, 157.7, 145.2, 141.4, 140.9, 140.2, 138.9, 135.0, 128.8, 127.9, 127.1, 127.1, 126.9, 52.1, 41.1, 31.9, 16.9, 16.8, 16.3, 16.0. **HRMS (ESI-TOF) m/z:** $[M+Na]^+$ Calcd for $[C_{30}H_{33}NaO^+]$: 431.2351, found 431.2349.



(2,3,4,5,6-pentamethylphenyl)((7aR)-1-phenyl-2,4,5,6,7,7a-hexahydro-1H-inden-3-yl)methanone (10): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colorless liquid was isolated. Yield = 62% (0.062 mmol, 23.1 mg). d.r. = 60:40. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.35 – 7.16 (m, 8H), 7.10 (s, 1H), 7.09 (s, 1H), 3.82 (d, *J* = 8.4 Hz, 1H), 3.75 (s, 1H), 3.12 – 3.06 (m, 1H), 3.03 (t, *J* = 7.6 Hz, 1H), 2.95 (d, *J* = 14.5 Hz, 1H), 2.48 (s, 1H), 2.31 – 1.99 (m, 36H), 1.87 (s, 3H), 1.76 – 1.63 (m, 4H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 211.8, 211.0, 147.9, 141.2, 140.6, 138.2, 135.5, 133.2, 133.1, 131.8, 128.6, 128.6, 128.5, 128.3, 127.5, 126.7, 126.2, 126.1, 72.3, 47.2, 44.6, 44.5, 33.5, 29.8, 29.5, 26.3, 26.3, 25.6, 23.4, 23.0, 18.0, 17.2, 17.1, 16.8, 16.8, 16.1, 16.1, 16.1. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{27}H_{34}O]$: 373.2531, found 373.2528

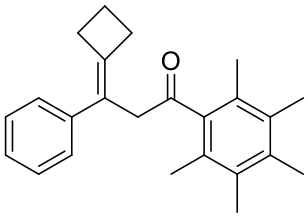


4.9 Reaction of 1-phenyl cyclobutyl methanol 2' with 1a



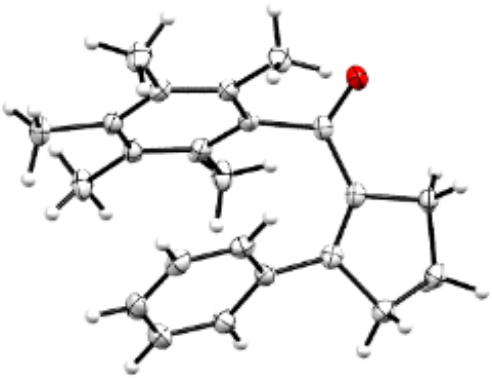
1a **2'** **3u**, 70% 20% recovered

The reaction of 1-phenyl cyclobutyl methanol with 1a under the same condition produced exocyclic cylobutyl alkene 3u in 70% yield. The structure of 3u was confirmed by single-crystal XRD (CCDC 2376543).



3-cyclobutylidene-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one (3u): The compound was purified by column chromatography using EtOAc / hexane (2:98), and a colourless liquid was isolated. Yield = 70% (0.07 mmol, 27.2 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 4H), 7.22 – 7.17 (m, 1H), 3.75 (s, 2H), 2.94 – 2.88 (m, 2H), 2.80 – 2.74 (m, 2H), 2.24 (s, 3H), 2.18 (s, 6H), 2.06 (s, 6H), 2.01 (t, *J* = 7.8 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 209.0, 143.2, 140.6, 139.9, 135.4, 133.1, 128.2, 127.6, 127.3, 126.3, 123.8, 48.0, 32.1, 31.1, 17.4, 16.9, 16.8, 16.0. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{24}H_{29}NO]$: 333.2218, found 333.2218

4.10 Single crystal X-ray data for 3a



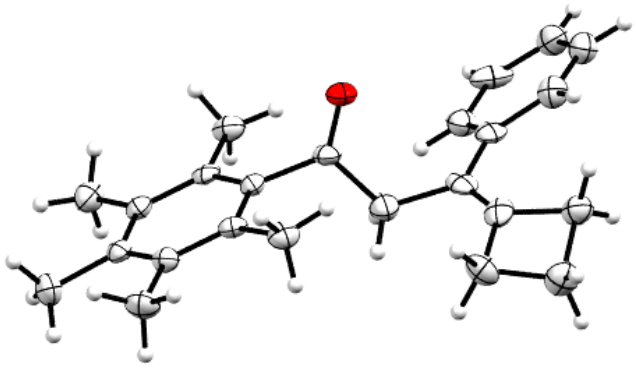
3a CCDC 2237272

Table S1a Crystal data and structure refinement for 3a

Identification code	BIPKSKKC145-2_auto
Empirical formula	$C_{23}H_{26}O$
Formula weight	318.44
Temperature/K	100.4(9)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.03845(7)
b/Å	13.58231(12)
c/Å	16.53779(14)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1805.61(3)
Z	4
ρ_{calc}g/cm^3	1.171
μ/mm^{-1}	0.529
F(000)	688.0
Crystal size/mm^3	0.002 × 0.002 × 0.001
Radiation	Cu Kα (λ = 1.54184)

2Θ range for data collection/°	8.424 to 136.38
Index ranges	-9 ≤ h ≤ 9, -15 ≤ k ≤ 16, -19 ≤ l ≤ 18
Reflections collected	26187
Independent reflections	3295 [R_{int} = 0.0987, R_{sigma} = 0.0352]
Data/restraints/parameters	3295/0/223
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0361, wR_2 = 0.0965
Final R indexes [all data]	R_1 = 0.0366, wR_2 = 0.0970
Largest diff. peak/hole / e $Å^{-3}$	0.17/-0.16
Flack parameter	0.07(17)

Melting point: 52-54 °C



3u CCDC 2376543

Table S1b Crystal data and structure refinement for 3u.

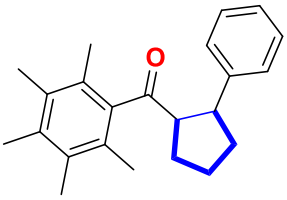
Identification code	bip_ksk_kd120a_final
Empirical formula	$C_{48}H_{56}O_2$
Formula weight	664.92
Temperature/K	298
Crystal system	monoclinic
Space group	$P2_1$
a/Å	13.057(2)
b/Å	7.9795(14)
c/Å	18.629(3)
α/°	90
β/°	106.871(6)
γ/°	90
Volume/$Å^3$	1857.3(6)
Z	2
$\rho_{calc}g/cm^3$	1.189
μ/mm^{-1}	0.070
F(000)	720.0
Crystal size/mm^3	0.002 × 0.002 × 0.001
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.252 to 25.018
Index ranges	-15 ≤ h ≤ 15, -9 ≤ k ≤ 9, -22 ≤ l ≤ 22
Reflections collected	69872
Independent reflections	6567 [R_{int} = 0.1340, R_{sigma} = 0.0759]
Data/restraints/parameters	6567/1/462
Goodness-of-fit on F^2	1.030

Final R indexes [I>=2σ (I)]	R_1 = 0.0635, wR_2 = 0.1361
Final R indexes [all data]	R_1 = 0.0796, wR_2 = 0.1453
Largest diff. peak/hole / e Å^{-3}	0.53/-0.20
Flack parameter	-0.1(10)

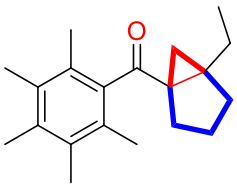
5. Derivatization of the final product

5.1 Characterization data of the derivatives of the final product

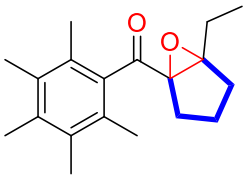
(2,3,4,5,6-pentamethylphenyl)((1S,2R)-2-phenylcyclopentyl)methanone (11): In a 15 mL reaction tube, Pd/C (2 mol%) and **3a** (0.1 mmol) were taken, followed by the addition of ethanol (0.5 mL). The reaction mixture was kept under 1 atm hydrogen with a balloon filled with H_2 gas and was stirred for 12 h at room temperature. The reaction mixture was then filtered and evaporated. The compound was purified by flash column chromatography. Yield = 70% (0.07 mmol, 22.3 mg). dr = 60:40. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.5 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 2H), 7.20 – 7.13 (m, 2H), 3.67 – 3.57 (m, 1H), 3.41 (q, *J* = 7. 9 Hz, 1H), 2.45 – 2.34 (m, 1H), 2.20 (s, 5H), 2.10 (s, 8H), 2.00 (dd, *J* = 13.9, 7.3 Hz, 2H), 1.92 – 1.66 (m, 6H**). ^{13}C NMR** (126 MHz, $CDCl_3$) δ 213.3, 212.1, 145.3, 141.9, 140.7, 140.6, 135.5, 135.4, 133.0, 133.0, 129.3, 128.8, 128.3, 128.0, 127.8, 127.7, 126.2, 126.1, 62.5, 58.5, 49.5, 47.6, 35.9, 31.2, 30.9, 29.8, 29.4, 25.9, 23.1, 16.8, 16.7, 16.0. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{23}H_{30}O]$: 321.2218, found 321.2228.



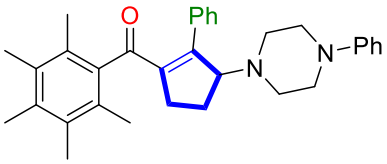
(2,3,4,5,6-pentamethylphenyl)((1R,5R)-5-phenylbicyclo[3.1.0]hexan-1-yl)methanone (12): In a 15 mL reaction tube, NaH (0.153 mmol, 1.02 equiv.) was taken in 0.2 mL THF (1.6 M) and Me_3SIO (0.172 mmol, 1.15 equiv.) were then added and stirred for 30 min. Then a DMSO (0.15 mL, 1M) solution of **3l** (0.15 mmol) was added dropwise. The reaction mixture was stirred for 16 h at 55 °C. It was then quenched with NH_4Cl (2 mL) and washed with Et_2O (5 mL). The organic part was then concentrated under vacuum and purified by flash column chromatography. Yield = 62%. dr, >99:1. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.22 (s, 3H), 2.17 (d, *J* = 5.2 Hz, 6H), 2.13 (s, 3H), 1.98 (s, 3H), 1.92 (dt, *J* = 14.9, 7.5 Hz, 2H), 1.74 (dd, *J* = 10.2, 4.2 Hz, 2H), 1.64 – 1.59 (m, 2H), 1.55 (d, *J* = 2.9 Hz, 2H), 1.19 – 1.10 (m, 2H), 1.06 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.7, 162.0, 140.9, 136.8, 134.9, 132.9, 128.1, 38.7, 33.9, 30.2, 29.8, 23.1, 17.2, 16.8, 16.1, 12.3**. HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{20}H_{30}O]$: 285.2218, found 285.2207.



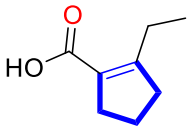
((1S,5R)-5-ethyl-6-oxabicyclo[3.1.0]hexan-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone (13):
To a stirred room temperature solution of **3l** (0.10 mmol) in *t*-BuOH (1 mL), NaOH (5 equiv.) and t-BuOOH (~5.5 M in decane, 5 equiv.) were added successively. The resulting suspension was heated to 85 °C and stirred for 16 h. The reaction mixture was then cooled to RT, and diluted with sat. aq. NH_4Cl (5 mL), extracted with Et_2O (3 x 5 mL), dried over Na_2SO_4, filtered, and concentrated in vacuo. The compound was purified by flash column chromatography, and a white solid was obtained. Yield = 84%. dr >99:1. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.22 (s, 3H), 2.17 (s, 6H), 2.10 (s, 6H), 2.09 – 2.02 (m, 3H), 1.79 – 1.66 (m, 3H), 1.63 – 1.54 (m, 2H), 1.43-1.35 (m, 1H), 1.07 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 208.4, 138.1, 136.2, 133.2, 128.9, 77.9, 74.2, 29.8, 29.3, 22.5, 18.5, 17.6, 16.9, 16.1, 10.6. **HRMS (ESI-TOF) m/z:**$[M+Na]^+$ Calcd for $[C_{19}H_{26}O_2]$: 309.1830, found 309.1842.



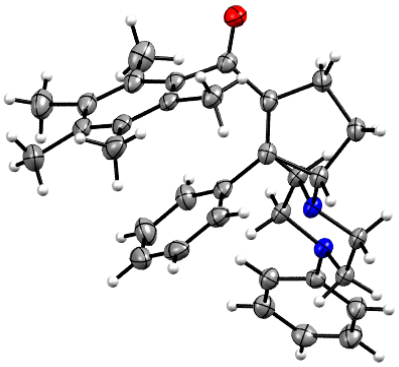
(S)-(2,3,4,5,6-pentamethylphenyl)(2-phenyl-3-(4-phenylpiperazin-1-yl)cyclopent-1-en-1-yl)methanone (14): In a 5 ml reaction tube, **3a** (0.2 mmol) and Br_2 (2 equiv.) in 0.2 mL DCM was stirred for 5 min followed by addition of 4-phenyl piperazine (3 equiv.). The reaction mixture was stirred for 24 h at 80 °C. The mixture was then quenched with $Na_2S_2O_4$ solution. After purification of the through-column chromatography, a brown color was obtained. Yield = 63% (0.126 mmol, 50.72 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.25 – 7.19 (m, 2H), 6.97 – 6.92 (m, 1H), 6.91 – 6.84 (m, 4H), 6.83 – 6.77 (m, 3H), 4.18 (s, 1H), 3.07-3.02 (m, 4H), 2.89-2.86 (m, 2H), 2.70-2.67 (m, 2H), 2.60-2.56 (m, 2H), 2.13 – 2.06 (m, 1H), 2.02 (s, 3H), 2.00 – 1.97 (m, 1H), 1.93 (d, *J* = 2.5 Hz, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 201.0, 154.5, 151.6, 142.0, 139.7, 136.2, 135.0, 132.4, 129.1, 128.3, 127.1, 126.4, 126.3, 119.7, 116.1, 49.6, 48.7, 32.5, 20.9, 17.7, 16.5, 15.7. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_{33}H_{40}N_2O]$: 479.3062, found 479.3078.



2-ethylcyclopent-1-ene-1-carboxylic acid (15a): In a 15 ml reaction tube **3l** (0.1 mmol), HFIP (0.88 mL) and HCl (12 M, 0.13 mL) were added. The reaction mixture was heated to 65 °C for 16 h. The solution was then cooled to RT, diluted with water, extracted with DCM (2 x 10 mL), and dried over Na_2SO_4. The compound was purified by flash column chromatography. Yield = 75% (0.075 mmol, 10 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.64 (t, *J* = 7.6 Hz, 4H), 2.58 – 2.50 (m, 2H), 1.83 (p, *J* = 7.7 Hz, 2H), 1.05 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.0, 164.8, 126.0, 38.2, 33.6, 23.5, 21.5, 12.6. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ Calcd for $[C_8H_{12}O_2]$: 479.0837, found 479.0858.



5.2 Single Crystal X-Ray data of 14.



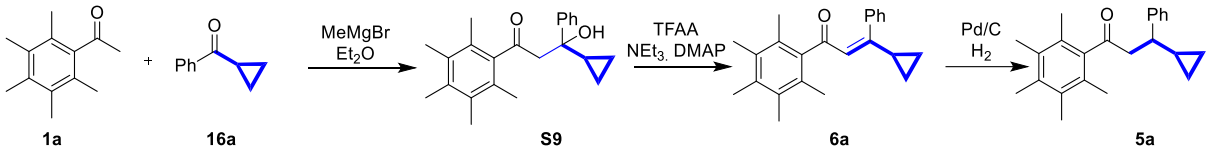
X-ray of **14**
CCDC = 2237255

Table S2 Crystal data and structure refinement for 14

Identification code	KSK-KC 93_auto
Empirical formula	$C_{33}H_{38}N_2O$
Formula weight	478.65
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.8634(3)
b/Å	23.6728(7)
c/Å	8.7931(3)
α/°	90
β/°	99.616(3)
γ/°	90
Volume/Å^3	2639.99(14)
Z	4
ρ_{calc}g/cm^3	1.204
μ/mm^{-1}	0.552
F(000)	1032.0
Crystal size/mm^3	0.002 × 0.002 × 0.001
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.97 to 136.848
Index ranges	-15 ≤ h ≤ 15, -28 ≤ k ≤ 28, -10 ≤ l ≤ 10
Reflections collected	37941
Independent reflections	4821 [R_{int} = 0.0752, R_{sigma} = 0.0290]
Data/restraints/parameters	4821/0/331
Goodness-of-fit on F^2	1.075
Final R indexes [I>=2σ (I)]	R_1 = 0.0457, wR_2 = 0.1164
Final R indexes [all data]	R_1 = 0.0521, wR_2 = 0.1222
Largest diff. peak/hole / e Å^{-3}	0.56/-0.20

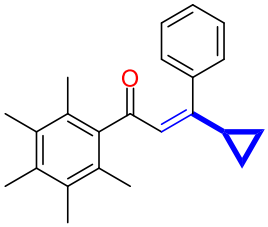
Melting point:125-127 °C

6. Synthesis of the intermediates 5a and 6a.[7]

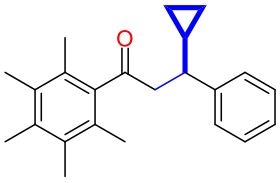


In a 50 mL Schlenk tube pentamethylacetophenone (**1a**, 5 .26 mmol) was taken in 12 mL Et_2O cooled to 0 °C and MeMgBr (3 M, 5.26 mmol) was added dropwise. The mixture was heated at 40 °C and stirred for 1 h, and a white precipitate formed. To this mixture was added 1-cyclopropane-1-phenyl-1-one (**16a**) (1.10 equiv.) in Et_2O (4 mL) dropwise. The reaction mixture was stirred for 3h and quenched with NH_4Cl solution (10 mL). The mixture was extracted with Et_2O: H_2O (60 mL:20 mL), and the organic part was evaporated under vacuum. The compound was purified through column chromatography using Et_2O/ Hexane (5:95), afforded **S9**. (Yield = 45%) as a white solid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.24 (d, *J* = 7.5 Hz, 1H), 4.81 (s, 1H), 3.49 – 3.43 (m, 1H), 3.35 – 3.29 (m, 1H), 2.24 – 2.13 (m, 10H), 2.12 – 1.78 (m, 6H), 1.29 – 1.22 (m, 1H), 0.66 – 0.58 (m, 1H), 0.50 – 0.41 (m, 2H), 0.33 – 0.25 (m, 1H).
Taking **S9** (2 mmol) in DCM was added Et_3N (4.3 equiv.) and DMAP (0.11 equiv.) sequentially. The mixture was cooled to 0 °C, and a solution of TFAA (2 equiv.) in DCM (5 mL) was added dropwise. The reaction mixture was warmed to RT slowly over 16 h, after which aq. NH_4Cl (20 mL), H_2O (5 mL), and Et_2O (20 mL) were added sequentially. The organic layer was separated and evaporated in reduced pressure. The compound **6a** was purified through column chromatography using 2% Et_2O/Hexane and was isolated with 30 % yield.
The intermediate **6a** was then hydrogenated to **5a** using H_2 and Pd/C as a catalyst in the ethanol medium.

6.1 Characterization data of 5a and 6a

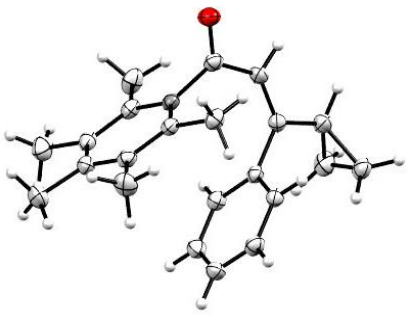


3-cyclopropyl-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylprop-2-en-1-one (6a): Yield = 30%, white solid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.01 (d, *J* = 5.2 Hz, 3H), 6.82 (d, *J* = 5.0 Hz, 2H), 6.40 (s, 1H), 2.05 (s, 3H), 1.99 (s, 12H), 1.72 (dd, *J* = 8.6, 4.0 Hz, 1H), 0.86 – 0.78 (m, 2H), 0.56 – 0.49 (m, 2H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.6, 161.7, 140.4, 136.4, 134.7, 132.4, 128.0, 127.1, 126.8, 126.7, 20.8, 17.7, 16.5, 15.8, 7.4. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{23}H_{27}O]$: 319.2026, found 319.2081.



(S)-3-cyclopropyl-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one (5a): Yield = 90%. White solid.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 4H), 7.28 – 7.16 (m, 2H), 3.30 – 3.12 (m, 2H), 3.02 (t, *J* = 6.4 Hz, 1H), 2.84 – 2.74 (m, 1H), 2.25 (d, *J* = 2.7 Hz, 3H), 2.18 (s, 6H), 1.96 (s, 6H), 1.12 (dt, *J* = 10.1, 4.8 Hz, 1H), 0.91 (t, *J* = 7.4 Hz, 1H), 0.66 – 0.55 (m, 1H), 0.50 – 0.35 (m, 2H), 0.25 (dt, *J* = 9.3, 4.9 Hz, 1H)..**^{13}C NMR** (126 MHz, $CDCl_3$) δ 210.2, 209.9, 145.2, 140.6, 135.4, 133.1, 128.4, 128.39, 128.0, 127.97, 127.5, 126.3, 53.0, 52.7, 44.3, 39.7, 38.7, 29.8, 20.7, 18.0, 16.9, 16.8, 16.0, 14.1, 5.6, 4.4. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{23}H_{29}O]$: 321.2218, found 321.2228.

6.2 Single X-Ray data of 6a



X-ray of **6a**
CCDC = 2237258

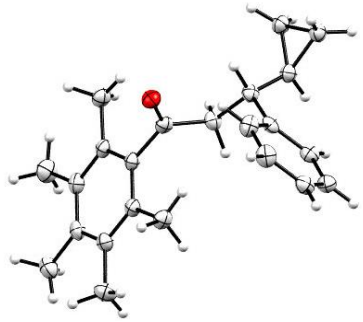
Table S3. Crystal data and structure refinement for 6a

Identification code	BIPKSK_INT_auto
Empirical formula	$C_{46}H_{52}O_2$
Formula weight	636.87
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1

a/Å	9.0547(2)
b/Å	10.15893(15)
c/Å	20.6100(3)
α/°	103.7839(13)
β/°	96.8936(18)
γ/°	92.5400(16)
Volume/Å^3	1822.70(6)
Z	2
ρ_{calc}g/cm^3	1.160
μ/mm^{-1}	0.524
F (000)	688.0
Crystal size/mm^3	0.002 × 0.001 × 0.001
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.456 to 136.62
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 9, -24 ≤ l ≤ 24
Reflections collected	19809
Independent reflections	6602 [R_{int} = 0.0594, R_{sigma} = 0.0438]
Data/restraints/parameters	6602/0/444
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0488, wR_2 = 0.1357
Final R indexes [all data]	R_1 = 0.0518, wR_2 = 0.1388
Largest diff. peak/hole / e Å^{-3}	0.31/-0.24

Melting point: 55-57 °C

6.3 Single X-Ray data of 5a



X-ray of **5a**
CCDC = 2237269

Table S4 Crystal data and structure refinement for 5a.

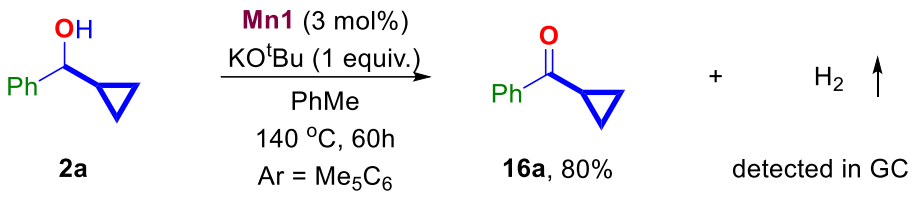
Identification code	KSK- KC PDT_auto
Empirical formula	$C_{23}H_{28}O$
Formula weight	320.45
Temperature/K	99.99(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	16.63527(13)
b/Å	10.05280(9)
c/Å	21.90982(17)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3664.00(5)
Z	8
ρ_{calc}g/cm^3	1.162
μ/mm^{-1}	0.522
F(000)	1392.0
Crystal size/mm^3	0.002 × 0.002 × 0.001
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.07 to 136.814
Index ranges	-20 ≤ h ≤ 20, -12 ≤ k ≤ 12, -26 ≤ l ≤ 25

Reflections collected	36854
Independent reflections	3335 [R_{int} = 0.1229, R_{sigma} = 0.0323]
Data/restraints/parameters	3335/0/223
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0458, wR_2 = 0.1261
Final R indexes [all data]	R_1 = 0.0474, wR_2 = 0.1277
Largest diff. peak/hole / e $Å^{-3}$	0.33/-0.25

Melting point: 52-54 °C

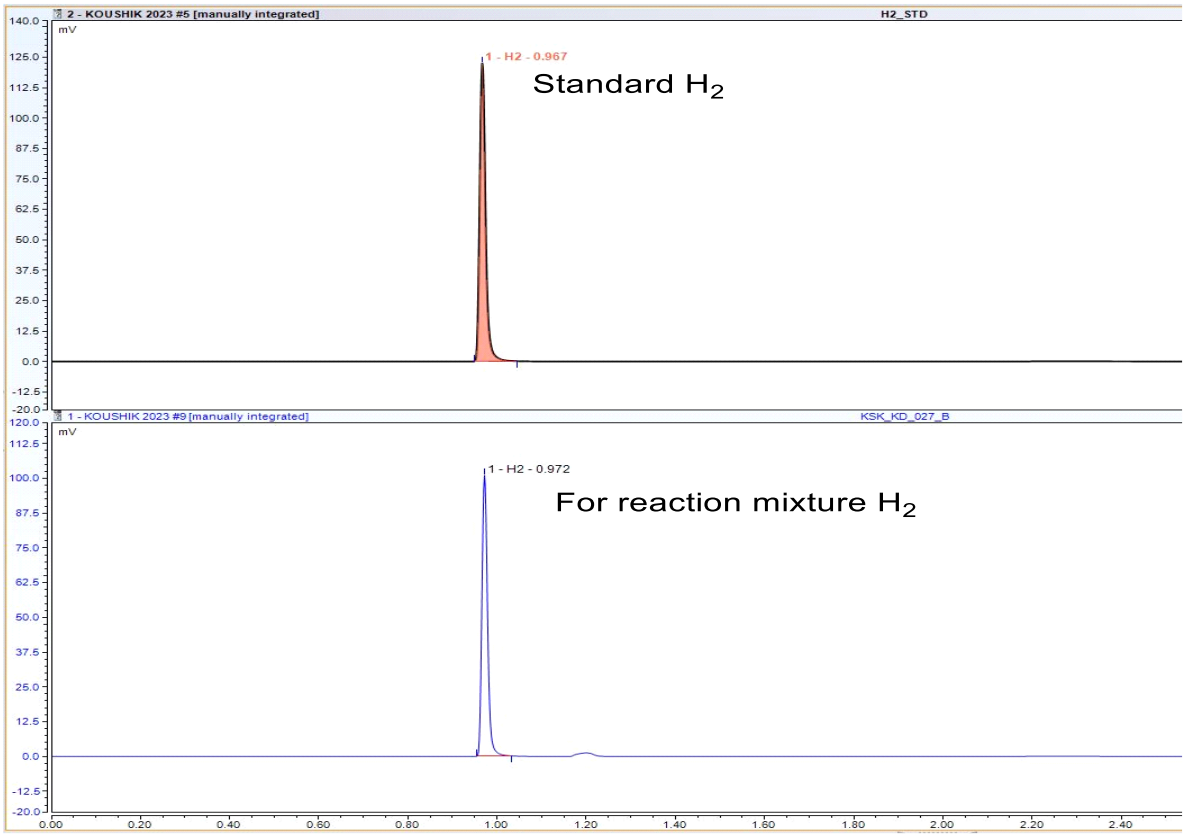
7. Controlled experiment and mechanistic study

7.1 Dehydrogenation of 2a



2a **16a**, 80% detected in GC

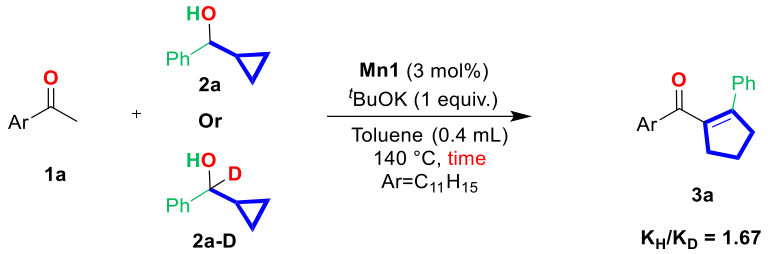
In a 15 ml reaction tube, under an inert atmosphere, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken and kept in a vacuum for 5 min. After flashing with Ar-gas, **2a** (0.2 mmol) in toluene (0.4 mL) was added. The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred for 60 h. After completion, the headspace of the reaction mixture was analyzed by GC. Hydrogen gas was detected. The reaction mixture was then quenched with water (1 mL) and worked up. The compound **16a** was isolated with 80% yield.

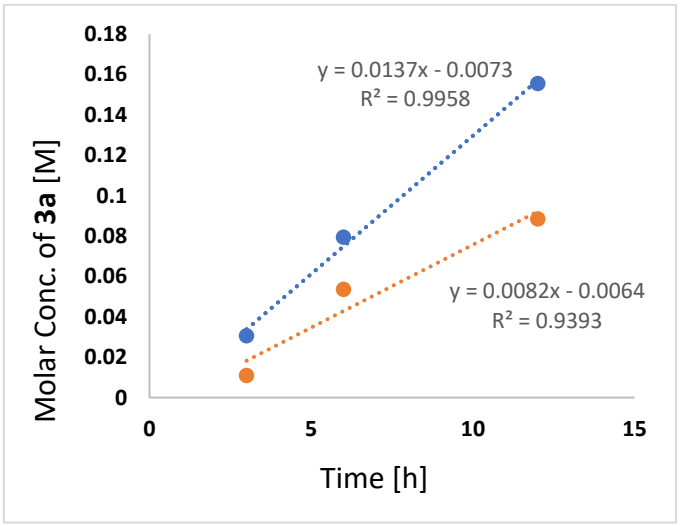


7.2 Kinetic isotope effect

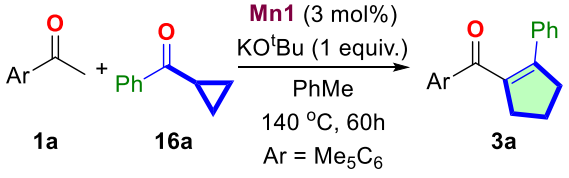
Initially, we carried out the reaction with the standard reaction condition, and data was collected at different time intervals.

In a 15 mL reaction tube, **1a** (0.1 mmol) and deuterated **2a** (0.2 mmol) were added into the reaction of **Mn1** (3 mol%), K^{t}OBu (1 equiv.), and toluene (0.4 mL) under nitrogen atmosphere and stirred at 140 ℃. We set up a few reactions, and after 3 h time interval, the reaction mixture was quenched by the addition of 1M HCl. Followed by the addition of mesitylene as the internal standard into the reaction mixture and transfer for the GCMS analysis. We have determined the primary kinetic isotope effect from the initial rate equation of the reactions. It is observed that the **KIE**=1.67.





7.3 Reaction of 1a with the intermediate 16a



entry	change	% yield of **3a**
1	no	61
2	without **Mn1**	56
3	without ^{t}BuOK	0
4	with TEMPO (1 equiv)	0

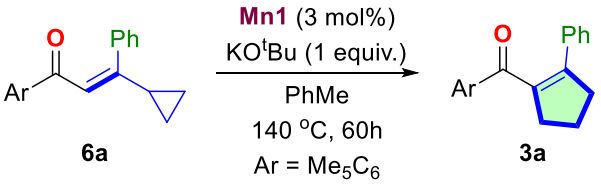
Entry-1. In a 15 ml reaction tube, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken and kept in a vacuum for 5 min. After flashing with Ar, toluene (0.4 mL) was added, followed by the stepwise addition of the ketone (**16a**, 0.4 mmol) and pentamethylacetophenone (**1a**, 0.2 mmol). The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred (250 rpm) for 60 h. After that, the reaction was quenched by adding 2-3 drops of water. It was then passed through a small Na_2SO_4 pad and evaporated under a vacuum. Purification via column chromatography using AcOEt/hexane mixture as an eluent produced **3a** in 61% yield.

Entry-2. In a 15 ml reaction tube, KO^{t}Bu (1 equiv.) was taken and kept in a vacuum for 5 min. After flashing with Ar, toluene (0.4 mL) was added, followed by the stepwise addition of the ketone (**16a**, 0.4 mmol) and pentamethylacetophenone (**1a**, 0.2 mmol). The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred (250 rpm) for 60 h. After that, the reaction was quenched by adding 2-3 drops of water. It was then passed through a small Na_2SO_4 pad and evaporated under a vacuum. Purification via column chromatography using AcOEt/hexane mixture as an eluent produced **3a** in 56% yield.

Entry-3. In a 15 ml reaction tube, **Mn1** (3 mol%) was taken and kept in a vacuum for 5 min. After flashing with Ar, toluene (0.4 mL) was added, followed by the stepwise addition of the ketone (**16a**, 0.4 mmol) and pentamethylacetophenone (**1a**, 0.2 mmol). The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred (250 rpm) for 60 h. After that, the reaction was quenched by adding 2-3 drops of water. It was then passed through a small Na_2SO_4 pad and evaporated under a vacuum. Purification via column chromatography using AcOEt/hexane mixture as an eluent produced **3a** in 61% yield.

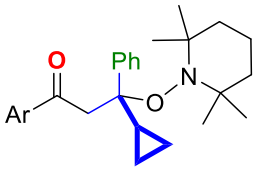
Entry-4. In a 15 ml reaction tube, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken and kept in a vacuum for 5 min. After flashing with Ar, toluene (0.4 mL) was added, followed by the stepwise addition of the ketone (**16a**, 0.4 mmol), pentamethylacetophenone (**1a**, 0.2 mmol), and TEMPO (0.2 mmol). The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred (250 rpm) for 60 h. After that, the reaction was quenched by adding 2-3 drops of water. It was then passed through a small Na_2SO_4 pad and evaporated under a vacuum. The TLC and GC analysis indicated that the product **3a** did not form. Formation of the vinylcyclopropane intermediate **6a** is noticed in about 10% yield.

7.4 Rearrangement of the vinylcyclopropane 6a



entry	change	% yield of **3a**
1	no	59
2	without **Mn1**	55
3	without ^{t}BuOK	0
4	with TEMPO (1 equiv)	0

plausible structure of **C_R-TEMPO** adduct (Ar = Me_5C_6)



HRMS m/z
$[M+H]^+$ Calcd for $[C_{32}H_{46}NO_2]$: 476.3524
found 476.3529

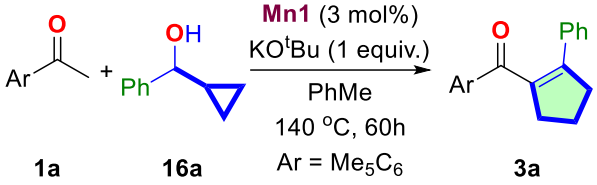
Entry-1. In a 15 mL reaction tube, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken under an inert atmosphere. Toluene (0.4 mL) was added to the mixture with continuous stirring at 250 rpm. The intermediate **6a** (0.1 mmol) was then added. The reaction mixture was stirred for 72 h at 140 °C. After that, it was cooled to room temperature and quenched with water. The compound was then purified by column chromatography using hexane and hexane (98:2) to obtain 59% yield of **3a**

Entry-2. In a 15 mL reaction tube, KO^{t}Bu (1 equiv.) was taken under an inert atmosphere. Toluene (0.4 mL) was added to the mixture with continuous stirring at 250 rpm. The intermediate **6a** (0.1 mmol) was then added. The reaction mixture was stirred for 72 h at 140 °C. After that, it was cooled to room temperature and quenched with water. The mixture compound was then purified by column chromatography using hexane and hexane (98:2) to obtain 55% yield of **3a**.

Entry-3. In a 15 mL reaction tube, intermediate **6a** (0.1 mmol) and toluene were taken and heated at 140 °C for 72 h. No conversion of the intermediate **6a** happened, as indicated by GCMS analysis of the crude reaction mixture using mesitylene as the internal standard. The reaction mixture was purified by flashed chromatography. We have recovered **6a** in 70% yield. *E*/*Z* isomerization happens *E*/*Z* = 55:45.

Entry-4. In a 15 mL reaction tube, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken under an inert atmosphere. Toluene (0.4 mL) was added to the mixture with continuous stirring at 250 rpm. The intermediate **6a** (0.1 mmol) was then added. Into this reaction mixture TEMPO (1 equiv.) was added. The reaction mixture was stirred for 72 h at 140 °C. After that, it was cooled to room temperature and quenched with water. No conversion of the intermediate **6a** happened, as indicated by GCMS analysis of the crude reaction mixture using mesitylene as the internal standard. HRMS analysis of the reaction mixture identified TEMPO adduct with molecular formula $C_{32}H_{46}NO_2$. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{32}H_{47}NO_2]$: 476.3524, found 476.3529.

7.5 Quenching experiment in the presence of TEMPO and BHT



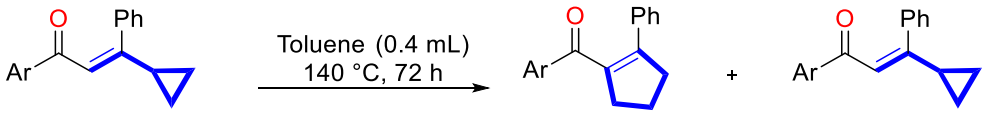
1a **16a** **3a**

entry	change	% yield of **3a**
1	no	90
2	with TEMPO (1 equiv)	0
3	with BHT (1 equiv)	0

Entry-2. In a 15 ml reaction tube, under an inert atmosphere, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken and kept in a vacuum for 5 min. After flashing with Ar-gas, toluene (0.4 mL) was added, followed by the stepwise addition of Cyclopropane-derived alcohol (**2a**, 2 equiv.) and pentamethylacetophenone (**1a**, 0.1 mmol), followed by the addition of TEMPO (1 equiv.).The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred for 72 h with stirring 250 rpm. After completion of the reaction, it was quenched with 2-3 drops of water and sent for HRMS analysis. The HRMS data confirmed that the reaction intermediate formed insitu of the reaction medium is trapped by TEMPO, giving the TEMPO adduct m/z value. The GCMS analysis of the reaction mixture indicated that **3a** did not form. HRMS analysis of the reaction mixture identified TEMPO adduct with molecular formula $C_{32}H_{46}NO_2$. **HRMS (ESI-TOF) m/z:** $[M+H]^+$ Calcd for $[C_{32}H_{47}NO_2]$: 476.3524, found 476.3529.

Entry-3. In a 15 ml reaction tube, under an inert atmosphere, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken and kept in a vacuum for 5 min. After flashing with Ar, toluene (0.4 mL) was added, followed by the stepwise addition of cyclopropane-derived alcohol (**2a**, 2 equiv.) and pentamethylacetophenone (**1a**, 0.1 mmol), followed by the addition of BHT (1 equiv.).The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred for 72 h with stirring 250 rpm. After completion of the reaction, it was quenched with 2-3 drops of water. The GCMS analysis of the reaction mixture indicated that **3a** did not form.

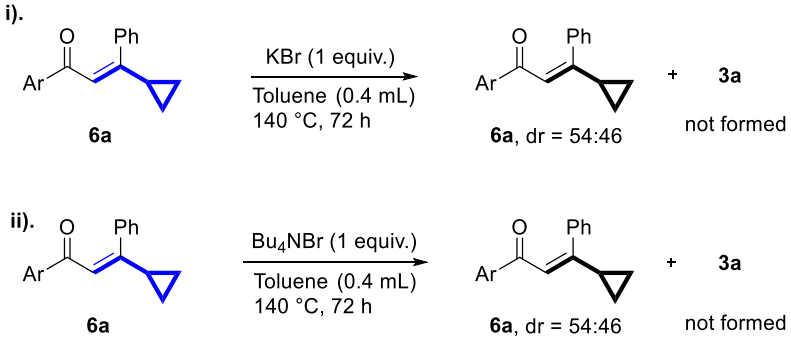
7.6 Thermal rearrangement of vinylcyclopropane 6a



6a **3a**, not formed **6a**, 70% *E/Z* = 55:45

In a 15 mL reaction tube, intermediate **6a** (0.1 mmol) and toluene were taken and heated at 140 °C for 72 h. No conversion of the intermediate **6a** happened, as indicated by GCMS analysis of the crude reaction mixture using mesitylene as the internal standard. The reaction mixture was purified by flashed chromatography. We have recovered **6a** in 70% yield. *E*/*Z* isomerization happens *E*/*Z* = 55:45.

7.7 Addition of nucleophile to 6a



7.7.1. In a 15 mL reaction tube, KBr (1 equiv.) was taken under an inert atmosphere. Toluene (0.4 mL) was added to the mixture with continuous stirring at 250 rpm. The intermediate **6a** (0.1 mmol) was then added. The reaction mixture was stirred for 72 h at 140 °C. After that, it was cooled to room temperature and quenched with water. No conversion of the intermediate **6a** happened, as indicated by GCMS analysis of the crude reaction mixture using mesitylene as the internal standard. The reaction mixture was purified by flashed chromatography. We have recovered **6a** in 71% yield. *E/Z* isomerization happens *E/Z* = 55:45.

7.7.2. In a 15 mL reaction tube, Bu_4NBr (1 equiv.) was taken under an inert atmosphere. Toluene (0.4 mL) was added to the mixture with continuous stirring at 250 rpm. The intermediate **6a** (0.1 mmol) was then added. The reaction mixture was stirred for 72 h at 140 °C. After that, it was cooled to room temperature and quenched with water. No conversion of the intermediate **6a** happened, as indicated by GCMS analysis of the crude reaction mixture using mesitylene as the internal standard. The reaction mixture was purified by flashed chromatography. We have recovered **6a** in 70% yield. *E/Z* isomerization happens *E/Z* = 55:45.

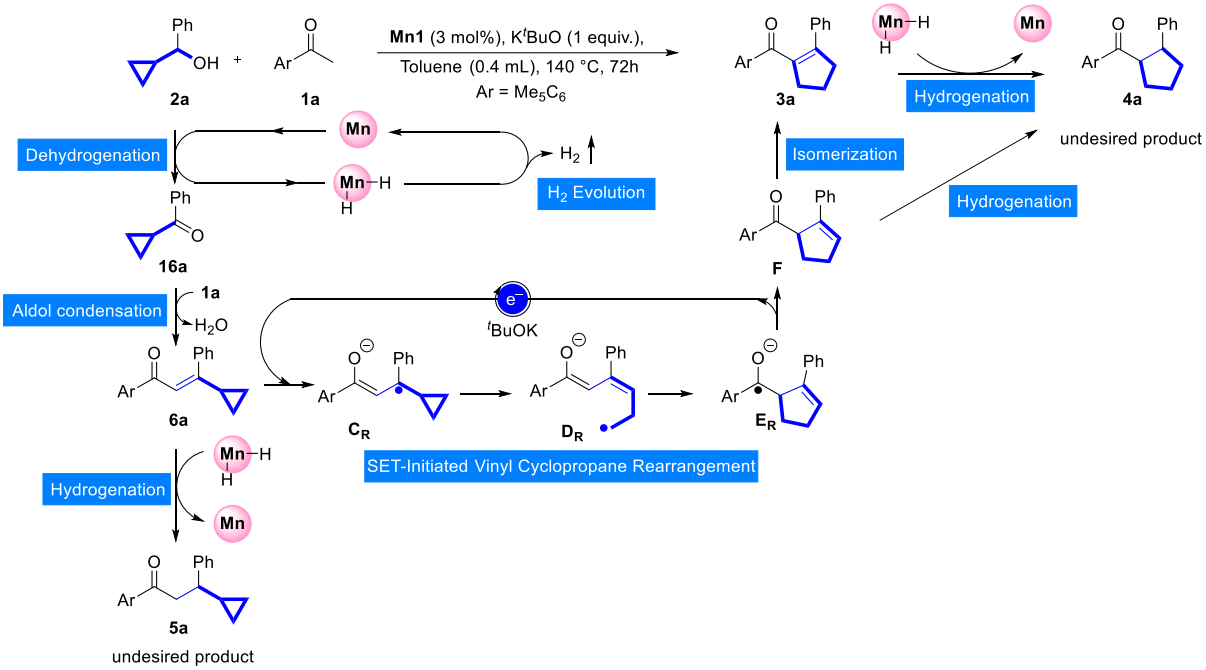
These two observations indicate that the reaction does not proceed by ionic pathways with a nucleophilic attack by a bromide ion to **6a**.

7.8 Evolution of hydrogen gas.

In a 15 ml reaction tube, **Mn1** (3 mol%) and KO^{t}Bu (1 equiv.) were taken and kept in a vacuum for 5 min. After flashing with Ar, toluene (2 mL) was added, followed by the stepwise addition of **2a** (2 equiv.) and **1a** (0.5 mmol). The tube was closed, and the mixture was placed in a preheated bath at 140 °C and stirred (250 rpm) for 60 h.

After cooling at room temp. H_2 gas was detected using GC-TCD along with a 60% yield of the desired product.

7.9 Proposed reaction mechanism



8. Computational Details

All calculations were carried out using the Gaussian09 suite of programme.[11] The geometries of all stationary states were optimized with hybrid exchange-correlation B3LYP functional,[12] overlayed with Grimme's empirical dispersion D3(BJ) correction term,[13] employing the IOp(3/124=40) keyword, in conjunction with Pople's 6-31G(d,p) basis sets for C, H, N, O; an added diffuse function with the 6-31+G(d,p) basis set on P and S whereas double-ζ LANL2DZ in combination with LANL2 effective core potential were used to express atom-centred basis set on K, Br, and Mn.[14-16] This basis set combination is named as B1. B3LYP has been the chosen functional for all the optimizations as it has been reported to correctly describe the geometry of species studied in the catalytic reactions of analogous Manganese complexes[17, 18] as well as correctly account for the electronic structure and thereby energies of open-shell radical species.[19] Harmonic frequencies were computed to characterize the structures as a minimum (all real frequencies) and transition state (one imaginary mode) and also to extract thermo-chemical information at the experimental temperature (413.15K). Intrinsic reaction coordinate scans were conducted to connect the transition states with relevant intermediates on either side. The solvent effect was introduced by utilizing Truhlar and coworkers' universal SMD solvation model, utilizing the dielectric constant of toluene (ε=2.3741).[20] Further, the electronic energies were refined by single-point calculations with Ahlrichs' all electron def2-TZVPP basis sets[21] at B3LYP-D3(BJ)/SMD(Toluene)/def2-TZVPP, M06/SMD(Toluene)/def2-TZVPP[22] and TPSSh-D3(BJ)/SMD(Toluene)/def2-TZVPP[23] on top of the B3LYP-D3(BJ)/B1 optimized geometries. For hydrogenation and H_2 evolution case of complex **MnV** mentioned in S8.5 (Figure S5 c, d), SMD solvation model with 1- pentanol as solvent (ε=5.78) instead was incorporated during geometry optimizations.

Notably, we have performed all the geometry optimizations in the SMD solvent model. However, the entropy of each solute was obtained through the Sakur−Tetrode equation, which essentially treats the molecules as an ideal gas. Since in the ideal gas model, the damping of translational and rotational degrees of freedom in the solvent phase gets ignored, the entropy is overestimated. This is in line with observations by Wertz[24] and Spickermann[25] that the entropy of a solute should be estimated to be 0.46S(g) or 0.67S(g), where S(g) is the entropy of the solute in gas phase. Furthermore, experiments by Yu and Houk[26] have demonstrated that the ideal gas model could overestimate the entropic contribution for bimolecular reaction by 50−70%. Hence, to compensate for such a situation, and based on previous reports,[27-29] we have computed the solution phase entropy of each solute species scaled by an empirical factor of 0.5 times the entropy obtained from the rigid-rotor model and corrected the solution phase Gibbs free energy according to equation (1).

$$G_{\mathrm{SMD}}^{0.5} = E_{\mathrm{SMD}} + H_{\mathrm{corr(SMD)}} + 0.5\,(G_{\mathrm{corr(SMD)}} - H_{\mathrm{corr(SMD)}}) \quad (1)$$

E_{SMD} = solvent phase energy obtained after optimization using the SMD solvent model

$H_{\mathrm{corr(SMD)}}$ = enthalpic correction obtained in the solution phase

$G_{\mathrm{corr(SMD)}}$ = Gibbs free energy correction obtained in the solution phase

$G_{SMD}^{0.5}$ = solution phase corrected free energy

The free energy activation barrier equation (2) and free energy change at each reaction step equation (3) has been determined using the solution phase corrected free energy.

$$\Delta G_{0.5}^{\ddagger} = G_{(SMD)}^{0.5}(Ts) - G_{(SMD)}^{0.5}(r) \quad (2)$$

$$\Delta G_{0.5} = G_{(SMD)}^{0.5}(p) - G_{(SMD)}^{0.5}(r) \quad (3)$$

$\Delta G_{0.5}^{\ddagger}$ = free energy activation barrier

$\Delta G_{0.5}$ = free energy change of a reaction step

Ts = transition state of a reaction step

p = product of a reaction step

r = reactant of a reaction step

However, for H_2(g) we have taken the gas-phase entropy, i.e., 1.0 scaling factor has been applied to the entropy obtained from gas-phase quantum chemical calculations.[30, 31] This accounts for correcting the solution phase Gibbs free energy by 7-18 kcal/mol. It must be noted that the application of the correction scheme does not overrule our proposed reaction mechanism. For validation, we have provided zero-point corrected total energy values in Table S5 and S6 for reactions shown in the main text Figure 1 and Figure 2.

Table S5. Relative zero-point corrected energy and Gibbs free energy in kcal/mol for the metal-assisted pathway as reported in Figure 1b (main text).

Species	ΔE(ZPE)	ΔG
RCMn1	0.0	0.0
RCMn2	9.9	9.2
TS1	17.4	18.2
INT1	18.5	19.5
TS2 [a]	19.8	21.1
MnH2 [b]	14.8	-6.6
TS3 [c]	15.1	15.1
Mn1a	28.0	-5.6

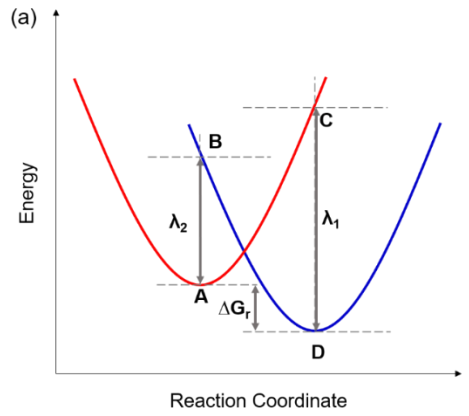
[a] **16a** released after here is not shown. [b] **2a** added here is not shown. and [c] **2a**, **H_2** released after here are not shown.

Table S6. Relative zero-point corrected energy (ΔE(ZPE)), and relative Gibbs free energy of reaction (ΔG_r) in kcal/mol for the metal unassisted pathway are reported in Figure 2 (main text).

Species	ΔE(ZPE)	ΔG_r
A+16a	0.0	0.0
TS4	5.4	15.0
17a [a]	1.6	11.3
TS5 [b]	-9	11.8
6a [c]	-2.9	6.7
C_R [d]	-23.1	-14.4
$TS6_R$	-7.1	1.8
D_R	-10.8	-2.3
$TS7_R$	-0.1	9.3
E_R [e]	-26.6	-17.4
F [f]	-46.8	-37.8
3a	-45.8	-37.1

[a] **2a** added here is not shown. [b] **2a⁻…H₂O** released after here is not shown. [c] **E_R** added here is not shown. [d] **F** radical released here is not shown. [e] **6a** added here is not shown. [f] **C_R** released here is not shown.

The SET activation barriers ($\Delta G_{SET}^{\ddagger}$) presented in the manuscript (Figure 2) are calculated using the Marcus theory. The key concept of Marcus theory and formula used are represented in Figure S4.



(b)

$$\lambda = \lambda_i + \lambda_o \quad \text{..... (1)}$$

$$\lambda_i = \frac{\lambda_1 + \lambda_2}{2} \quad \text{..... (2)}$$

$$\lambda_0 = 332\left(\frac{1}{2r_1} + \frac{1}{2r_2} - \frac{1}{R}\right)\left(\frac{1}{\epsilon_{op}} - \frac{1}{\epsilon_{sp}}\right) \quad \text{..... (3)}$$

$$\Delta G^0 = -nFE^0 \quad \text{..... (4)}$$

$$E^0 = -\frac{\Delta G_r}{F} \quad \text{..... (5)}$$

$$\Delta G^{\ddagger}_{SET} = \frac{(\lambda + \Delta G_r)^2}{4\lambda} \quad \text{..... (6)}$$

Figure S1. (a) The key concept of Marcus theory and (b) formula used for ($\Delta G_{SET}^{\ddagger}$ calculation.

- A = E_R(G_R) is the energy of the reactant in the reactant geometry
- B = E_P(G_R) is the energy of the product in the reactant geometry
- C = E_R(G_P) is the energy of the reactant in the product geometry
- D = E_P(G_P) is the energy of the product in the product geometry
- ΔG_r = Difference in Gibbs free energy of reaction
- λ = Total reorganization energy
- λ_i = Inner sphere reorganization energy
- λ_o = Outer sphere reorganization energy
- r_1 = radius of single electron donor species
- r_2 = radius of single electro acceptor species
- ϵ_{op} = optical dielectric constant of solvent molecule
- ϵ_{sp} = static dielectric constant of solvents molecule
- ΔG^0, E^0 and F= standard Gibbs free energy difference standard electrode potential and Faraday constant respectively

8.1 Relative energetics for the metal-assisted and unassisted pathways at different levels of theory.

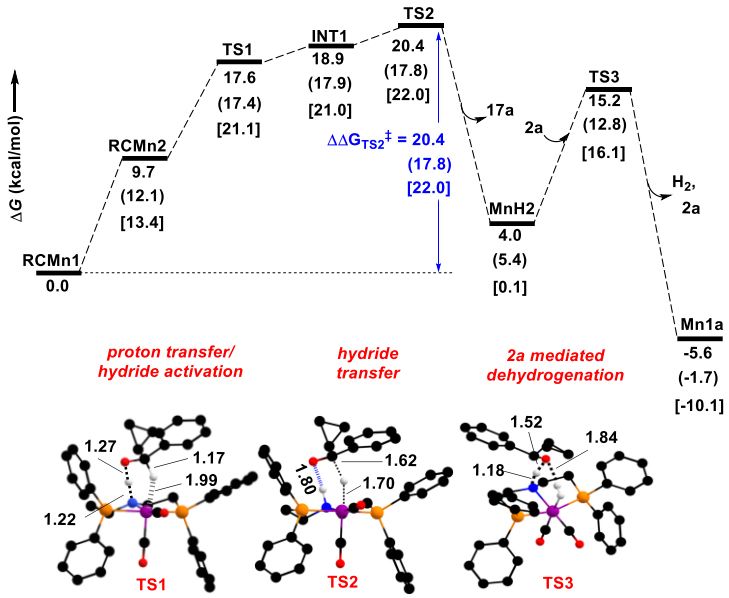


Figure S2. Reaction-free energy profile (in kcal/mol) for the metal-assisted C-H activation of alcohol (**2a**) to ketone (**16a**) by **Mn1** complex at B3LYP-D3(BJ)/SMD(Toluene)/def2-TZVPP, TPSSh-D3(BJ)/SMD(Toluene)/def2-TZVPP and M06L/SMD(Toluene)/def2-TZVPP level of theory. The last two levels are given in parentheses and brackets, respectively. Color coding of optimized geometry of **TS1**, **TS2** and **TS3** shown in Figure S1: C(black), H(white), O(red), P(orange), N(blue), Mn(purple). Distances shown are in units of Å. Unimportant hydrogen atoms are not shown for clarity.

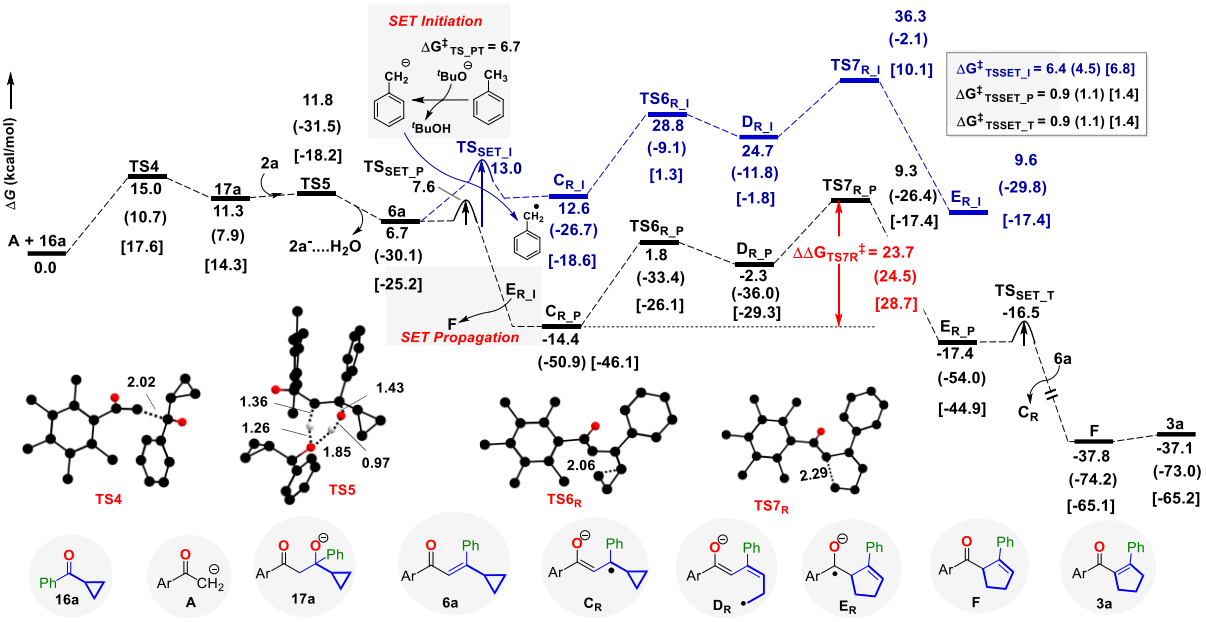
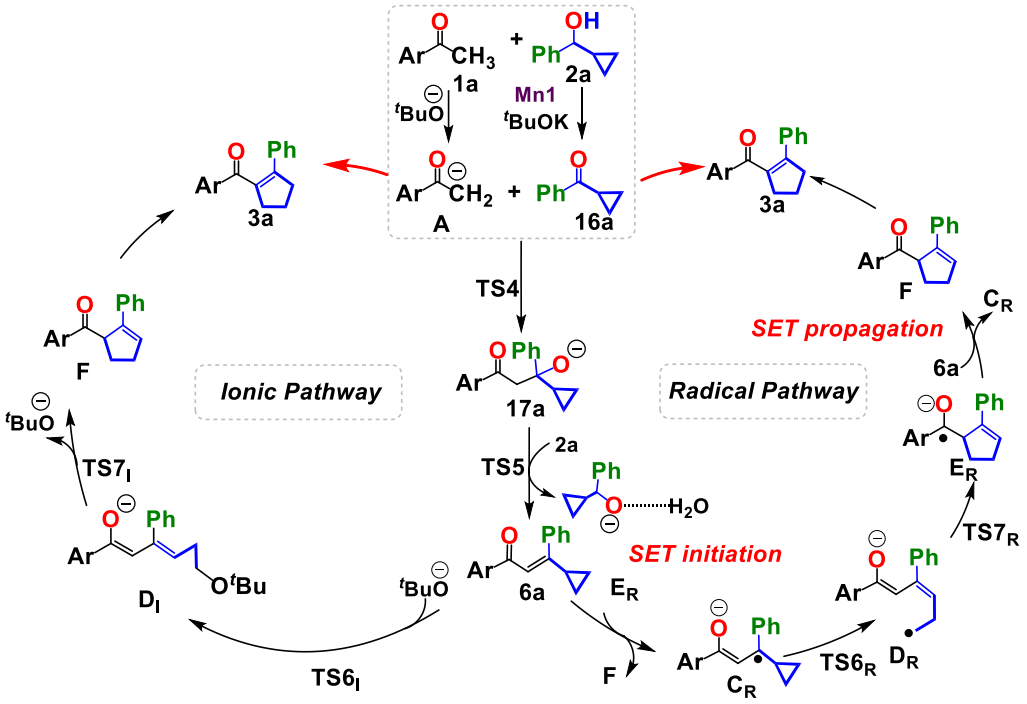


Figure S3. Reaction-free energy profile (in kcal/mol) for the metal-unassisted pathway at B3LYP-D3(BJ)/SMD(Toluene)/def2-TZVPP, TPSSh-D3(BJ)/SMD(Toluene)/def2-TZVPP and M06L/SMD(Toluene)/def2-TZVPP level of theory. The last two levels are given in parentheses and brackets, respectively. Color coding of optimized geometry of **TS4**, **TS5**, **TS6$_R$** and **TS7$_R$** shown in Figure S2: C(black), H(white), O(red), P(orange), N(blue), Mn(purple). Distances shown are in units of Å. Unimportant hydrogen atoms are not shown for clarity. Subscript R denotes radical pathway.

8.2 Alternative pathways explored for 3a formation from A and 16a in the metal unassisted pathways.



Scheme S1. Schematic representation of different pathways for **3a** formation.

As mentioned in the main text, different pathways are explored for the metal unassisted reaction (Scheme S1). The free energies in Figure S4 are shown from the key common intermediate **6a**.

We have investigated the formation of **3a** from intermediate **6a** with single electron transfer (SET) and nucleophilic attack pathways, as shown in Scheme S1 and Figure S3. The SET initiation can occur either through *in situ* generated radical anion, $PhCH_2^-$ or $^tBuO^-$. Due to the predominantly high barrier of the ring-closure transition state, **TS7R** ($\Delta G^‡$ = 56.4 kcal/mol) in the $^tBuO^-$ / $^tBuO^•$ mediated pathway (Figure S3), this pathway has been ruled out. Additionally, the formation of a highly stable intermediate, **DI** raises the rate-determining barrier for the formation of the a β,γ-unsaturated 5-membered neutral cyclopentene, **F**, in the S_N2 pathway to 36.0 kcal/mol while the $PhCH_2^-$/$PhCH_2^•$ mediated pathway shows the highest barrier of 36.3 kcal/mol. However, the *in situ* generated radical anion **ER** initiated SET requires only 23.7 kcal/mol. Computationally calculated single electron transfer activation barriers sheds light on favourability of SET propagation through **ER** ($\Delta G_{SET}^‡$ = 0.9 kcal/mol) and further trend in energies against other pathways (see S8.3 for details of calculation). Hence, it is the most feasible mechanistic pathway for the formation of **3a**.

It is unlikely on the metal complex to direct the rearrangement of **6a** in the radical pathway. The precursor catalyst **Mn1** is the source of Br^- anion, which can mediate S_N2 based ring opening and ring closing rearrangement reactions forming cyclopentene product. However, we found that the kinetic barrier for the ring closing elementary step turned out to be 28.1 kcal/mol. This is again higher than the *in situ* generated radical anion **ER** propagated SET pathway of ring closing via **TS7R** (23.7 kcal/mol). This rules out the role of Mn in the second part of the hypothesized mechanism.

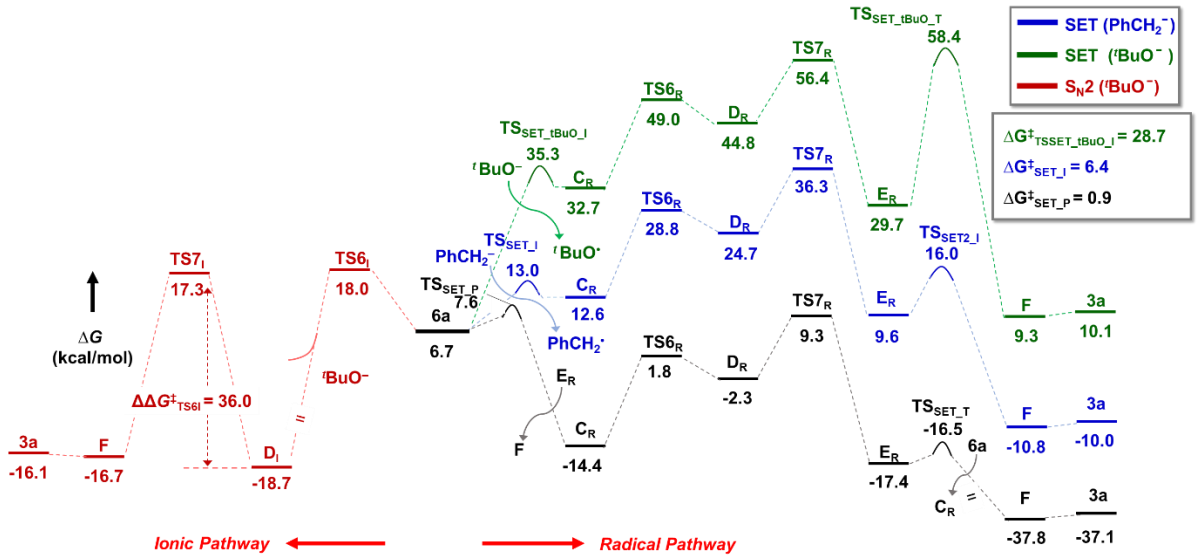


Figure S4. Comparative reaction free energy profiles (in kcal/mol) for the formation of **3a** with **A** and **16a** in the metal unassisted pathways at B3LYP/def2-TZVPP. (Energies of transition states $TS6_R$, $TS7_R$, intermediates (C_R, D_R, E_R) and product (**3a**) are different in different paths due to involvement of different SET electron donors or electrophile in each case)

Table S7. Relative Gibbs free energy in kcal/mol for the metal unassisted SET pathway with $PhCH_2^-$/$PhCH_2^\bullet$ pair with different functionals, SMD(Toluene) and def2-TZVPP basis set.

Species	B3LYP	TPSSh	M06L
6a	6.6	-30.0	-25.2
C_R	12.6	-26.7	-18.6
$TS6_R$	28.8	-9.1	1.3
D_R	24.7	-11.8	-1.8
$TS7_R$	36.3	-2.1	10.1
E_R	9.6	-29.8	-17.4
F	-10.8	-49.9	-37.6
3a	-10.0	-48.8	-37.7

Table S8. Relative Gibbs free energy in kcal/mol for the metal unassisted SET pathway with $^tBuO^-$/$^tBuO^\bullet$ pair with different functionals, SMD(Toluene) and def2-TZVPP basis set.

Species	B3LYP	TPSSh	M06L
6a	6.6	-30.0	-25.2
C_R	32.7	-7.9	-0.6
$TS6_R$	49.0	9.6	19.3
D_R	44.8	7.0	16.2
$TS7_R$	56.4	16.6	28.1
E_R	29.7	-11.0	0.5
F	9.3	-31.1	-19.7
3a	10.1	-30.0	-19.8

Table S9. Relative Gibbs free energy in kcal/mol for the metal unassisted S_N2 with $^tBuO^-$ anion with different functional, SMD(Toluene) and def2-TZVPP basis set.

Species	B3LYP	TPSSh	M06L
6a	6.6	-30.0	-25.2
TS6$_I$	18.0	-22.4	-14.1
D$_I$	-18.7	-56.7	-45.3
TS7$_I$	17.3	-23.5	-8.7
F	-16.7	-53.3	-44.2
3a	-16.1	-52.2	-44.3

8.3 Why hydrogenation of 3a is less feasible?

We have carried out additional computations to understand why the final α,β-unsaturated cyclopentene product **3a** does not undergo hydrogenation despite forming a metal-hydride species, **MnH$_2$**. We also investigated the reason for slower rates of hydrogenation of **6a**. At first, we calculated the hydricity of the monohydride and substrates. The ability of a metal hydride to transfer its hydrogen to any system can be quantified through its hydricity value, which measures the strength of the metal-hydrogen bond. The calculated hydricity of our manganese mono-hydride system, **MnH2**, is 44.6 kcal/mol, which is fairly low and susceptible to donation. This agrees to the calculated hydride dissociation energy (46.4 kcal/mol) of the corresponding Mn-hydride complex of Beller's **Mn2**. The hydricity of **6a** and **3a** are 120.5 and 86.0 kcal/mol, respectively, which suggests the possibility of a facile hydride transfer from the manganese monohydride. At this stage, the mono hydride **MnH2** has two choices: hydrogenation of product **3a**, or dehydrogenation of the metal hydride system itself. The activation barrier for hydrogenation of **6a** was found to be 29.3 kcal/mol (Figure S5a), and **3a** hydrogenation takes place at the expense of 19.2 kcal/mol (Figure S5b). The self-dehydrogenation of **MnH2** occurs at a kinetic barrier of 24.3 kcal/mol through the transition state **TS3$_{self}$**. Interestingly, **2a** alcohol-assisted dehydrogenation of **MnH2** (proposed in the main text, Figure 1) occurs at an incredibly lower activation barrier than any of the other possibilities ($\Delta\Delta G^{\ddagger}_{TS3}$ =11.1 kcal/mol). Hence, unlike previous reports,[7] the alcohol-assisted dehydrogenation process should predominate over hydrogenation of the *in situ* generated alkenes. Furthermore, in the absence of **MnH2**, a simple reduction of **3a** in a concerted way with released molecular H_2 at 1,4 position requires a predominantly high barrier of 41.0 kcal/mol (**TS9$_{_H2}$**), which is very unlikely at given reaction conditions. This explains the absence of hydrogenated products of the targeted cyclopentene.

Encouraged by the findings of our curious case, we further analyzed dehydrogenation vs. hydrogenation possibilities of a previously reported catalyst here, mentioned as **MnV**.[17, 18b] The hydricity of **MnV** is 34.8, which supports the calculated barrier for the otherwise difficult hydride transfer (HT) to **3a** ($\Delta\Delta G^{\ddagger}_{TSMnV3}$ =4.6 kcal/mol). Similarly, for **5**, the HT takes place at 3.8 kcal/mol (Figure S5c and S5d). However, self-dehydrogenation **TSMnV2$_{self}$** and diol-assisted dehydrogenation **TSMnV2$_{5\text{-}ass}$** are 20.6 and 18.6 kcal/mol, respectively (Figure S5d). Hence, **MnV** mono hydride favors the hydrogenation of alkene products over dehydrogenation. Incidentally, these two Mn pincer complexes hydrogenate through metal-ligand cooperativity. **MnV** mono hydride has the advantage of a labile thiophene end, which easily detaches itself for the incoming substrate, thus facilitating hydrogenation. On the other hand, in **MnH2**, the metal is coordinated with amine and phosphine ligands through a rigid, non-labile backbone. Thus, combined electronic (hydricity) and steric effects play a crucial role in hydrogenation performance.

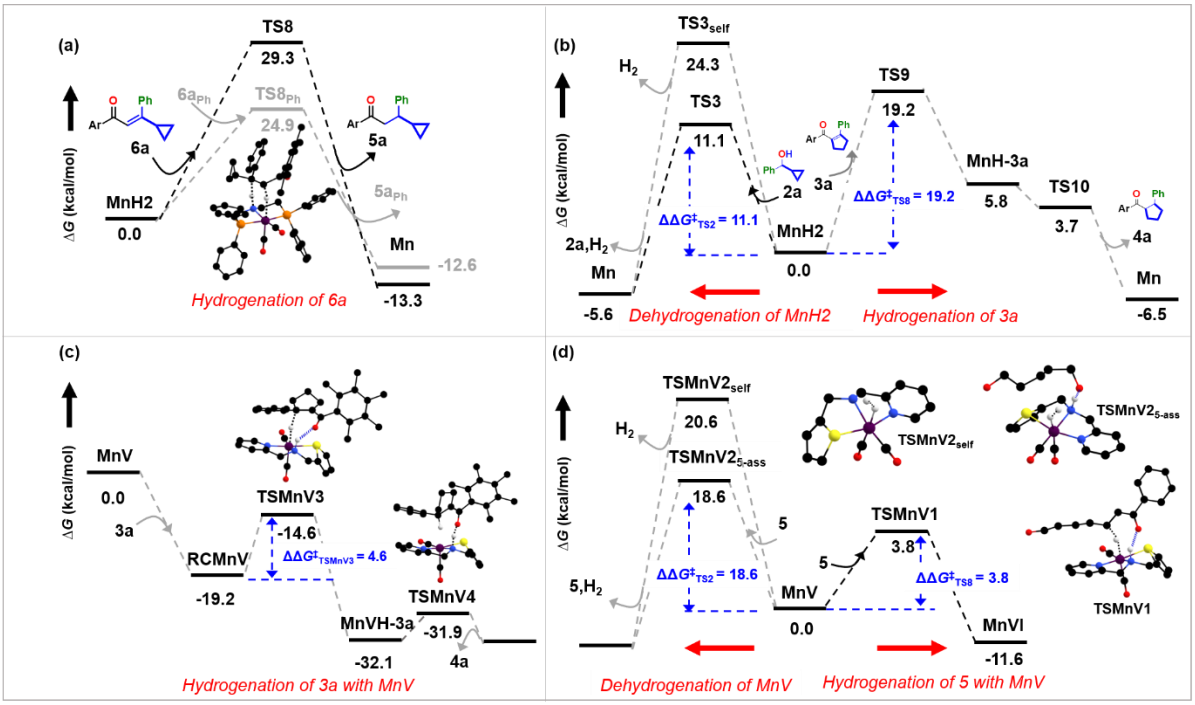


Figure S5. Reaction free energy profiles (in kcal/mol) for the hydrogenation of (a) hydrogenation of **6a** and **6aPh** (b) dehydrogenation of **MnH2** vs hydrogenation of **3a** (c) hydrogenation of **3a** with **MnV** and (d) dehydrogenation of **MnV** vs hydrogenation of **5** with **MnV** at B3LYP-D3(BJ)/SMD(Toluene)/def2-TZVPP. Colour coding for the optimized geometries of **TS8**, **TS8$_{Ph}$**, **TS9**, **TS10** **TS3$_{self}$**, **TS3**, **TSMnV2$_{self}$**, **TSMnV2$_{5\text{-}ass}$**, **TSMnV1**, **TSMnV3**, and **TSMnV4**: C(black), H(white), O(red), P(orange), N(blue), Mn(purple). Distances shown are in units of Å. Unimportant hydrogen atoms are not shown for clarity.

8.4 IRC of important transition states

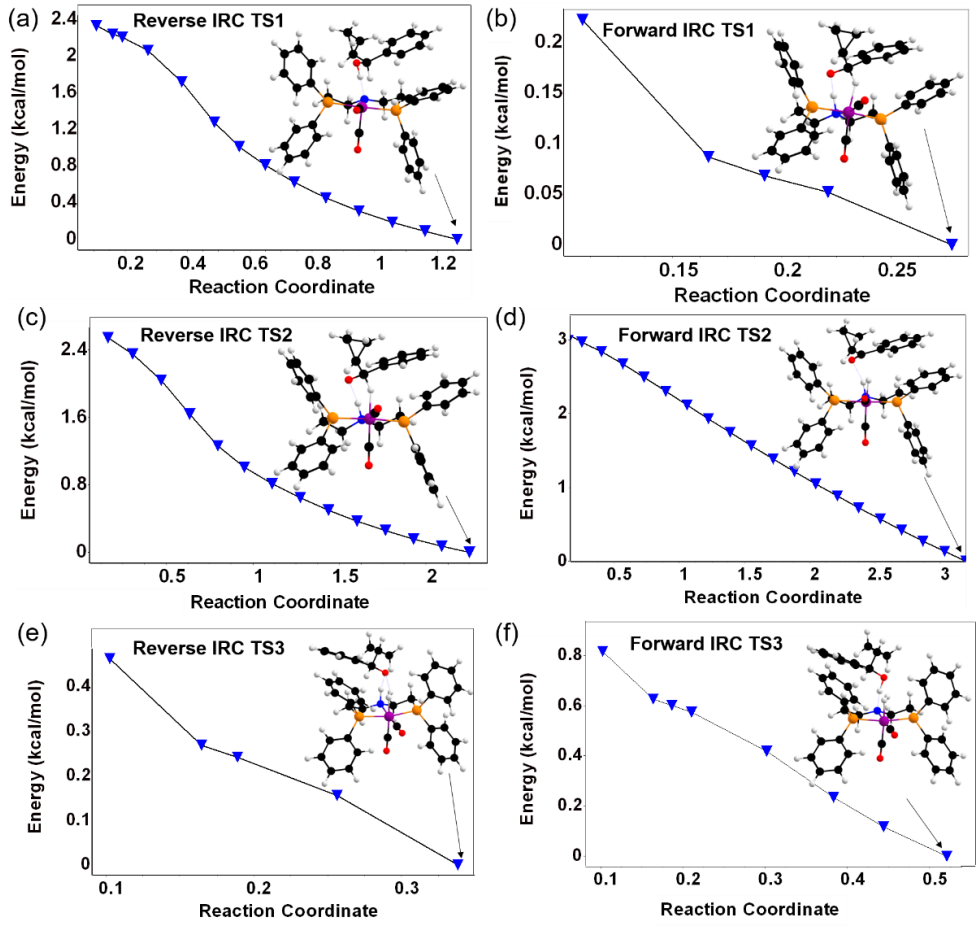


Figure S6. Dehydrogenation of **2a**, (a) Reverse IRC and (b) Forward IRC along transition state TS1, (c) Reverse IRC and (d) Forward IRC along transition state TS2, (e) Reverse IRC and (f) Forward IRC along transition state TS3. Colour coding: C(black), H(white), O(red), P(orange), N(blue), Mn(purple). Distances shown are in unit of Å.

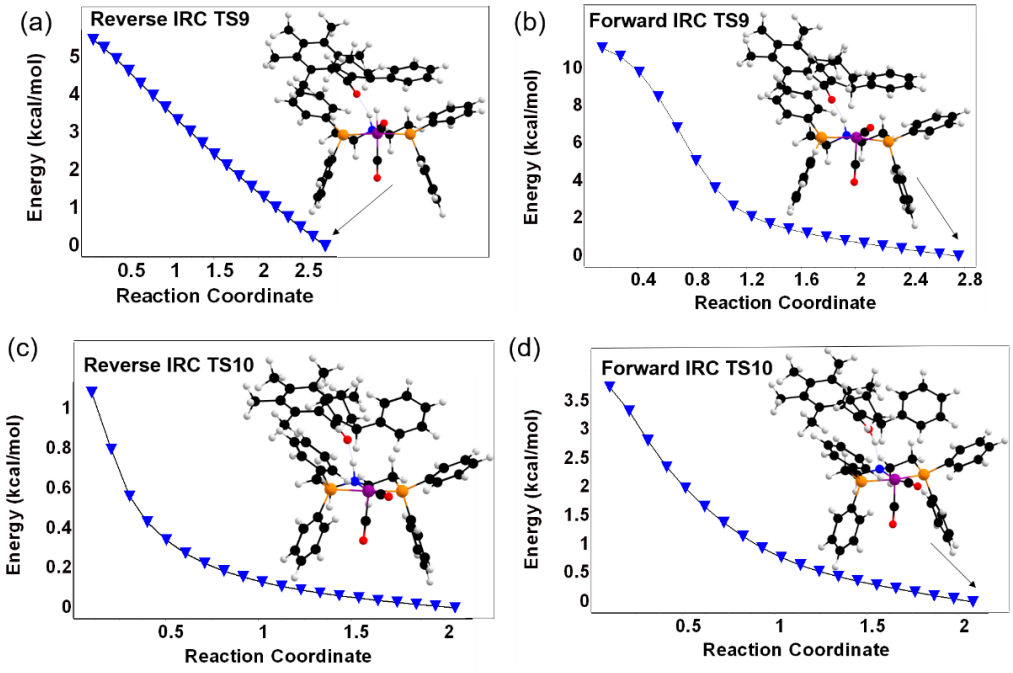
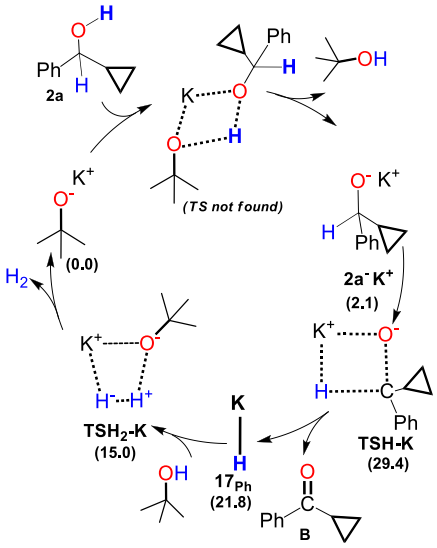


Figure S7. Hydrogenation of **3a**, (a) Reverse IRC and (b) Forward IRC along transition state TS9, (c) Reverse IRC and (d) Forward IRC along transition state TS10. Colour coding: C(black), H(white), O(red), P(orange), N(blue), Mn(purple). Distances shown are in units of Å.

8.5 Dehydrogenation of $2a_{Ph}$ with the assistance of ^{t}BuOK.



Scheme S2. Probable mechanistic path for dehydrogenation of $\mathbf{2a_{Ph}}$ with ^{t}BuOK with reaction Gibbs free energy in kcal/mol at B3LYP-D3(BJ)/SMD(Toluene)/Def2-TZVPP level of theory.

Dub and Tkachenko have reported that self-dehydrogenation of tert-butyl phenyl methanol to pivalophenone takes place reversibly at a predominantly high energetic requirement with $\Delta G^{\ddagger}$ = 79 kcal/mol at M06-2X-D3/def2-QZVP level at two different temperatures (25 and 210°C).[32] However, ^{t}BuOK is proposed to be a catalyst during the hydrogenation of pivalophenone with H_2. On a similar note, we tried to investigate the possibility of a base-catalyzed dehydrogenation of the cyclopropyl alcohol. ^{t}BuOK-assisted deprotonation of dehydrogenation of alcohol is a feasible process with ΔG = 2.1 kcal/mol. Thereafter, we found that C-H activation of the cyclopropyl alkoxide with K^{+} takes place at 29.4 kcal/mol. Notably, the metal-assisted β-hydride elimination takes place at 20.4 kcal/mol and is predicted to overcome the ^{t}BuOK-assisted pathway.

8.6 XYZ coordinates of all intermediates and transition states.

XYZ coordinates, and respective electronic and Gibbs free energies are reported at the B3LYP/D3BJ/SMD (toluene) level of theory with the following basis sets for specific atoms were employed:

6-31G(d,p) basis sets on C, H, N, O; 6-31+G(d,p) basis set on P and S, and double-ζ LANL2DZ in combination with LANL2 effective core potential on K, Br, and Mn.

Gibbs free energies and electronic energies are in the units of Hartree (Eh).

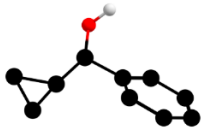
Unimportant hydrogen atoms are removed for clarity in the structural images of species.

^{t}BuOK

G = -833.0855201 Eh

E = -833.1558131 Eh

8	-0.077124000	-0.000209000	-0.920301000
6	0.974535000	-0.000036000	-0.064151000
6	1.865926000	1.257557000	-0.264896000
1	1.261712000	2.161075000	-0.103933000
1	2.226645000	1.277150000	-1.300807000
1	2.735359000	1.295687000	0.408763000
6	1.866125000	-1.257548000	-0.264505000
1	2.226063000	-1.277689000	-1.300667000
1	2.736045000	-1.294894000	0.408556000
1	1.262367000	-2.161191000	-0.102479000
6	0.511029000	0.000243000	1.433691000
1	-0.096392000	0.898695000	1.631868000
1	-0.099358000	-0.896460000	1.630776000
1	1.336607000	-0.001535000	2.159804000
19	-2.330408000	-0.000024000	-0.058437000



2a

G = -463.5583126 Eh

E = -463.6980346 Eh

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8	1.257034000	1.898225000	-0.642389000
1	1.290230000	-0.009047000	-1.488299000
6	1.872368000	-0.045243000	0.556840000
1	1.635799000	0.364196000	1.536851000
6	3.313827000	-0.373822000	0.261958000
1	4.054448000	-0.173750000	1.032253000
1	2.367110000	-2.045082000	1.425060000
6	2.314790000	-1.485091000	0.494939000
1	1.998534000	-2.072213000	-0.364618000
1	3.664242000	-0.208615000	-0.754640000
6	-0.469273000	0.197793000	-0.286775000
6	-1.251086000	1.082546000	0.466578000
1	-0.802906000	2.006766000	0.819310000
6	-2.585123000	0.781538000	0.750888000
1	-3.183590000	1.476087000	1.334624000
6	-3.150137000	-0.409497000	0.286249000
1	-4.188175000	-0.643774000	0.505897000
6	-2.375098000	-1.296276000	-0.467354000
1	-2.810177000	-2.220766000	-0.837704000
6	-1.043086000	-0.991010000	-0.753631000
1	-0.441395000	-1.675558000	-1.346936000
1	0.616025000	2.268748000	-1.265242000

^{t}BuOH

G = -233.7088858 Eh

E = -233.7998428 Eh

8	0.049467000	-0.000166000	1.454395000
1	0.985589000	0.000004000	1.699157000
6	-0.006748000	0.000000000	0.018568000
6	0.676197000	1.260727000	-0.524551000
1	0.199877000	2.156352000	-0.110871000
1	1.738065000	1.271968000	-0.244501000
1	0.616400000	1.303998000	-1.618345000
6	0.676121000	-1.260678000	-0.524751000
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1	1.737882000	-1.272173000	-0.244257000
1	0.199516000	-2.156397000	-0.111622000
1	-1.635173000	-0.000064000	-1.413965000
6	-1.494497000	0.000080000	-0.327698000
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1	-1.980493000	0.889150000	0.089069000

KBr

G = -3174.25769 Eh

E = -3174.221812 Eh

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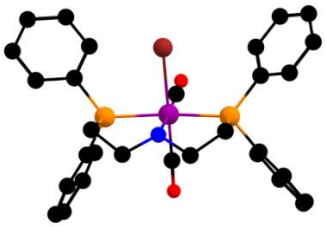
35	0.000000000	0.000000000	1.084713000



Mn1 (Singlet)

G = -5774.249466 Eh

E = -5774.654814 Eh

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6	-1.218197000	0.810348000	2.855152000
15	2.280360000	0.013036000	0.438151000
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1	-1.225213000	0.742893000	3.952488000
1	1.309237000	1.771695000	2.627030000
1	-1.198081000	1.870151000	2.578704000
6	0.028809000	-0.189643000	-1.628752000
8	0.050547000	-0.340040000	-2.784879000
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6	3.151153000	1.550695000	-0.063168000
6	3.139975000	1.870424000	-1.432017000
6	3.766896000	2.431445000	0.835402000
1	2.645067000	1.207328000	-2.137210000
1	3.777030000	2.217205000	1.899201000
6	3.748463000	3.036580000	-1.892131000
6	4.368823000	3.607045000	0.373305000
1	3.734875000	3.269305000	-2.953209000
1	4.839693000	4.283745000	1.081176000
6	4.364730000	3.909523000	-0.988835000
1	4.832655000	4.822391000	-1.346391000
6	3.408547000	-1.285618000	-0.189491000
6	2.976133000	-2.170134000	-1.185576000
6	4.725012000	-1.370754000	0.291538000
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1	5.842326000	-3.960827000	-1.611283000
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6	-3.081166000	-1.962509000	-1.288650000
6	-4.598398000	-1.501753000	0.543034000
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6	-5.461968000	-2.496418000	0.079490000
1	-3.694071000	-3.515022000	-2.647501000
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6	-5.140583000	-3.217325000	-1.074065000
1	-5.812410000	-3.990983000	-1.435569000
6	-3.128016000	1.617696000	-0.183396000
6	-2.801099000	2.067143000	-1.473714000
6	-4.088698000	2.321795000	0.556564000

1	-2.045820000	1.541174000	-2.050245000
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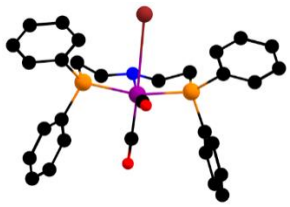

Mn1 (Triplet)

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E = -5774.607577 Eh

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1	-1.199629000	0.440745000	3.875648000
1	1.321941000	1.685773000	2.609790000
1	-1.322196000	1.685593000	2.609858000
6	-0.000149000	-0.197585000	-1.747048000
8	-0.000245000	-0.491715000	-2.875422000
1	0.000027000	-0.911016000	2.221293000
6	3.091939000	1.610402000	-0.072828000
6	3.054839000	2.007146000	-1.422391000
6	3.636826000	2.481955000	0.880096000
1	2.614336000	1.347600000	-2.165732000
1	3.669387000	2.201649000	1.927857000
6	3.567154000	3.244185000	-1.809070000
6	4.139042000	3.728059000	0.490748000
1	3.536622000	3.537071000	-2.854687000
1	4.556247000	4.397112000	1.238263000
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1	4.498260000	5.077786000	-1.151933000
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6	2.971691000	-2.417993000	-0.909587000
6	4.870769000	-0.988120000	-0.403334000
1	1.903732000	-2.607243000	-0.866994000
1	5.268928000	-0.056830000	-0.009907000
6	3.840366000	-3.362518000	-1.461670000
6	5.731991000	-1.935878000	-0.957160000
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1	6.801477000	-1.745557000	-0.980916000
6	5.216378000	-3.123746000	-1.486232000
1	5.887988000	-3.859821000	-1.919643000
6	2.435471000	-0.147474000	2.188605000
1	3.388854000	0.202685000	2.596971000
1	2.338796000	-1.216459000	2.408404000
6	-2.435533000	-0.147784000	2.188695000
1	-2.338691000	-1.216764000	2.408435000
1	-3.388942000	0.202241000	2.597115000
6	-0.000108000	2.200311000	-0.099848000
8	0.000279000	3.349359000	-0.103917000
35	-0.000108000	-3.001299000	1.210498000
6	-3.486907000	-1.229108000	-0.372492000
6	-2.971670000	-2.417856000	-0.909943000
6	-4.870820000	-0.988067000	-0.403681000
1	-1.903715000	-2.607115000	-0.867230000
1	-5.269033000	-0.056860000	-0.010107000
6	-3.840263000	-3.362253000	-1.462371000
6	-5.731961000	-1.935695000	-0.957861000
1	-3.438009000	-4.283798000	-1.873367000
1	-6.801443000	-1.745361000	-0.981750000
6	-5.216269000	-3.123453000	-1.487109000

1	-5.887814000	-3.859423000	-1.920803000
6	-3.091915000	1.610410000	-0.072445000
6	-3.054895000	2.007337000	-1.421960000
6	-3.636571000	2.481930000	0.880650000
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6	-3.567031000	3.244519000	-1.808417000
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1	-3.536556000	3.537541000	-2.853997000
1	-4.555621000	4.397199000	1.239170000
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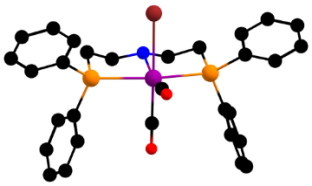

Mn1 (Quintet)

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E = -5774.593054 Eh

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6	1.225468000	0.648743000	2.648440000
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15	2.604360000	0.026400000	0.280759000
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1	1.225648000	0.633045000	3.750502000
1	-1.222218000	0.630040000	3.753048000
1	1.245483000	1.699390000	2.333375000
1	-1.245825000	1.697623000	2.336949000
6	-0.016844000	-0.909945000	-2.195569000
8	-0.035574000	-1.326740000	-3.267284000
1	0.001796000	-0.957171000	2.332006000
6	3.301980000	1.694396000	-0.026830000
6	3.352648000	2.129228000	-1.363641000
6	3.743981000	2.560295000	0.984582000
1	2.989446000	1.478109000	-2.155503000
1	3.706622000	2.253586000	2.024723000
6	3.853818000	3.390775000	-1.681630000
6	4.233508000	3.830560000	0.665564000
1	3.890300000	3.710977000	-2.719011000
1	4.569884000	4.492157000	1.459213000
6	4.293620000	4.246045000	-0.666023000
1	4.674510000	5.233093000	-0.912476000
6	3.979077000	-1.114829000	-0.136246000
6	3.660768000	-2.430204000	-0.513564000
6	5.323756000	-0.710121000	-0.097602000
1	2.620631000	-2.745663000	-0.543130000
1	5.574435000	0.310392000	0.177874000
6	4.680139000	-3.329911000	-0.833640000
6	6.336888000	-1.612712000	-0.425762000
1	4.426551000	-4.346447000	-1.121322000
1	7.374936000	-1.292429000	-0.396842000
6	6.016395000	-2.923297000	-0.792901000
1	6.806548000	-3.623478000	-1.050197000
6	2.463217000	-0.095825000	2.131672000
1	3.371279000	0.260400000	2.630201000
1	2.367602000	-1.165704000	2.350579000
6	-2.461480000	-0.099005000	2.135370000
1	-2.363956000	-1.169072000	2.352542000
1	-3.369292000	0.255190000	2.635797000
6	0.000690000	1.820831000	-0.674112000
8	0.001127000	2.940457000	-0.959290000
35	0.004779000	-2.924834000	0.613264000
6	-3.975136000	-1.117334000	-0.135883000
6	-3.651564000	-2.430495000	-0.516471000
6	-5.321184000	-0.717270000	-0.098018000
1	-2.610182000	-2.741977000	-0.545383000
1	-5.575662000	0.301649000	0.179898000
6	-4.667301000	-3.332883000	-0.840419000
6	-6.330663000	-1.622504000	-0.430164000
1	-4.409828000	-4.347743000	-1.130546000
1	-7.369883000	-1.305991000	-0.401882000

6	-6.005015000	-2.930951000	-0.800429000
1	-6.792353000	-3.633168000	-1.060790000
6	-3.304406000	1.693867000	-0.019286000
6	-3.353055000	2.132395000	-1.354972000
6	-3.750143000	2.556019000	0.993700000
1	-2.986650000	1.484325000	-2.147840000
1	-3.714270000	2.246384000	2.033024000
6	-3.856115000	3.393824000	-1.670412000
6	-4.241499000	3.826217000	0.677269000
1	-3.891058000	3.716920000	-2.706942000
1	-4.580749000	4.484932000	1.472087000
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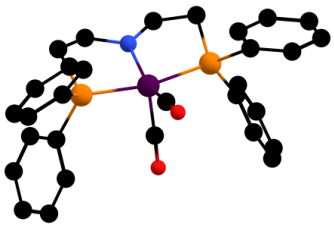

Mn1a

G = -3199.380962 Eh

E = -3199.775904 Eh

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6	1.198749000	-0.658320000	2.900510000
15	-2.260540000	0.082870000	0.518570000
15	2.260582000	0.082685000	0.518651000
1	-1.067735000	-0.397221000	3.963481000
1	1.067652000	-0.397680000	3.963487000
1	-1.366716000	-1.748605000	2.865547000
1	1.366357000	-1.748982000	2.865383000
6	0.000143000	1.270795000	-1.064464000
8	0.000178000	2.047744000	-1.937403000
6	-3.162234000	-1.386753000	-0.093443000
6	-3.293654000	-1.553477000	-1.483080000
6	-3.648587000	-2.386104000	0.761554000
1	-2.902493000	-0.795548000	-2.156700000
1	-3.546006000	-2.284389000	1.837036000
6	-3.917510000	-2.685921000	-2.003973000
6	-4.262500000	-3.527567000	0.236342000
1	-4.016887000	-2.799352000	-3.079821000
1	-4.632404000	-4.296523000	0.908999000
6	-4.402811000	-3.677135000	-1.144475000
1	-4.882316000	-4.563120000	-1.551091000
6	-3.289357000	1.504146000	-0.020991000
6	-2.713064000	2.784028000	0.029163000
6	-4.623940000	1.370780000	-0.433159000
1	-1.674754000	2.891916000	0.330185000
1	-5.076956000	0.385938000	-0.487976000
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6	-5.368624000	2.499465000	-0.785512000
1	-3.003096000	4.895011000	-0.276455000
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6	-4.789963000	3.769731000	-0.725736000
1	-5.370096000	4.645941000	-1.001790000
6	-2.423215000	0.079147000	2.358282000
1	-3.373455000	-0.334907000	2.713283000
1	-2.375567000	1.132651000	2.655346000
6	2.423249000	0.078616000	2.358368000
1	2.375836000	1.132082000	2.655603000
1	3.373399000	-0.335706000	2.713295000
6	0.000022000	-1.264116000	-0.876118000
8	0.000020000	-2.200590000	-1.572613000
6	3.289376000	1.504084000	-0.020628000
6	4.623978000	1.370848000	-0.432775000
6	2.713009000	2.783925000	0.029690000
1	5.077044000	0.386037000	-0.487731000
1	1.674674000	2.891701000	0.330679000
6	5.368609000	2.499626000	-0.784943000
6	3.460798000	3.910458000	-0.315084000
1	6.400349000	2.384882000	-1.106129000

1	3.002926000	4.894967000	-0.275634000
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1	5.369965000	4.646132000	-1.000922000
6	3.162256000	-1.386811000	-0.093691000
6	3.293778000	-1.553155000	-1.483365000
6	3.648442000	-2.386448000	0.761065000
1	2.902725000	-0.795008000	-2.156804000
1	3.545766000	-2.285031000	1.836566000
6	3.917586000	-2.685501000	-2.004524000
6	4.262304000	-3.527813000	0.235582000
1	4.017047000	-2.798634000	-3.080396000
1	4.632081000	-4.296993000	0.908053000
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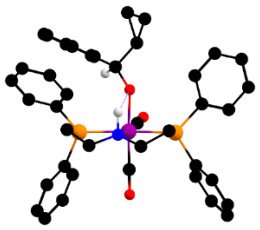

RCMn1

G = -3662.936172 Eh

E = -3663.513984 Eh

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6	-1.486319000	0.333920000	2.895906000
15	1.733170000	1.256021000	0.161179000
15	-2.591860000	-0.236348000	0.423551000
1	1.014815000	0.789126000	3.792166000
1	-1.306087000	0.038903000	3.940746000
1	0.553564000	2.164798000	2.765898000
1	-1.884680000	1.355310000	2.898178000
6	-0.554823000	0.417322000	-1.777981000
8	-0.623795000	0.318000000	-2.939625000
6	1.932210000	3.072820000	-0.050652000
6	1.592316000	3.611665000	-1.303044000
6	2.369438000	3.933973000	0.963612000
1	1.220868000	2.956860000	-2.087242000
1	2.624292000	3.546575000	1.944841000
6	1.708281000	4.979801000	-1.541292000
6	2.472940000	5.309353000	0.727795000
1	1.443994000	5.381891000	-2.515400000
1	2.807746000	5.967584000	1.524987000
6	2.148829000	5.833507000	-0.524262000
1	2.231033000	6.901261000	-0.706672000
6	3.191472000	0.649545000	-0.775381000
6	3.030526000	0.251130000	-2.110170000
6	4.470970000	0.626582000	-0.202398000
1	2.042260000	0.253207000	-2.558950000
1	4.609726000	0.925847000	0.832015000
6	4.131894000	-0.173398000	-2.857402000
6	5.570906000	0.201317000	-0.948565000
1	3.994366000	-0.489120000	-3.887705000
1	6.556306000	0.178749000	-0.491506000
6	5.402742000	-0.201909000	-2.276530000
1	6.258408000	-0.537076000	-2.856066000
6	2.136074000	0.917096000	1.936958000
1	2.956408000	1.524885000	2.330184000
1	2.442752000	-0.133676000	1.979444000
6	-2.467028000	-0.637409000	2.236125000
1	-2.057237000	-1.652563000	2.276739000
1	-3.432336000	-0.650606000	2.750818000
6	-1.012098000	2.205313000	0.088272000
8	-1.390622000	3.302801000	0.210808000
6	-3.316638000	-1.766315000	-0.288324000
6	-4.523814000	-1.755747000	-1.005490000
6	-2.629365000	-2.981160000	-0.116243000
1	-5.059676000	-0.824419000	-1.156160000
1	-1.663443000	-2.975333000	0.375490000
6	-5.044203000	-2.942569000	-1.529301000
6	-3.162740000	-4.163633000	-0.631373000
1	-5.979738000	-2.920135000	-2.081693000

1	-2.627798000	-5.097613000	-0.486819000
6	-4.370227000	-4.150046000	-1.335464000
1	-4.779792000	-5.073811000	-1.735233000
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6	-3.977114000	1.750236000	-0.928556000
6	-4.958725000	1.168444000	1.203463000
1	-3.190460000	1.626040000	-1.667684000
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6	-4.999071000	2.673867000	-1.149590000
6	-5.972932000	2.106188000	0.989884000
1	-5.009706000	3.256996000	-2.066034000
1	-6.745494000	2.244479000	1.741297000
6	-5.996587000	2.857228000	-0.187654000
1	-6.786949000	3.583889000	-0.353766000
1	0.083859000	-0.640069000	1.974470000
1	1.509918000	-1.485685000	-1.174237000
8	0.044150000	-1.449659000	0.277445000
6	1.068021000	-2.118104000	-0.390994000
6	2.204498000	-2.481473000	0.561974000
6	1.931167000	-2.789172000	1.902354000
6	3.534707000	-2.511076000	0.127450000
6	2.959949000	-3.113072000	2.789572000
6	4.569893000	-2.832926000	1.010242000
6	4.286876000	-3.133224000	2.345256000
1	0.898143000	-2.760222000	2.235037000
1	3.760855000	-2.248369000	-0.901696000
1	2.729567000	-3.351133000	3.825318000
1	5.597872000	-2.833763000	0.657301000
1	5.091092000	-3.379876000	3.033536000
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6	0.513552000	-3.347265000	-1.125935000
6	0.424310000	-4.706692000	-0.480571000
1	1.174487000	-4.911360000	-2.587039000
1	2.452892000	-4.428192000	-1.368477000
1	-0.322806000	-3.069700000	-1.764732000
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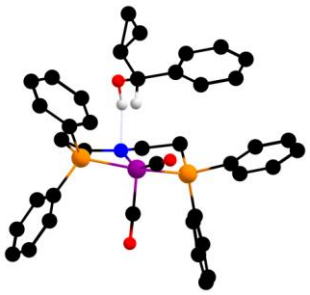

RCMn2

G = -3662.921449 Eh

E = -3663.496837 Eh

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6	-1.274495000	1.073796000	2.745718000
15	2.143572000	0.806125000	0.286786000
15	-2.415776000	0.658184000	0.291298000
1	0.942391000	0.148816000	3.684617000
1	-1.182764000	0.669026000	3.766538000
1	1.301589000	1.762604000	3.058312000
1	-1.296749000	2.170895000	2.844855000
6	-0.075758000	-0.020106000	-1.602693000
8	-0.014369000	-0.539638000	-2.650807000
6	2.875711000	2.492078000	0.340860000
6	2.926089000	3.228555000	-0.854477000
6	3.367137000	3.073347000	1.518656000
1	2.542960000	2.793720000	-1.773084000
1	3.341404000	2.525931000	2.454382000
6	3.462634000	4.515181000	-0.872809000
6	3.897191000	4.367469000	1.500208000
1	3.497145000	5.070778000	-1.805673000
1	4.273294000	4.806474000	2.420322000
6	3.948034000	5.089174000	0.306534000
1	4.362389000	6.093316000	0.293773000
6	3.373199000	-0.103472000	-0.721982000
6	3.225810000	-0.154221000	-2.116010000
6	4.490007000	-0.708521000	-0.127398000

1	2.363340000	0.302253000	-2.588063000
1	4.611877000	-0.685023000	0.950903000
6	4.182142000	-0.799950000	-2.902107000
6	5.444212000	-1.354764000	-0.914739000
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1	6.302389000	-1.825465000	-0.443138000
6	5.292634000	-1.400948000	-2.303043000
1	6.035290000	-1.905049000	-2.915346000
6	2.289003000	0.147414000	1.995521000
1	3.242339000	0.377011000	2.482649000
1	2.191557000	-0.940838000	1.913497000
6	-2.578670000	0.559175000	2.137432000
1	-2.688596000	-0.501265000	2.377192000
1	-3.452785000	1.109344000	2.499137000
6	-0.205874000	2.342090000	-0.780117000
8	-0.266031000	3.403074000	-1.260335000
6	-3.451947000	-0.732851000	-0.310236000
6	-3.176973000	-1.351484000	-1.537981000
6	-4.531285000	-1.197413000	0.459601000
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6	-3.960841000	-2.419074000	-1.983497000
6	-5.310724000	-2.266805000	0.016115000
1	-3.729308000	-2.896006000	-2.931445000
1	-6.136350000	-2.621201000	0.626857000
6	-5.025289000	-2.881091000	-1.206959000
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6	-4.426900000	2.122942000	-1.097205000
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6	-5.119806000	3.295865000	-1.413674000
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1	-5.924946000	3.263636000	-2.142690000
1	-3.468715000	5.470237000	0.619376000
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1	-5.325788000	5.409557000	-1.035943000
8	-0.853051000	-2.087743000	2.019254000
6	-0.640750000	-2.643080000	0.727499000
6	0.786349000	-3.133888000	0.553563000
6	1.516796000	-3.612199000	1.648651000
6	1.386875000	-3.123715000	-0.712277000
6	2.821298000	-4.084956000	1.478714000
6	2.690376000	-3.593204000	-0.884487000
6	3.409885000	-4.078603000	0.210620000
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1	0.834514000	-2.727017000	-1.558848000
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1	3.154012000	-3.551684000	-1.865255000
1	4.427660000	-4.435045000	0.078430000
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6	-1.699753000	-3.713729000	0.509839000
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1	-0.561690000	-4.917559000	-0.990074000
1	-2.702855000	-3.301113000	0.573150000
1	-0.560056000	-5.366789000	1.472963000
1	-2.374187000	-5.626008000	1.452964000
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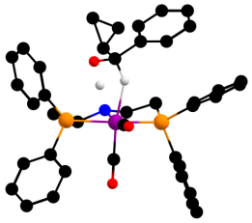

TS1

G = -3662.907128 Eh

E = -3663.480094 Eh

ν = - 764.4 cm^{-1}

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6	1.294335000	0.660925000	-2.831284000	1	3.461707000	0.450049000	-2.728760000
15	-1.987419000	0.988136000	-0.190535000	6	0.595838000	2.309525000	-0.111096000
15	2.541784000	0.127948000	-0.436277000	8	0.781258000	3.451016000	-0.244036000
1	-1.187117000	0.073171000	-3.687662000	6	3.570618000	-1.306276000	0.107943000
1	1.161400000	0.369632000	-3.884906000	6	3.437548000	-2.560180000	-0.512767000
1	-1.079280000	1.687522000	-2.963009000	6	4.481251000	-1.163217000	1.168765000
1	1.375594000	1.755944000	-2.799778000	1	2.666222000	-2.711226000	-1.260639000
6	0.417539000	0.498511000	1.769492000	1	4.596780000	-0.203589000	1.662351000
8	0.544334000	0.430688000	2.928187000	6	4.227564000	-3.634845000	-0.099747000
6	-2.458442000	2.761933000	-0.261166000	6	5.257092000	-2.247017000	1.587293000
6	-2.290524000	3.523845000	0.907202000	1	4.114922000	-4.597184000	-0.591154000
6	-2.945394000	3.384350000	-1.417886000	1	5.958248000	-2.119235000	2.407382000
1	-1.891201000	3.054561000	1.803397000	6	5.140387000	-3.482921000	0.947100000
1	-3.071370000	2.819449000	-2.335697000	1	5.750934000	-4.323055000	1.266488000
6	-2.620080000	4.877837000	0.922218000	6	3.655372000	1.527854000	0.001914000
6	-3.268141000	4.745508000	-1.403390000	6	3.403661000	2.259630000	1.172189000
1	-2.487877000	5.455012000	1.833074000	6	4.797991000	1.833491000	-0.753920000
1	-3.643618000	5.218155000	-2.306885000	1	2.528026000	2.033013000	1.770011000
6	-3.110632000	5.492194000	-0.234953000	1	5.034284000	1.262493000	-1.646066000
1	-3.363319000	6.548698000	-0.225260000	6	4.267311000	3.280945000	1.573391000
6	-3.291480000	0.317312000	0.907943000	6	5.654226000	2.864185000	-0.361309000
6	-2.993624000	-0.010953000	2.236792000	1	4.056074000	3.837528000	2.482128000
6	-4.604390000	0.164533000	0.437069000	1	6.530159000	3.094779000	-0.961415000
1	-1.980570000	0.093926000	2.607982000	6	5.390620000	3.590085000	0.803818000
1	-4.844906000	0.416349000	-0.591836000	1	6.058447000	4.390325000	1.110312000
6	-3.994571000	-0.497299000	3.082006000	1	0.227436000	-0.990855000	-1.950383000
6	-5.602258000	-0.322532000	1.281194000	1	-0.409686000	-1.288112000	0.047231000
1	-3.752610000	-0.757754000	4.108554000	8	0.444416000	-2.203204000	-1.617277000
1	-6.614219000	-0.446669000	0.905974000	6	-0.236266000	-2.332817000	-0.443293000
6	-5.297806000	-0.656391000	2.605090000	6	-1.651822000	-2.885616000	-0.633473000
1	-6.074697000	-1.037729000	3.261950000	6	-2.016403000	-3.443578000	-1.864515000
6	-2.338252000	0.306650000	-1.868293000	6	-2.607177000	-2.824787000	0.389137000
1	-3.257662000	0.697791000	-2.315894000	6	-3.310039000	-3.932238000	-2.069084000
1	-2.454747000	-0.774222000	-1.746024000	6	-3.901084000	-3.308269000	0.189487000
6	2.564182000	0.005769000	-2.290334000	6	-4.257762000	-3.863004000	-1.043785000
1	2.552279000	-1.058300000	-2.531793000	1	-1.269345000	-3.470009000	-2.650558000

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1	-3.579328000	-4.364642000	-3.029689000
1	-4.630384000	-3.234307000	0.990589000
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6	0.832566000	-4.547482000	0.477851000
1	0.481967000	-4.041789000	2.632289000
1	-1.043809000	-4.273365000	1.651067000
1	1.408010000	-2.481945000	0.980096000
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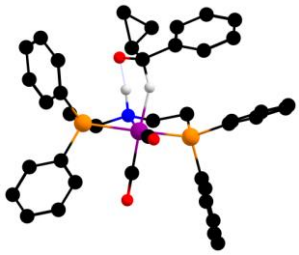

INT1

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E = -3663.481448 Eh

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6	-1.265783000	0.762794000	2.820021000
15	2.057556000	0.846567000	0.203273000
15	-2.514788000	0.222101000	0.416940000
1	1.206922000	0.074672000	3.731017000
1	-1.169536000	0.523575000	3.889479000
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1	-1.275034000	1.854007000	2.717732000
6	-0.335106000	0.455539000	-1.781234000
8	-0.434632000	0.379382000	-2.941494000
6	2.593254000	2.604583000	0.266926000
6	2.467703000	3.361438000	-0.910055000
6	3.094040000	3.219031000	1.421789000
1	2.058282000	2.900750000	-1.806167000
1	3.190845000	2.658618000	2.345961000
6	2.851541000	4.700783000	-0.934936000
6	3.471218000	4.566122000	1.397855000
1	2.751674000	5.273269000	-1.852846000
1	3.857002000	5.032135000	2.300468000
6	3.355346000	5.306894000	0.220934000
1	3.650338000	6.352257000	0.203532000
6	3.373528000	0.143009000	-0.860787000
6	3.100220000	-0.190704000	-2.193173000
6	4.676478000	-0.010455000	-0.363968000
1	2.094485000	-0.083286000	-2.583911000
1	4.899287000	0.250646000	0.666553000
6	4.114964000	-0.688127000	-3.015127000
6	5.688357000	-0.508085000	-1.184789000
1	3.891899000	-0.954358000	-4.044456000
1	6.692440000	-0.632945000	-0.789191000
6	5.408054000	-0.850048000	-2.511847000
1	6.195689000	-1.239533000	-3.150863000
6	2.362125000	0.181568000	1.898425000
1	3.300878000	0.528398000	2.342586000
1	2.414869000	-0.906771000	1.800885000
6	-2.550749000	0.143426000	2.275492000
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1	-3.433326000	0.629140000	2.699694000
6	-0.451705000	2.285766000	0.101714000
8	-0.581078000	3.436130000	0.223353000
6	-3.653537000	-1.141707000	-0.091927000
6	-3.614497000	-2.390241000	0.552048000
6	-4.558432000	-0.946390000	-1.149483000
1	-2.842260000	-2.587636000	1.289258000
1	-4.600194000	0.009021000	-1.662370000
6	-4.493119000	-3.404622000	0.165905000
6	-5.421131000	-1.972435000	-1.542574000
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1	-6.115078000	-1.804943000	-2.361721000
6	-5.399743000	-3.200548000	-0.877520000

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6	-5.471638000	3.123480000	0.298507000
1	-3.804402000	3.994188000	-2.538194000
1	-6.339804000	3.401502000	0.889756000
6	-5.161518000	3.827331000	-0.868702000
1	-5.785252000	4.658528000	-1.185570000
1	-0.238121000	-0.850115000	2.066179000
1	0.174247000	-1.280403000	-0.015832000
8	-0.672935000	-2.274853000	1.632574000
6	-0.017590000	-2.374823000	0.478046000
6	1.411980000	-2.914382000	0.622959000
6	1.814174000	-3.461857000	1.846623000
6	2.337322000	-2.851195000	-0.424845000
6	3.118605000	-3.933870000	2.020026000
6	3.641057000	-3.319498000	-0.258935000
6	4.037312000	-3.860957000	0.968336000
1	1.085289000	-3.491312000	2.649746000
1	2.035572000	-2.416295000	-1.369915000
1	3.418955000	-4.357190000	2.975544000
1	4.348158000	-3.239276000	-1.078960000
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6	-0.818593000	-3.052658000	-0.651326000
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1	-0.712371000	-4.007863000	-2.660609000
1	0.761227000	-4.332685000	-1.628692000
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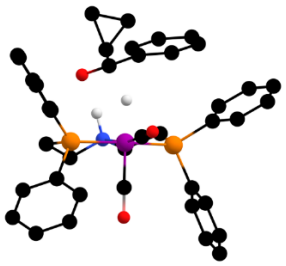

TS2

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E = -3663.4772 Eh

ν = - 446.3 cm^{-1}

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6	-1.220733000	0.745054000	2.865029000
15	2.052500000	0.811283000	0.164008000
15	-2.468167000	0.267167000	0.450616000
1	1.304872000	0.180825000	3.750318000
1	-1.129826000	0.506235000	3.935111000
1	1.204581000	1.708097000	2.848305000
1	-1.219835000	1.834718000	2.757127000
6	-0.372874000	0.479449000	-1.752241000
8	-0.509550000	0.382416000	-2.910234000
6	2.659739000	2.551331000	0.171251000
6	2.476311000	3.299831000	-1.003669000
6	3.260570000	3.164476000	1.278082000
1	1.986864000	2.843447000	-1.860820000
1	3.405007000	2.613731000	2.201846000
6	2.901054000	4.625101000	-1.074958000
6	3.676995000	4.498776000	1.210237000
1	2.754363000	5.189775000	-1.991550000
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6	3.502031000	5.229561000	0.034488000
1	3.826236000	6.265158000	-0.017733000
6	3.332674000	0.052490000	-0.910585000
6	3.000135000	-0.400361000	-2.192981000
6	4.664842000	-0.023706000	-0.476948000
1	1.970959000	-0.351098000	-2.531434000

1	4.934042000	0.334430000	0.512980000
6	3.985030000	-0.937993000	-3.026607000
6	5.647465000	-0.560933000	-1.308295000
1	3.716353000	-1.293566000	-4.017449000
1	6.675545000	-0.621944000	-0.961976000
6	5.308035000	-1.020667000	-2.585436000
1	6.072964000	-1.438564000	-3.234152000
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1	3.349708000	0.523069000	2.285805000
1	2.431703000	-0.908746000	1.799461000
6	-2.506800000	0.133960000	2.308305000
1	-2.526081000	-0.929075000	2.552772000
1	-3.386762000	0.609321000	2.749642000
6	-0.404678000	2.309071000	0.183695000
8	-0.502111000	3.463647000	0.320703000
6	-3.612436000	-1.061328000	-0.139733000
6	-4.318396000	-0.858106000	-1.338949000
6	-3.764709000	-2.283263000	0.534740000
1	-4.216403000	0.079393000	-1.876563000
1	-3.157826000	-2.503040000	1.403831000
6	-5.166022000	-1.845848000	-1.843282000
6	-4.627444000	-3.262375000	0.035267000
1	-5.703584000	-1.668655000	-2.770831000
1	-4.734487000	-4.201207000	0.571817000
6	-5.331661000	-3.048545000	-1.151616000
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1	-6.324075000	3.402755000	1.029342000
6	-5.134817000	3.908342000	-0.700245000
1	-5.759808000	4.749979000	-0.985794000
1	-0.143790000	-0.822246000	2.156983000
1	0.078301000	-1.125536000	-0.051987000
8	-0.816498000	-2.417269000	1.668273000
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6	2.216519000	-2.897000000	-0.301021000
6	3.083508000	-3.757407000	2.206377000
6	3.553025000	-3.243813000	-0.110724000
6	3.991022000	-3.675764000	1.145510000
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1	1.880585000	-2.534200000	-1.262860000
1	3.417240000	-4.096439000	3.183722000
1	4.252622000	-3.148706000	-0.935050000
1	5.033074000	-3.945043000	1.296451000
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6	-0.906923000	-3.120934000	-0.618818000
6	-1.333740000	-4.572518000	-0.600076000
1	-0.704493000	-3.965608000	-2.665788000
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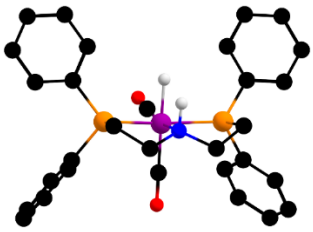

MnH2

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E = -3200.987637 Eh

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1	1.243298000	-0.624989000	4.028670000
1	-1.262237000	-1.721194000	2.625190000
1	1.262824000	-1.720732000	2.625445000
6	0.000149000	0.460528000	-1.506954000
8	0.000294000	0.785122000	-2.631307000
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6	-2.937122000	-1.696494000	-1.461856000
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1	-2.160805000	-1.190243000	-2.028272000
1	-4.424858000	-1.685531000	1.604710000
6	-3.638151000	-2.754916000	-2.038171000
6	-4.883715000	-3.045715000	0.011820000
1	-3.414247000	-3.057028000	-3.057472000
1	-5.635777000	-3.572564000	0.593054000
6	-4.612667000	-3.435039000	-1.300862000
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1	-5.349393000	4.682591000	-1.070128000
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1	2.388177000	1.142669000	2.679605000
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8	-0.000025000	-2.886449000	-0.147461000
6	3.253471000	1.573736000	-0.024085000
6	4.657089000	1.513846000	-0.035897000
6	2.614742000	2.761429000	-0.408597000
1	5.161259000	0.588409000	0.227574000
1	1.529374000	2.791560000	-0.411217000
6	5.407615000	2.630594000	-0.407271000
6	3.368306000	3.877880000	-0.781006000
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1	2.864267000	4.792764000	-1.080948000
6	4.763594000	3.815415000	-0.778089000
1	5.348801000	4.682728000	-1.071766000
6	3.210531000	-1.286607000	-0.144751000
6	2.937284000	-1.696880000	-1.461184000
6	4.191059000	-1.973377000	0.585769000
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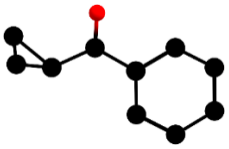

16a

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E = -462.4961818 Eh

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1	-0.339231000	-2.012935000	-0.135271000
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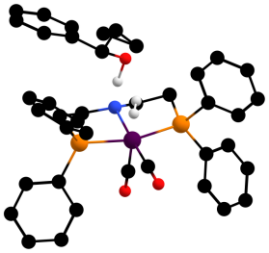
1	-2.762617000	-2.449234000	-0.092393000
1	-4.371945000	-0.560869000	0.052373000
6	3.178966000	-0.562536000	-0.688467000
6	1.923446000	-0.602074000	0.182653000
6	3.272088000	-0.172429000	0.746843000
1	3.587749000	-1.518195000	-1.006006000
1	3.209147000	0.235271000	-1.425656000
1	1.559866000	-1.578725000	0.479310000
1	3.363916000	0.886711000	0.970454000
1	3.748708000	-0.853227000	1.447045000



TS3

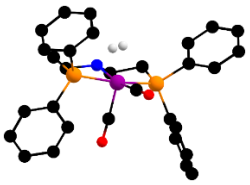
G = -3664.092981 Eh

E = -3664.681123 Eh

ν = -8825.5 cm^{-1}

25	-0.761479000	0.663706000	0.044805000
7	-0.077581000	-0.097898000	-1.816840000
6	-1.160687000	-0.429227000	-2.753987000
6	0.937065000	0.729388000	-2.480488000
15	-2.599960000	-0.621635000	-0.441183000
15	1.339552000	1.555871000	0.100362000
1	-0.747096000	-0.917516000	-3.651206000
1	1.341914000	0.202155000	-3.358627000
1	-1.676690000	0.484912000	-3.088119000
1	0.488920000	1.669215000	-2.839900000
6	-1.344880000	1.233586000	1.631099000
8	-1.749460000	1.623057000	2.654296000
6	-4.212968000	0.210747000	-0.681678000
6	-5.206679000	-0.336171000	-1.509971000
6	-4.478817000	1.403812000	0.006070000
1	-5.026894000	-1.270039000	-2.034251000
1	-3.721468000	1.829641000	0.654713000
6	-6.435353000	0.308729000	-1.659870000
6	-5.711989000	2.043793000	-0.136959000
1	-7.193835000	-0.120020000	-2.308890000
1	-5.904760000	2.967970000	0.400499000
6	-6.688982000	1.500753000	-0.974184000
1	-7.645107000	2.002914000	-1.092504000
6	-2.978261000	-2.038400000	0.662188000
6	-2.003951000	-3.041037000	0.822391000
6	-4.170538000	-2.105127000	1.398544000
1	-1.063438000	-2.986880000	0.274074000
1	-4.925152000	-1.333236000	1.282621000
6	-2.237788000	-4.098970000	1.702056000
6	-4.391603000	-3.165616000	2.282497000
1	-1.481152000	-4.869904000	1.817503000
1	-5.318556000	-3.208879000	2.847848000
6	-3.427869000	-4.164864000	2.433846000
1	-3.602111000	-4.989619000	3.119548000
6	-2.146197000	-1.380332000	-2.071751000
1	-3.019370000	-1.584180000	-2.698488000
1	-1.642987000	-2.325511000	-1.849171000
6	2.084002000	1.029246000	-1.513505000
1	2.651885000	0.114468000	-1.328288000
1	2.768843000	1.773215000	-1.930156000
6	-1.404940000	2.086440000	-0.815019000
8	-1.804970000	3.001521000	-1.408354000
6	2.515835000	0.947282000	1.373942000
6	3.869363000	0.721873000	1.081959000
6	2.040328000	0.682438000	2.667526000
1	4.249631000	0.897413000	0.080922000
1	0.992111000	0.842876000	2.900641000

6	4.731277000	0.234440000	2.067200000
6	2.903810000	0.198913000	3.652216000
1	5.774885000	0.052194000	1.826351000
1	2.523014000	-0.011325000	4.647530000
6	4.250311000	-0.028412000	3.352725000
1	4.919946000	-0.414376000	4.115953000
6	1.523432000	3.380699000	0.186870000
6	2.637673000	4.040713000	-0.355160000
6	0.541789000	4.131321000	0.851147000
1	3.413595000	3.477113000	-0.864841000
1	-0.322614000	3.631465000	1.275188000
6	2.761258000	5.426634000	-0.243790000
6	0.670756000	5.516915000	0.969466000
1	3.624560000	5.927006000	-0.673603000
1	-0.097360000	6.086948000	1.484444000
6	1.777681000	6.166701000	0.419067000
1	1.874173000	7.245439000	0.504370000
1	0.381908000	-1.214215000	-1.426304000
1	-0.040929000	-0.559108000	1.074754000
8	0.617995000	-2.310963000	-0.923572000
1	-0.126084000	-0.994677000	0.423651000
6	1.869912000	-2.329872000	-0.316138000
6	1.980324000	-3.508089000	0.642612000
1	1.957104000	-4.481400000	0.155209000
6	2.816090000	-3.379676000	1.893591000
1	3.365961000	-4.250576000	2.243553000
1	3.315154000	-2.429519000	2.071460000
6	1.305362000	-3.395201000	1.986537000
1	0.802389000	-2.457808000	2.212364000
1	0.819204000	-4.274056000	2.403020000
6	3.019391000	-2.325691000	-1.326229000
6	2.769490000	-2.489076000	-2.692632000
1	1.743077000	-2.649469000	-3.005503000
6	3.814437000	-2.437063000	-3.620664000
1	3.603936000	-2.565096000	-4.679811000
6	5.125824000	-2.218150000	-3.191487000
1	5.937919000	-2.172738000	-3.912426000
6	5.385866000	-2.056830000	-1.825678000
6	4.340276000	-2.111019000	-0.902475000
1	6.403719000	-1.886751000	-1.482716000
1	4.538938000	-1.974046000	0.155698000
1	2.020161000	-1.427437000	0.312691000



TS3$_{self}$

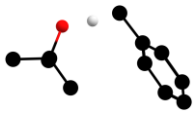
G = -3200.529234 Eh

E = -3200.94421 Eh

ν = -825.0 cm^{-1}

25	-0.000001000	0.087767000	0.244446000
7	-0.000009000	-0.087532000	2.363730000
6	-1.208743000	-0.662289000	2.918474000
6	1.208713000	-0.662322000	2.918463000
15	-2.257351000	0.110438000	0.521111000
15	2.257347000	0.110433000	0.521121000
1	-1.207604000	-0.587568000	4.020899000
1	1.207574000	-0.587631000	4.020889000
1	-1.300730000	-1.741305000	2.674691000
1	1.300679000	-1.741333000	2.674647000
6	0.000013000	0.573508000	-1.471694000
8	0.000022000	0.896673000	-2.593631000
6	-3.199458000	-1.313940000	-0.143821000
6	-2.949093000	-1.679055000	-1.477859000
6	-4.145425000	-2.039240000	0.593711000
1	-2.201156000	-1.137701000	-2.050608000
1	-4.352322000	-1.782339000	1.627234000
6	-3.641467000	-2.737238000	-2.064776000
6	-4.830412000	-3.108615000	0.007413000
1	-3.437755000	-3.007973000	-3.096972000
1	-5.556481000	-3.667172000	0.591753000

6	-4.583338000	-3.456256000	-1.321729000
1	-5.116162000	-4.286988000	-1.775917000
6	-3.256734000	1.553248000	-0.021041000
6	-2.603418000	2.742749000	-0.375675000
6	-4.659568000	1.500478000	-0.065664000
1	-1.518722000	2.776366000	-0.361159000
1	-5.173108000	0.575202000	0.180495000
6	-3.341625000	3.868377000	-0.749866000
6	-5.395075000	2.625230000	-0.442446000
1	-2.826333000	4.784886000	-1.024021000
1	-6.480043000	2.574836000	-0.475831000
6	-4.736785000	3.811566000	-0.781918000
1	-5.310601000	4.685556000	-1.077682000
6	-2.430291000	0.084128000	2.368986000
1	-3.376791000	-0.336169000	2.722717000
1	-2.390508000	1.133428000	2.684981000
6	2.430271000	0.084095000	2.368996000
1	2.390495000	1.133390000	2.685010000
1	3.376766000	-0.336215000	2.722726000
6	0.000004000	-1.672882000	-0.055481000
8	0.000006000	-2.829895000	-0.172148000
6	3.256749000	1.553240000	-0.021009000
6	4.659575000	1.500399000	-0.065815000
6	2.603454000	2.742814000	-0.375439000
1	5.173097000	0.575074000	0.180194000
1	1.518762000	2.776483000	-0.360792000
6	5.395094000	2.625152000	-0.442574000
6	3.341674000	3.868443000	-0.749601000
1	6.480056000	2.574702000	-0.476101000
1	2.826397000	4.785009000	-1.023592000
6	4.736828000	3.811559000	-0.781836000
1	5.310653000	4.685550000	-1.077579000
6	3.199442000	-1.313948000	-0.143821000
6	2.949067000	-1.679061000	-1.477858000
6	4.145414000	-2.039252000	0.593701000
1	2.201128000	-1.137705000	-2.050601000
1	4.352321000	-1.782351000	1.627222000
6	3.641433000	-2.737245000	-2.064782000
6	4.830393000	-3.108628000	0.007397000
1	3.437712000	-3.007977000	-3.096977000
1	5.556466000	-3.667187000	0.591730000
6	4.583307000	-3.456267000	-1.321744000
1	5.116126000	-4.286999000	-1.775937000
1	0.000012000	1.207653000	1.568722000
1	0.000013000	1.725258000	0.821212000



TS_PT

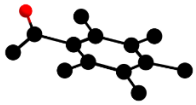
G = -504.737492 Eh

E = -504.922844 Eh

ν = -1282.09 cm^{-1}

8	-2.079909000	1.111913000	-0.364313000
6	-2.284994000	-0.261480000	-0.119518000
6	-2.080390000	-0.588086000	1.367578000
1	-2.707096000	0.064420000	1.985406000
1	-1.032300000	-0.436933000	1.646143000
1	-2.341378000	-1.632025000	1.577348000
6	-1.372607000	-1.127308000	-1.001449000
1	-0.320658000	-0.955122000	-0.755725000
1	-1.589078000	-2.192792000	-0.857460000
1	-1.528402000	-0.878083000	-2.057030000
6	-3.761412000	-0.489967000	-0.504476000
1	-4.418083000	0.126726000	0.117835000
1	-3.925749000	-0.232945000	-1.556091000
1	-4.015321000	-1.545932000	-0.354715000
1	-0.876155000	1.456783000	0.070982000
6	0.191558000	1.875974000	0.533374000
1	-0.025766000	2.044204000	1.591275000
6	1.275710000	0.910651000	0.278617000
6	1.660589000	-0.023044000	1.259775000
6	1.907706000	0.858527000	-0.979373000

1	1.180888000	0.008420000	2.234640000
1	1.613068000	1.568933000	-1.747574000
6	2.644666000	-0.974541000	0.995255000
6	2.890774000	-0.092066000	-1.244931000
1	2.932101000	-1.684005000	1.766335000
1	3.369424000	-0.117240000	-2.220031000
6	3.262364000	-1.014077000	-0.259223000
1	4.028182000	-1.756002000	-0.467120000
1	0.291805000	2.818790000	-0.013487000

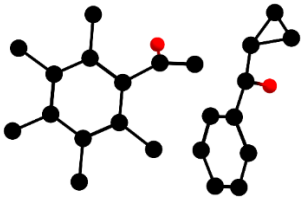


A

G = -580.9909895 Eh

E = -581.1902495 Eh

6	3.139497000	0.461587000	1.074418000
1	2.580877000	0.857233000	1.919925000
6	2.499697000	0.005670000	-0.062082000
8	3.022425000	-0.466852000	-1.126819000
6	0.960866000	0.021561000	-0.011844000
6	0.228493000	1.226030000	-0.037128000
6	0.264623000	-1.208468000	0.009972000
6	-1.183743000	1.201878000	-0.024409000
6	-1.141041000	-1.231326000	0.057719000
6	-1.870693000	-0.024801000	-0.001839000
1	4.227750000	0.450221000	1.135598000
6	-1.877521000	-2.553327000	0.186868000
1	-2.143270000	-2.982819000	-0.791283000
1	-1.270459000	-3.297401000	0.709522000
1	-2.808074000	-2.441780000	0.752884000
6	-3.387713000	-0.052461000	-0.061006000
1	-3.780649000	0.783615000	-0.647853000
1	-3.754972000	-0.970176000	-0.529826000
1	-3.851514000	0.008429000	0.935853000
6	-1.955939000	2.508526000	-0.035951000
1	-2.166912000	2.855607000	-1.059350000
1	-2.917702000	2.420445000	0.479136000
1	-1.395189000	3.306963000	0.458394000
6	0.935679000	2.566183000	-0.107306000
1	0.801379000	3.144840000	0.818697000
1	2.008766000	2.431539000	-0.247485000
1	0.534178000	3.182553000	-0.923839000
6	1.051785000	-2.505647000	0.008856000
1	1.242350000	-2.863186000	1.032092000
1	0.517685000	-3.302105000	-0.521431000
1	2.012414000	-2.341591000	-0.484098000



TS4

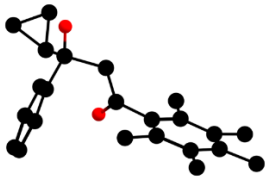
G = -1043.328921 Eh

E = -1043.679691 Eh

ν = -274.0 cm^{-1}

8	-3.332422000	-0.457600000	-1.896989000
6	-2.820866000	-0.528927000	-0.737114000
6	-2.621361000	0.785710000	0.016742000
6	-2.916139000	1.979531000	-0.656805000
6	-2.177355000	0.863113000	1.347563000
6	-2.749699000	3.218757000	-0.035667000
6	-2.011625000	2.100315000	1.971926000
6	-2.295649000	3.286604000	1.285064000
1	-3.262455000	1.894203000	-1.682235000
1	-1.915278000	-0.045135000	1.876130000
1	-2.976756000	4.133616000	-0.579849000
1	-1.655144000	2.139851000	2.999101000
1	-2.166466000	4.249140000	1.774976000
6	-4.795065000	-1.832648000	0.309883000
6	-3.298058000	-1.661645000	0.182463000
6	-3.971045000	-2.831379000	-0.476578000
1	-5.213910000	-2.134241000	1.268843000
1	-5.406704000	-1.143957000	-0.269274000
1	-2.673141000	-1.868436000	1.044846000

1	-4.041754000	-2.768135000	-1.559948000
1	-3.819404000	-3.825295000	-0.059239000
6	-0.914403000	-1.219814000	-0.999452000
1	-0.576063000	-0.741822000	-1.918750000
6	0.003987000	-1.190093000	0.113515000
8	-0.251960000	-1.707432000	1.222734000
1	-1.333829000	-2.208434000	-1.169970000
6	1.399347000	-0.586255000	-0.046520000
6	2.491850000	-1.450384000	0.207864000
6	1.639713000	0.762167000	-0.376620000
6	3.808128000	-0.954414000	0.164971000
6	2.961995000	1.253970000	-0.411335000
6	4.047406000	0.392740000	-0.173850000
6	3.202123000	2.724912000	-0.695351000
1	3.320863000	2.926234000	-1.770755000
1	2.365993000	3.337378000	-0.347606000
1	4.103469000	3.091375000	-0.194955000
6	5.470822000	0.904049000	-0.300867000
1	6.150502000	0.115202000	-0.636432000
1	5.540854000	1.717089000	-1.028885000
1	5.864987000	1.286711000	0.652753000
6	4.972124000	-1.868946000	0.502690000
1	5.363285000	-2.393620000	-0.382142000
1	5.804526000	-1.312519000	0.943361000
1	4.679400000	-2.635225000	1.225734000
6	2.274595000	-2.927877000	0.481914000
1	3.055658000	-3.529264000	0.003206000
1	2.296686000	-3.150172000	1.556837000
1	1.308106000	-3.270997000	0.110946000
6	0.504856000	1.707362000	-0.695057000
1	0.336876000	2.431332000	0.113079000
1	0.719288000	2.285237000	-1.602589000
1	-0.428612000	1.179067000	-0.849406000



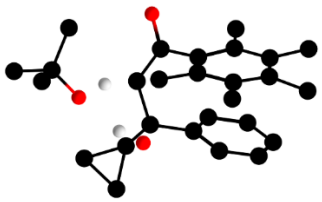
17a

G = -1043.334844 Eh

E = -1043.68686 Eh

8	-2.865853000	-0.740378000	-2.035398000
6	-2.434374000	-0.732379000	-0.781368000
6	-2.706851000	0.621838000	-0.051572000
6	-3.048541000	1.719233000	-0.851746000
6	-2.609687000	0.820946000	1.335460000
6	-3.260252000	2.984071000	-0.298562000
6	-2.829885000	2.082484000	1.897926000
6	-3.150561000	3.173233000	1.083479000
1	-3.136370000	1.516072000	-1.915695000
1	-2.333960000	-0.010176000	1.974375000
1	-3.516039000	3.824912000	-0.941715000
1	-2.748261000	2.214672000	2.975456000
1	-3.318724000	4.155075000	1.521368000
6	-4.464263000	-2.251031000	-0.174367000
6	-3.028073000	-1.885410000	0.085921000
6	-3.348211000	-3.164713000	-0.639969000
1	-5.096451000	-2.568749000	0.654059000
1	-4.945649000	-1.666309000	-0.955014000
1	-2.649571000	-1.978865000	1.100008000
1	-3.140619000	-3.138967000	-1.707367000
1	-3.201596000	-4.117090000	-0.131399000
6	-0.830802000	-0.943193000	-0.805932000
1	-0.443537000	-0.259381000	-1.567791000
6	0.033045000	-0.888141000	0.425424000
8	-0.311864000	-1.303261000	1.529570000
1	-0.711514000	-1.959280000	-1.210676000
6	1.453792000	-0.388452000	0.231641000
6	2.513424000	-1.304296000	0.386359000
6	1.702378000	0.953436000	-0.119267000

6	3.837183000	-0.870702000	0.176384000
6	3.026019000	1.370825000	-0.355125000
6	4.089119000	0.453912000	-0.228089000
6	3.329387000	2.800696000	-0.756992000
1	3.673106000	2.855297000	-1.799633000
1	2.457908000	3.450840000	-0.670640000
1	4.128310000	3.229184000	-0.139330000
6	5.506664000	0.903480000	-0.523512000
1	6.118185000	0.083745000	-0.911095000
1	5.526667000	1.703694000	-1.268358000
1	6.010451000	1.287982000	0.376105000
6	4.986827000	-1.838784000	0.378288000
1	5.252154000	-2.361649000	-0.552812000
1	5.887668000	-1.327109000	0.729752000
1	4.738871000	-2.604964000	1.117466000
6	2.258539000	-2.756547000	0.742894000
1	2.842428000	-3.423546000	0.097679000
1	2.555673000	-2.970237000	1.778742000
1	1.206919000	-3.029568000	0.651993000
6	0.557415000	1.940717000	-0.224898000
1	0.739424000	2.821904000	0.402487000
1	0.423675000	2.298101000	-1.253739000
1	-0.391158000	1.516185000	0.098140000



TS5

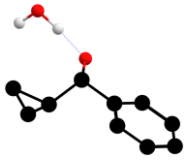
G = -1277.020879 Eh

E = -1277.49825 Eh

ν = -1134.0 cm^{-1}

8	-1.118716000	0.778657000	-1.504899000
6	-0.816677000	1.473735000	-0.287053000
6	0.674780000	1.818780000	-0.323197000
6	1.499573000	1.441849000	-1.389006000
6	1.243159000	2.547689000	0.731372000
6	2.858898000	1.764487000	-1.389792000
6	2.595830000	2.886224000	0.727669000
6	3.415553000	2.491762000	-0.335121000
1	1.067581000	0.866609000	-2.197798000
1	0.619815000	2.823779000	1.577002000
1	3.486547000	1.438937000	-2.216301000
1	3.014049000	3.446088000	1.561046000
1	4.472734000	2.746137000	-0.338033000
6	-1.919750000	3.512672000	-1.551721000
6	-1.586306000	2.813984000	-0.260968000
6	-3.016913000	2.876168000	-0.721473000
1	-1.853107000	4.598599000	-1.589982000
1	-1.630132000	2.992282000	-2.460611000
1	-1.317704000	3.444532000	0.583940000
1	-3.453021000	1.941141000	-1.060652000
1	-3.696986000	3.530100000	-0.177779000
6	-1.264753000	0.658015000	0.946490000
1	-2.399124000	0.097699000	0.446954000
6	-0.479830000	-0.411603000	1.542123000
8	-0.765929000	-0.894702000	2.653448000
1	-1.695867000	1.280915000	1.736599000
6	-4.255028000	-1.171384000	0.175522000
6	-3.669433000	-1.970737000	1.358488000
6	-4.665309000	-2.145694000	-0.943097000
1	-5.067987000	-1.584808000	-1.795714000
1	-3.786593000	-2.704646000	-1.287347000
1	-5.426309000	-2.864113000	-0.606959000
1	-2.846342000	-2.609096000	1.020349000
1	-4.432665000	-2.612979000	1.819740000
1	-3.261547000	-1.297736000	2.119914000
8	-3.318023000	-0.268704000	-0.341434000
1	-1.954469000	0.290060000	-1.350472000
6	-5.493814000	-0.389607000	0.657184000
1	-5.914307000	0.187352000	-0.175839000
1	-6.276900000	-1.049684000	1.056877000
1	-5.198580000	0.315578000	1.443211000

6	0.747740000	-0.961201000	0.826712000
6	2.009305000	-0.672386000	1.386700000
6	0.653090000	-1.736789000	-0.340407000
6	3.177494000	-1.070552000	0.713623000
6	1.828250000	-2.148428000	-1.001371000
6	3.087724000	-1.758887000	-0.512038000
6	1.715195000	-2.997779000	-2.252297000
1	2.607611000	-3.609033000	-2.414938000
1	0.861275000	-3.678908000	-2.190639000
1	1.566120000	-2.383000000	-3.152566000
6	4.346616000	-2.058200000	-1.304834000
1	4.821019000	-3.004738000	-1.004528000
1	4.138158000	-2.124494000	-2.376214000
1	5.091252000	-1.267423000	-1.172337000
6	4.531813000	-0.737766000	1.305694000
1	4.506575000	-0.770374000	2.398993000
1	5.305906000	-1.437317000	0.977474000
1	4.853025000	0.274885000	1.020514000
6	2.137116000	0.085380000	2.693253000
1	2.910123000	0.856669000	2.626086000
1	1.202463000	0.562776000	2.984778000
1	2.417265000	-0.595318000	3.510420000
6	-0.687866000	-2.165952000	-0.891095000
1	-0.828258000	-3.249031000	-0.753431000
1	-1.520995000	-1.650143000	-0.421026000
1	-0.758024000	-1.966004000	-1.965797000

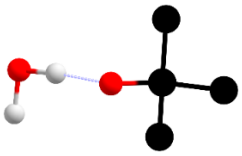


2a-H_2O

G = -539.4924561 Eh

E = -539.6387381 Eh

8	-3.583557000	-1.658679000	-0.679208000
1	-4.010151000	-1.315695000	0.115546000
6	-0.716494000	-0.297629000	-0.189060000
8	-1.160851000	-1.518685000	0.165896000
1	-2.594247000	-1.650211000	-0.375924000
6	-1.308132000	0.846020000	0.678726000
6	-1.605429000	2.199561000	0.074215000
1	-1.473021000	3.096827000	0.678008000
1	-1.374655000	2.334419000	-0.981655000
6	-2.734035000	1.249647000	0.425720000
1	-3.238802000	0.709942000	-0.373090000
1	-3.366679000	1.506990000	1.275090000
1	-0.973264000	0.828979000	1.716520000
6	0.824897000	-0.175445000	-0.138625000
6	1.510873000	0.974035000	-0.561147000
1	0.942584000	1.815933000	-0.949068000
6	2.904158000	1.048253000	-0.490611000
1	3.417729000	1.947570000	-0.826304000
6	3.641483000	-0.032620000	0.008333000
1	4.726773000	0.022039000	0.062519000
6	2.967683000	-1.183452000	0.429051000
1	3.533085000	-2.030569000	0.814497000
6	1.573130000	-1.250294000	0.352749000
1	1.007314000	-2.126755000	0.655927000
1	-0.990202000	0.010988000	-1.241671000



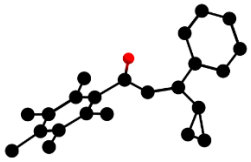
^{t}BuO^{-}-H_2O

G = -309.6369162 Eh

E = -309.7327052 Eh

1	-2.718761000	0.848465000	0.007091000
8	-2.605094000	-0.102825000	-0.112471000
1	-1.662144000	-0.127417000	-0.585513000
8	-0.289963000	-0.036851000	-1.143740000
6	0.539734000	-0.002167000	-0.065070000
6	0.268739000	1.256649000	0.814299000
1	-0.775028000	1.214947000	1.148103000
1	0.397020000	2.159285000	0.200398000

1	0.921350000	1.340611000	1.699192000
6	0.340309000	-1.251991000	0.842863000
1	0.978743000	-1.263333000	1.742123000
1	0.546849000	-2.159740000	0.258676000
6	2.021834000	0.037896000	-0.523596000
1	2.186497000	0.925440000	-1.149982000
1	2.741999000	0.061054000	0.310821000
1	2.232639000	-0.846685000	-1.139784000
1	-0.712410000	-1.277532000	1.147586000

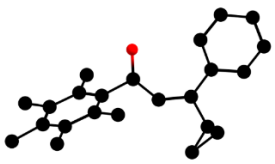


6a

G = -967.408114 Eh

E = -967.751939 Eh

6	-2.145139000	0.960146000	0.131219000
6	-3.217933000	-0.017197000	-0.177264000
6	-4.238710000	-0.247668000	0.763760000
6	-3.294843000	-0.658538000	-1.424397000
6	-5.287871000	-1.120972000	0.478068000
6	-4.354962000	-1.514751000	-1.717183000
6	-5.350993000	-1.754638000	-0.765790000
1	-4.195556000	0.252013000	1.726555000
1	-2.521797000	-0.476552000	-2.159941000
1	-6.057776000	-1.301472000	1.223181000
1	-4.402562000	-1.997378000	-2.689296000
1	-6.172997000	-2.427622000	-0.994084000
6	-2.338446000	2.348190000	2.329452000
6	-2.634654000	2.185521000	0.836430000
6	-1.750265000	3.305503000	1.332113000
1	-3.146204000	2.682848000	2.975881000
1	-1.670506000	1.610075000	2.766083000
1	-3.641575000	2.476060000	0.547598000
1	-0.680341000	3.262125000	1.151696000
1	-2.170110000	4.306500000	1.274819000
6	-0.821512000	0.796782000	-0.128992000
6	-0.093990000	-0.423398000	-0.541765000
8	-0.609062000	-1.461626000	-0.946405000
1	-0.161278000	1.621314000	0.117977000
6	1.404325000	-0.348009000	-0.333492000
6	1.994443000	-1.192139000	0.626624000
6	2.180630000	0.548143000	-1.093419000
6	3.384579000	-1.122341000	0.839010000
6	3.566936000	0.624844000	-0.860810000
6	4.160037000	-0.186618000	0.126992000
6	4.435068000	1.575472000	-1.659964000
1	5.364078000	1.090057000	-1.978586000
1	3.931707000	1.943879000	-2.555402000
1	4.722680000	2.452619000	-1.062978000
6	5.640507000	-0.050164000	0.420742000
1	6.244251000	-0.731027000	-0.196926000
1	5.995978000	0.964563000	0.223106000
1	5.864272000	-0.277526000	1.466593000
6	4.041870000	-2.055517000	1.836444000
1	3.488415000	-2.993421000	1.929813000
1	5.062524000	-2.308295000	1.536040000
1	4.098695000	-1.610718000	2.840755000
6	1.158408000	-2.145657000	1.457240000
1	1.473829000	-2.127849000	2.506089000
1	0.094623000	-1.906855000	1.420022000
1	1.266290000	-3.179741000	1.104127000
6	1.548386000	1.404773000	-2.174502000
1	1.692213000	2.474712000	-1.977743000
1	2.002386000	1.195982000	-3.151160000
1	0.476026000	1.228130000	-2.276081000



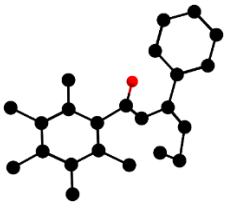
C_R

G = -967.4800103 Eh

E = -967.8162353 Eh

6	2.190877000	0.769722000	0.102352000

6	3.332515000	-0.119381000	0.120628000
6	4.666475000	0.398170000	0.137692000
6	3.218788000	-1.541919000	0.160108000
6	5.780160000	-0.434132000	0.200992000
6	4.340068000	-2.359932000	0.220169000
6	5.639696000	-1.826618000	0.246920000
1	4.825134000	1.469553000	0.096328000
1	2.221907000	-1.971199000	0.104436000
1	6.773440000	0.012884000	0.213308000
1	4.201209000	-3.440096000	0.245420000
1	6.511211000	-2.475035000	0.297705000
6	3.014155000	2.979158000	-1.069112000
6	2.528701000	2.239588000	0.168676000
6	1.666730000	3.302346000	-0.466800000
1	3.820639000	3.704248000	-0.966897000
1	3.025622000	2.414458000	-1.998410000
1	3.040200000	2.555338000	1.082405000
1	0.783508000	2.974120000	-1.008299000
1	1.549256000	4.250009000	0.055811000
6	0.804115000	0.464533000	0.111346000
6	-0.002375000	-0.693178000	-0.062973000
8	0.325283000	-1.888127000	-0.331767000
1	0.186737000	1.346692000	0.267611000
6	-1.504796000	-0.427298000	0.010853000
6	-2.265750000	-0.505282000	-1.174274000
6	-2.146246000	-0.174147000	1.240033000
6	-3.658523000	-0.307274000	-1.133171000
6	-3.541988000	0.025077000	1.278558000
6	-4.293392000	-0.006337000	0.088892000
6	-4.233112000	0.282719000	2.604055000
1	-5.244897000	-0.134927000	2.621261000
1	-3.683010000	-0.160524000	3.438096000
1	-4.323657000	1.358989000	2.816722000
6	-5.780346000	0.294257000	0.120805000
1	-6.385795000	-0.606723000	0.303446000
1	-6.026591000	1.011291000	0.909986000
1	-6.123882000	0.725739000	-0.823897000
6	-4.477668000	-0.411077000	-2.405869000
1	-3.985140000	-1.043703000	-3.148548000
1	-5.465407000	-0.843119000	-2.213994000
1	-4.640092000	0.571318000	-2.875138000
6	-1.585767000	-0.773590000	-2.502632000
1	-1.831091000	-1.775438000	-2.881576000
1	-1.913164000	-0.054582000	-3.264708000
1	-0.500414000	-0.718419000	-2.414957000
6	-1.353000000	-0.128481000	2.531504000
1	-1.518738000	0.813074000	3.071906000
1	-1.652470000	-0.939201000	3.211091000
1	-0.282684000	-0.221279000	2.342514000



TS6$_R$

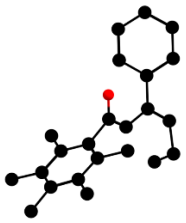
G = -967.4539954 Eh

E = -967.7876684 Eh

ν = -578.9 cm^{-1}

6	2.282992000	0.969827000	0.201586000
6	3.256008000	-0.099041000	-0.121853000
6	4.540512000	0.202028000	-0.624646000
6	2.959571000	-1.461242000	0.105867000
6	5.488904000	-0.794849000	-0.860432000
6	3.904122000	-2.456602000	-0.130275000
6	5.179422000	-2.135081000	-0.612879000
1	4.786571000	1.235897000	-0.850530000
1	1.973706000	-1.724163000	0.465127000
1	6.467708000	-0.522986000	-1.250771000
1	3.643541000	-3.495181000	0.063235000
1	5.912361000	-2.916032000	-0.801616000
6	2.033905000	3.376669000	1.107800000
6	2.814817000	2.174503000	0.706447000
6	2.060611000	2.845600000	2.499983000

1	2.568142000	4.324129000	0.976692000
1	1.042557000	3.438319000	0.649596000
1	3.888891000	2.244301000	0.848082000
1	1.381586000	2.047970000	2.777785000
1	2.897498000	3.065239000	3.154952000
6	0.866284000	0.765312000	0.147890000
6	0.119219000	-0.181056000	-0.588672000
8	0.533132000	-1.063287000	-1.387845000
1	0.261572000	1.479078000	0.703188000
6	-1.389204000	-0.162661000	-0.331453000
6	-2.227755000	0.814406000	-0.894470000
6	-1.940071000	-1.217955000	0.425640000
6	-3.622209000	0.745807000	-0.686379000
6	-3.330471000	-1.298844000	0.615965000
6	-4.169026000	-0.290113000	0.092406000
6	-3.938731000	-2.467223000	1.371454000
1	-4.943397000	-2.701295000	1.006140000
1	-3.337859000	-3.373129000	1.254888000
1	-4.024456000	-2.269971000	2.450751000
6	-5.659119000	-0.316909000	0.381565000
1	-6.221183000	-0.901893000	-0.362648000
1	-5.869011000	-0.757370000	1.361048000
1	-6.085088000	0.690584000	0.386455000
6	-4.532859000	1.790915000	-1.302931000
1	-4.079565000	2.251985000	-2.184006000
1	-5.488912000	1.358770000	-1.616456000
1	-4.762436000	2.604031000	-0.597540000
6	-1.644653000	1.944673000	-1.719317000
1	-1.969300000	2.923676000	-1.342336000
1	-0.553851000	1.921275000	-1.697719000
1	-1.969054000	1.885840000	-2.768279000
6	-0.988179000	-2.227636000	1.035602000
1	-1.432756000	-2.777824000	1.869162000
1	-0.635342000	-2.943376000	0.283467000
1	-0.101509000	-1.704750000	1.410712000



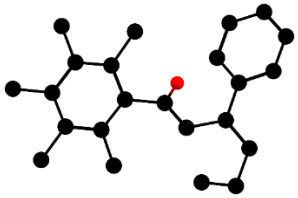
D_R

G = -967.4624321 Eh

E = -967.7934961 Eh

6	2.315065000	0.955870000	-0.161662000
6	3.251280000	-0.205030000	-0.061046000
6	4.419159000	-0.263392000	-0.840645000
6	3.026686000	-1.243456000	0.860956000
6	5.342426000	-1.302343000	-0.692304000
6	3.945972000	-2.278715000	1.015357000
6	5.112307000	-2.315132000	0.240714000
1	4.589136000	0.516582000	-1.577426000
1	2.113765000	-1.227578000	1.444065000
1	6.235577000	-1.323444000	-1.313100000
1	3.750564000	-3.067435000	1.738568000
1	5.824302000	-3.129017000	0.356689000
6	2.125094000	3.495885000	-0.388502000
6	2.894406000	2.196030000	-0.307575000
6	1.979242000	4.007450000	1.014766000
1	2.665324000	4.223175000	-1.011176000
1	1.145797000	3.319722000	-0.854410000
1	3.975509000	2.284554000	-0.223741000
1	1.355285000	3.438029000	1.701204000
1	2.799019000	4.568632000	1.462295000
6	0.893384000	0.767800000	-0.035597000
6	0.150318000	-0.408880000	-0.261919000
8	0.558672000	-1.547595000	-0.608819000
1	0.306756000	1.651828000	0.199501000
6	-1.367830000	-0.269088000	-0.111244000
6	-2.154153000	-0.255417000	-1.280478000
6	-1.985028000	-0.261659000	1.152650000
6	-3.557407000	-0.244308000	-1.185880000
6	-3.392286000	-0.241432000	1.247485000

6	-4.177702000	-0.203726000	0.080033000
6	-4.057073000	-0.265465000	2.611131000
1	-5.004299000	-0.813830000	2.589895000
1	-3.420227000	-0.746029000	3.358447000
1	-4.277896000	0.747617000	2.980685000
6	-5.688780000	-0.099371000	0.179969000
1	-6.178004000	-1.085390000	0.192411000
1	-5.996743000	0.423140000	1.090308000
1	-6.107993000	0.455082000	-0.665323000
6	-4.403343000	-0.288701000	-2.444928000
1	-3.881094000	-0.804139000	-3.255688000
1	-5.345899000	-0.819536000	-2.277447000
1	-4.658450000	0.716966000	-2.812298000
6	-1.474374000	-0.234383000	-2.635525000
1	-1.387744000	-1.242305000	-3.063547000
1	-2.028768000	0.383125000	-3.351311000
1	-0.463025000	0.170720000	-2.550628000
6	-1.145801000	-0.278380000	2.415578000
1	-1.484748000	0.481086000	3.131504000
1	-1.206840000	-1.249426000	2.928543000
1	-0.098061000	-0.076315000	2.184525000



$TS7_R$

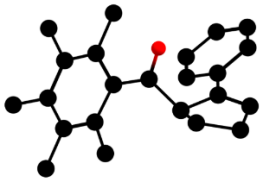
G = -967.4404526 Eh

E = -967.7768556 Eh

ν = -320.3 cm^{-1}

6	-2.417526000	1.103883000	-0.334786000
6	-3.039771000	-0.242665000	-0.269775000
6	-4.358186000	-0.422958000	0.190381000
6	-2.341571000	-1.381355000	-0.710537000
6	-4.958131000	-1.682324000	0.194457000
6	-2.935128000	-2.642823000	-0.701355000
6	-4.250471000	-2.802946000	-0.253200000
1	-4.899571000	0.438731000	0.570791000
1	-1.317021000	-1.255165000	-1.043087000
1	-5.975555000	-1.793181000	0.563768000
1	-2.367008000	-3.505834000	-1.041771000
1	-4.713739000	-3.786727000	-0.242234000
6	-2.534885000	3.552085000	-0.605123000
6	-3.177145000	2.185415000	-0.621538000
6	-1.285740000	3.489249000	0.230379000
1	-2.282938000	3.870766000	-1.633047000
1	-3.274603000	4.296031000	-0.248206000
1	-4.230666000	2.084877000	-0.881657000
1	-1.426585000	3.413382000	1.307459000
1	-0.427540000	4.079886000	-0.081022000
6	-0.940867000	1.263170000	-0.206797000
6	-0.238024000	0.489313000	0.762074000
8	-0.772701000	0.057159000	1.827451000
1	-0.401263000	1.509790000	-1.120580000
6	1.207642000	0.119709000	0.451640000
6	1.579004000	-1.245771000	0.363696000
6	2.192296000	1.109669000	0.234454000
6	2.888248000	-1.600353000	-0.014100000
6	3.501103000	0.749562000	-0.147162000
6	3.860621000	-0.605920000	-0.247850000
6	4.522440000	1.834069000	-0.438052000
1	5.238412000	1.519327000	-1.203848000
1	4.041013000	2.746678000	-0.800549000
1	5.103212000	2.110907000	0.455131000
6	5.290065000	-0.997699000	-0.575748000
1	5.456711000	-1.118368000	-1.657437000
1	6.003845000	-0.247410000	-0.222795000
1	5.564191000	-1.945623000	-0.102807000
6	3.255453000	-3.064636000	-0.173358000
1	2.386578000	-3.669036000	-0.446769000
1	4.010275000	-3.209566000	-0.952780000
1	3.663301000	-3.493034000	0.755095000
6	0.580920000	-2.350239000	0.659851000

1	1.027072000	-3.101089000	1.325113000
1	-0.307905000	-1.949554000	1.143907000
1	0.282251000	-2.881595000	-0.255283000
6	1.874809000	2.570364000	0.475885000
1	2.690128000	3.060919000	1.023144000
1	1.733394000	3.131026000	-0.458714000
1	0.954692000	2.675799000	1.047950000



E_R

G = -967.4830557 Eh

E = -967.8224967 Eh

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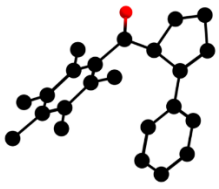
6	2.454943000	0.786111000	-0.538049000
6	3.511856000	1.689209000	-0.322118000
6	1.228897000	1.295245000	-1.005761000
6	3.357136000	3.052059000	-0.575832000
6	1.072327000	2.660968000	-1.255289000
6	2.133038000	3.545205000	-1.043155000
1	4.451772000	1.312889000	0.072380000
1	0.395679000	0.620315000	-1.156432000
1	4.186241000	3.732143000	-0.395104000
1	0.113087000	3.030539000	-1.608541000
1	2.007227000	4.608864000	-1.230352000
6	3.573055000	-2.816686000	-0.110793000
6	3.765769000	-1.341820000	-0.362188000
6	2.148313000	-2.868132000	0.487709000
1	3.642046000	-3.381954000	-1.055881000
1	4.332511000	-3.243551000	0.560024000
1	4.724446000	-0.908597000	-0.639290000
1	2.213072000	-2.796511000	1.578732000
1	1.601897000	-3.779250000	0.222233000
6	1.424734000	-1.577632000	0.017207000
6	0.487896000	-0.971980000	1.081617000
8	1.046042000	-0.710797000	2.198868000
1	0.889957000	-1.746422000	-0.925028000
6	-0.872218000	-0.603099000	0.703206000
6	-1.478677000	0.634356000	1.138217000
6	-1.662897000	-1.452849000	-0.162450000
6	-2.718663000	1.035803000	0.633669000
6	-2.898182000	-1.021094000	-0.664504000
6	-3.452259000	0.216049000	-0.269115000
6	-3.675463000	-1.907899000	-1.624314000
1	-4.214023000	-1.311058000	-2.368298000
1	-3.016729000	-2.587490000	-2.172181000
1	-4.426308000	-2.529068000	-1.110102000
6	-4.816281000	0.647156000	-0.770376000
1	-4.778024000	1.211127000	-1.719598000
1	-5.474189000	-0.211375000	-0.945523000
1	-5.327667000	1.290470000	-0.046536000
6	-3.291632000	2.392676000	1.009778000
1	-2.516928000	3.088308000	1.340116000
1	-3.802098000	2.859009000	0.159007000
1	-4.032352000	2.324099000	1.822608000
6	-0.718528000	1.573530000	2.059472000
1	-1.372161000	1.984100000	2.840548000
1	0.109113000	1.043953000	2.531483000
1	-0.306840000	2.428393000	1.501381000
6	-1.246665000	-2.895490000	-0.393876000
1	-0.581546000	-3.220548000	0.412185000
1	-2.117301000	-3.564064000	-0.394066000
1	-0.712505000	-3.076146000	-1.340112000



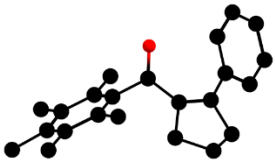
F

G = -967.444981 Eh

E = -967.791835 Eh

6	2.484855000	0.006386000	-0.379903000

6	1.767484000	1.260307000	-0.664679000
6	2.268754000	2.499172000	-0.216414000
6	0.550142000	1.258662000	-1.367395000
6	1.582476000	3.684811000	-0.465049000
6	-0.141702000	2.445561000	-1.611991000
6	0.367897000	3.664345000	-1.161013000
1	3.193674000	2.525121000	0.351389000
1	0.124857000	0.320838000	-1.703750000
1	1.986819000	4.626032000	-0.102345000
1	-1.087565000	2.411937000	-2.145317000
1	-0.174201000	4.587931000	-1.344070000
6	4.155998000	-1.553866000	0.285766000
6	3.753595000	-0.122281000	0.048779000
6	3.032240000	-2.345518000	-0.424360000
1	5.152832000	-1.787192000	-0.109135000
1	4.173601000	-1.773457000	1.362134000
1	4.427152000	0.712018000	0.221803000
1	2.788097000	-3.280709000	0.085921000
1	3.336869000	-2.575506000	-1.450768000
6	1.826888000	-1.380327000	-0.471943000
6	0.904046000	-1.538098000	0.746126000
8	1.326350000	-1.986740000	1.799930000
1	1.233918000	-1.486422000	-1.384547000
6	-0.508855000	-1.044950000	0.585478000
6	-0.924005000	0.118156000	1.255439000
6	-1.366446000	-1.728327000	-0.297072000
6	-2.221670000	0.613830000	1.022002000
6	-2.666644000	-1.238319000	-0.509967000
6	-3.102481000	-0.082575000	0.172310000
6	-3.601271000	-1.952720000	-1.464766000
1	-4.204690000	-1.240848000	-2.036470000
1	-3.056264000	-2.569049000	-2.183181000
1	-4.300540000	-2.613481000	-0.932289000
6	-4.530145000	0.397703000	-0.002384000
1	-4.618918000	1.136614000	-0.811816000
1	-5.204302000	-0.428495000	-0.241824000
1	-4.907119000	0.868032000	0.909611000
6	-2.639936000	1.909006000	1.686291000
1	-1.805185000	2.615257000	1.722160000
1	-3.457089000	2.399925000	1.152777000
1	-2.969950000	1.747838000	2.722695000
6	0.005079000	0.885051000	2.169253000
1	-0.473387000	1.074233000	3.137614000
1	0.937600000	0.353913000	2.357295000
1	0.253258000	1.860170000	1.732916000
6	-0.918417000	-3.009910000	-0.975145000
1	-1.669085000	-3.798058000	-0.848434000
1	-0.776336000	-2.875448000	-2.055818000
1	0.017869000	-3.393873000	-0.562165000



3a

G = -967.4433226 Eh

E = -967.7895756 Eh

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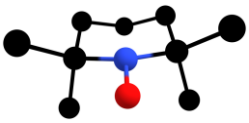
6	3.345544000	-0.034484000	0.037964000
6	4.389683000	0.915945000	0.084048000
6	3.443987000	-1.080400000	-0.900714000
6	5.467091000	0.845755000	-0.795650000
6	4.530726000	-1.152962000	-1.772583000
6	5.544028000	-0.192772000	-1.728668000
1	4.346196000	1.725612000	0.805176000
1	2.658680000	-1.821966000	-0.937958000
1	6.249535000	1.598372000	-0.749599000
1	4.586495000	-1.970276000	-2.486576000
1	6.387470000	-0.253763000	-2.411093000
6	2.502822000	0.802446000	2.327002000
6	1.301493000	0.408297000	3.199451000
6	2.244505000	0.084564000	1.006486000
1	2.517714000	1.888686000	2.149033000
1	3.473033000	0.537748000	2.760540000

1	1.060592000	1.153396000	3.963683000
6	0.922804000	-0.248261000	0.925757000
6	0.142574000	-0.793805000	-0.206059000
8	0.577339000	-1.573443000	-1.051200000
6	-1.307358000	-0.361394000	-0.264823000
6	-1.609906000	0.977178000	-0.573000000
6	-2.322007000	-1.304769000	-0.017378000
6	-2.956285000	1.380023000	-0.642534000
6	-3.667249000	-0.896316000	-0.103532000
6	-3.981140000	0.433881000	-0.445890000
1	1.516548000	-0.541351000	3.702801000
6	-4.790854000	-1.877134000	0.162847000
1	-5.571623000	-1.425049000	0.784479000
1	-5.273482000	-2.195621000	-0.771988000
1	-4.442481000	-2.777294000	0.671715000
6	-5.432036000	0.844238000	-0.596569000
1	-5.861618000	1.182441000	0.357762000
1	-5.547037000	1.662355000	-1.312388000
1	-6.047710000	0.012403000	-0.949044000
6	-3.301892000	2.826872000	-0.930812000
1	-2.496005000	3.501322000	-0.631281000
1	-3.488391000	2.998002000	-2.000954000
1	-4.202797000	3.135695000	-0.392488000
6	-0.506041000	1.979341000	-0.851735000
1	0.450929000	1.495869000	-1.056939000
1	-0.750812000	2.597587000	-1.721927000
1	-0.356601000	2.662594000	-0.004055000
6	-1.990494000	-2.732813000	0.369707000
1	-2.449643000	-3.446243000	-0.325094000
1	-0.917837000	-2.926872000	0.371132000
1	-2.378231000	-2.967255000	1.369517000
1	-0.360736000	1.140408000	1.973639000
1	-0.581343000	-0.525013000	2.497082000



TEMPO

G = -483.7732864 Eh

E = -483.9655024 Eh

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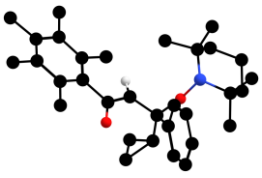
6	-1.242385000	1.386492000	-0.515212000
6	-1.318883000	-0.072395000	-0.030556000
1	2.162255000	1.892152000	-0.199655000
1	1.228447000	1.391367000	-1.613793000
1	0.000309000	3.154833000	-0.366593000
1	0.000472000	2.159229000	1.088426000
1	-2.161816000	1.892606000	-0.198641000
1	-1.228764000	1.391952000	-1.613292000
7	-0.000068000	-0.754524000	-0.239349000
8	-0.000158000	-2.032003000	-0.091173000
6	-1.691804000	-0.145725000	1.460782000
1	-1.055434000	0.497052000	2.074551000
1	-2.731139000	0.174331000	1.596295000
1	-1.590903000	-1.177772000	1.809742000
6	-2.365237000	-0.832325000	-0.853543000
1	-2.456642000	-1.863074000	-0.504867000
1	-3.334022000	-0.330732000	-0.754300000
1	-2.083448000	-0.844770000	-1.912073000
6	1.691778000	-0.145051000	1.460761000
1	1.057326000	0.500496000	2.073650000
1	1.588187000	-1.176349000	1.811134000
1	2.731985000	0.172381000	1.595736000
6	2.365064000	-0.833104000	-0.853298000
1	2.456298000	-1.863695000	-0.504099000
1	2.083213000	-0.846070000	-1.911802000
1	3.333950000	-0.331647000	-0.754363000



C_R_TEMPO

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E = -1451.786451 Eh

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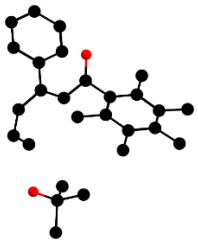
6	1.007229000	0.837049000	0.810018000
6	1.460630000	1.710751000	-0.360896000
6	1.995468000	2.992370000	-0.192423000
6	1.370814000	1.199907000	-1.663784000
6	2.461569000	3.729853000	-1.283650000
6	1.845458000	1.924055000	-2.756102000
6	2.403979000	3.193638000	-2.571598000
1	2.048615000	3.424463000	0.800128000
1	0.917027000	0.227849000	-1.798305000
1	2.871198000	4.725137000	-1.124751000
1	1.772121000	1.501847000	-3.756099000
1	2.772139000	3.762844000	-3.422309000
6	0.233219000	2.593032000	2.586257000
6	1.228897000	1.546563000	2.151496000
6	0.324648000	1.279108000	3.327358000
1	0.615953000	3.487195000	3.075502000
1	-0.599096000	2.753653000	1.906011000
1	2.273626000	1.746708000	2.385882000
1	-0.481575000	0.568071000	3.176678000
1	0.773235000	1.279067000	4.319353000
6	-0.403425000	0.366876000	0.606604000
6	-1.421503000	1.127964000	0.049862000
8	-1.372956000	2.311858000	-0.413919000
1	-0.683560000	-0.544346000	1.115095000
6	-2.770683000	0.412375000	-0.065791000
6	-3.165004000	-0.093942000	-1.320704000
6	-3.633957000	0.297512000	1.038370000
6	-4.399393000	-0.755139000	-1.458863000
6	-4.881894000	-0.344400000	0.895703000
6	-5.277123000	-0.846352000	-0.357945000
6	-5.801399000	-0.488820000	2.093919000
1	-6.364743000	-1.427474000	2.060900000
1	-5.241522000	-0.477686000	3.032935000
1	-6.537632000	0.327737000	2.148815000
6	-6.646911000	-1.479918000	-0.519938000
1	-6.644031000	-2.553294000	-0.274452000
1	-7.385397000	-1.005113000	0.133802000
1	-7.017684000	-1.384330000	-1.544495000
6	-4.781214000	-1.377550000	-2.789460000
1	-3.895162000	-1.666428000	-3.361095000
1	-5.386947000	-2.279367000	-2.653463000
1	-5.362575000	-0.688645000	-3.421082000
6	-2.237015000	0.065102000	-2.510117000
1	-1.629307000	-0.836554000	-2.675448000
1	-2.799356000	0.249273000	-3.433013000
1	-1.565396000	0.910134000	-2.348824000
6	-3.234839000	0.874291000	2.381647000
1	-4.045607000	1.476694000	2.812081000
1	-3.004223000	0.086122000	3.113111000
1	-2.348321000	1.501290000	2.289553000
6	4.005178000	-0.746377000	-0.065965000
6	4.676768000	-1.488615000	1.111752000
1	5.759423000	-1.311162000	1.068957000
1	4.303293000	-1.040672000	2.041032000
6	4.367340000	-2.985583000	1.123915000
1	4.801182000	-3.470568000	0.239659000
1	4.825371000	-3.462220000	2.000392000
6	2.850928000	-3.180339000	1.147921000
1	2.587750000	-4.246359000	1.123023000
1	2.458570000	-2.764993000	2.084453000
6	2.129083000	-2.460674000	-0.015247000
6	2.412637000	-3.164916000	-1.361343000
1	2.147132000	-2.507559000	-2.194439000
1	1.797113000	-4.069239000	-1.427324000
1	3.449246000	-3.480254000	-1.483493000
6	0.622537000	-2.587320000	0.232644000
1	0.368959000	-2.237419000	1.232336000
1	0.045992000	-2.000004000	-0.485800000
1	0.341894000	-3.644679000	0.152121000

6	4.297702000	0.751279000	0.102308000
1	5.382527000	0.867606000	0.220808000
1	3.985261000	1.320378000	-0.774012000
1	3.805774000	1.160922000	0.983269000
6	4.656979000	-1.137445000	-1.410053000
1	4.016962000	-0.820593000	-2.238668000
1	5.616993000	-0.615998000	-1.501169000
1	4.865701000	-2.202705000	-1.508871000



TS6$_I$

G = -1200.532196 Eh

E = -1200.979024 Eh

ν = -490.5 cm^{-1}

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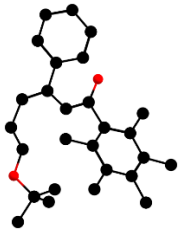
6	-3.547634000	-0.212191000	0.122590000
6	-4.745850000	0.041978000	0.808304000
6	-3.552915000	-1.179956000	-0.896046000
6	-5.913831000	-0.659822000	0.497492000
6	-4.718564000	-1.870145000	-1.218279000
6	-5.905171000	-1.615737000	-0.519655000
1	-4.750765000	0.785996000	1.599825000
1	-2.631063000	-1.373614000	-1.433423000
1	-6.828604000	-0.457123000	1.049019000
1	-4.704085000	-2.610099000	-2.014671000
1	-6.813223000	-2.159682000	-0.767544000
6	-1.452557000	2.926083000	1.079281000
6	-2.498098000	1.997484000	0.501246000
6	-1.297644000	2.984336000	-0.366815000
1	-1.835584000	3.824284000	1.563602000
1	-0.658486000	2.441254000	1.645392000
1	-3.507756000	2.379732000	0.394135000
1	-0.644685000	2.292762000	-0.875715000
1	-1.804306000	3.739535000	-0.947763000
6	-1.060668000	-0.004864000	0.493583000
6	-0.714427000	-1.396843000	0.638405000
8	-1.498804000	-2.334094000	0.866458000
1	-0.211221000	0.669638000	0.499531000
8	0.379542000	4.490910000	-0.717591000
6	1.619022000	3.944922000	-0.823241000
6	1.979749000	3.028647000	0.388003000
1	1.295972000	2.173666000	0.426891000
1	1.862595000	3.599968000	1.318155000
1	3.006537000	2.633343000	0.344607000
6	2.680550000	5.082689000	-0.874537000
1	2.599039000	5.692089000	0.034934000
1	3.714930000	4.713015000	-0.958577000
1	2.470830000	5.733577000	-1.733306000
6	1.783999000	3.094326000	-2.118757000
1	1.105700000	2.231180000	-2.097445000
1	1.514136000	3.711144000	-2.985860000
1	2.805996000	2.711184000	-2.264688000
6	0.772810000	-1.686020000	0.461649000
6	1.718051000	-1.134357000	1.347975000
6	1.194764000	-2.479806000	-0.625143000
6	3.092068000	-1.366505000	1.141213000
6	2.570248000	-2.700478000	-0.831562000
6	3.516709000	-2.175139000	0.071012000
6	3.038052000	-3.497483000	-2.034697000
1	3.211949000	-4.555278000	-1.786292000
1	2.304773000	-3.472644000	-2.843969000
1	3.976734000	-3.102288000	-2.435824000
6	4.989785000	-2.492730000	-0.104648000
1	5.499400000	-2.563803000	0.860782000
1	5.136256000	-3.447345000	-0.617045000
1	5.512349000	-1.723464000	-0.692085000
6	4.098112000	-0.729575000	2.079266000
1	4.245157000	-1.326761000	2.991912000
1	5.075829000	-0.605044000	1.607062000

1	3.763546000	0.262507000	2.396874000
6	1.290410000	-0.313354000	2.549136000
1	1.822356000	-0.641609000	3.450791000
1	1.522762000	0.751216000	2.408920000
1	0.219113000	-0.393808000	2.739065000
6	0.193066000	-3.074012000	-1.597990000
1	0.222986000	-2.554052000	-2.566157000
1	0.420316000	-4.128098000	-1.797002000
1	-0.822641000	-3.025937000	-1.207726000



D_I

G = -1200.556932 Eh

E = -1201.049902 Eh

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6	-3.646057000	0.026985000	0.111904000
6	-4.853946000	0.391837000	0.728753000
6	-3.673268000	-1.032935000	-0.812279000
6	-6.050797000	-0.262808000	0.423359000
6	-4.864764000	-1.683589000	-1.124614000
6	-6.062976000	-1.304766000	-0.506156000
1	-4.840620000	1.190578000	1.465177000
1	-2.741815000	-1.324534000	-1.283687000
1	-6.971560000	0.036493000	0.919750000
1	-4.859980000	-2.496536000	-1.847543000
1	-6.990800000	-1.821009000	-0.741871000
6	-1.264354000	3.013646000	0.734474000
6	-2.464061000	2.135118000	0.495913000
6	-0.457245000	3.264933000	-0.547330000
1	-1.558988000	3.984149000	1.156830000
1	-0.582830000	2.538267000	1.453072000
1	-3.421677000	2.620673000	0.320215000
1	-0.241660000	2.302757000	-1.020880000
1	-1.054635000	3.851291000	-1.262330000
6	-1.117729000	0.071793000	0.411937000
6	-0.857539000	-1.286423000	0.669018000
8	-1.665227000	-2.214601000	0.946486000
1	-0.232541000	0.688697000	0.317673000
8	0.743299000	3.981248000	-0.240643000
6	1.976498000	3.457258000	-0.757480000
6	2.282404000	2.064462000	-0.183548000
1	1.571071000	1.309080000	-0.527137000
1	2.252690000	2.094568000	0.910593000
1	3.281500000	1.739320000	-0.496680000
6	3.032263000	4.455927000	-0.279150000
1	3.038143000	4.499937000	0.815681000
1	4.029007000	4.158087000	-0.623949000
1	2.809747000	5.457375000	-0.664765000
6	1.949702000	3.415481000	-2.292086000
1	1.188803000	2.715523000	-2.653458000
1	1.724509000	4.411350000	-2.691565000
1	2.920248000	3.090682000	-2.685442000
6	0.627518000	-1.643840000	0.503567000
6	1.023058000	-2.428650000	-0.601369000
6	1.592598000	-1.171869000	1.415814000
6	2.390868000	-2.666412000	-0.834976000
6	2.961174000	-1.431600000	1.191135000
6	3.359720000	-2.148807000	0.049193000
6	4.013156000	-0.922975000	2.159138000
1	4.531481000	-0.036922000	1.763713000
1	3.583689000	-0.639096000	3.121713000
1	4.781275000	-1.680674000	2.353078000
6	4.830520000	-2.376366000	-0.240348000
1	5.035499000	-2.347626000	-1.315641000
1	5.461642000	-1.618756000	0.231755000
1	5.175067000	-3.357450000	0.121574000
6	2.859872000	-3.456707000	-2.041094000
1	3.379873000	-2.812367000	-2.765034000
1	3.574441000	-4.238050000	-1.752003000
1	2.037506000	-3.938273000	-2.572403000

6	-0.022321000	-2.966411000	-1.562152000
1	0.022272000	-2.456125000	-2.534714000
1	0.130444000	-4.035663000	-1.755961000
1	-1.023052000	-2.855066000	-1.144275000
6	1.174095000	-0.387541000	2.645499000
1	1.502760000	-0.891257000	3.565366000
1	1.620534000	0.615703000	2.654765000
1	0.091876000	-0.264969000	2.687598000

TS7$_I$

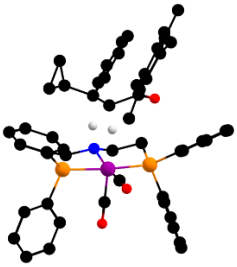
G = -1200.533666 Eh

E = -1200.983011 Eh

ν = -595.3 cm^{-1}

6	-2.550306000	0.755405000	-0.611098000
6	-3.821642000	0.176708000	-0.119730000
6	-4.940713000	0.987466000	0.156985000
6	-3.961566000	-1.209807000	0.071506000
6	-6.153127000	0.435047000	0.567750000
6	-5.171676000	-1.765367000	0.485874000
6	-6.279123000	-0.948400000	0.731083000
1	-4.846450000	2.065653000	0.066542000
1	-3.100574000	-1.846947000	-0.091701000
1	-6.998589000	1.087372000	0.774152000
1	-5.247737000	-2.841342000	0.624563000
1	-7.221006000	-1.380333000	1.059941000
6	-1.102349000	2.469251000	-1.563208000
6	-2.471117000	1.972357000	-1.190961000
6	-0.038321000	1.762238000	-0.739264000
1	-0.891609000	2.305152000	-2.632493000
1	-1.002806000	3.547197000	-1.398593000
1	-3.346213000	2.580235000	-1.415171000
1	-0.016439000	1.935025000	0.325784000
1	0.772177000	1.213809000	-1.184774000
6	-1.247118000	0.037112000	-0.587023000
6	-0.788588000	-0.703838000	0.550937000
8	-1.331611000	-0.693657000	1.674437000
1	-0.899010000	-0.322832000	-1.554092000
8	1.201151000	3.401173000	-1.016916000
6	2.321558000	3.451511000	-0.223972000
6	3.198395000	4.636857000	-0.701971000
1	2.623641000	5.569380000	-0.633633000
1	3.474553000	4.487651000	-1.753528000
1	4.118943000	4.747535000	-0.108766000
6	3.177308000	2.158375000	-0.324701000
1	3.431637000	1.973197000	-1.376645000
1	4.113189000	2.231505000	0.249651000
1	2.620083000	1.291121000	0.041643000
6	1.966373000	3.695910000	1.267358000
1	1.363159000	4.609302000	1.348190000
1	1.372980000	2.864604000	1.662459000
1	2.856189000	3.808421000	1.905508000
6	0.560450000	-1.393138000	0.378609000
6	0.755078000	-2.411411000	-0.578651000
6	1.639150000	-0.965520000	1.182836000
6	2.042752000	-2.948939000	-0.780119000
6	2.922487000	-1.509754000	0.978453000
6	3.132991000	-2.468728000	-0.029658000
6	4.072720000	-1.032780000	1.841974000
1	4.474809000	-0.076730000	1.475916000
1	3.748865000	-0.866727000	2.874130000
1	4.895361000	-1.751781000	1.869703000
6	4.533853000	-2.978114000	-0.310670000
1	4.625334000	-3.373647000	-1.325224000
1	5.273304000	-2.177796000	-0.208329000
1	4.828871000	-3.781919000	0.380382000
6	2.276644000	-4.039097000	-1.809185000
1	2.781708000	-3.646265000	-2.703485000
1	2.915957000	-4.834373000	-1.408432000

1	1.346806000	-4.502719000	-2.142385000
6	-0.410279000	-2.967221000	-1.377149000
1	-0.260710000	-2.841405000	-2.457438000
1	-0.530115000	-4.043607000	-1.194325000
1	-1.349003000	-2.478872000	-1.119040000
6	1.471235000	0.090689000	2.257239000
1	1.524862000	-0.364493000	3.256541000
1	2.270436000	0.835953000	2.199505000
1	0.510665000	0.597688000	2.193828000



TS8

G = -4167.912314 Eh

E = -4168.711739 Eh

ν = -499.1 cm^{-1}

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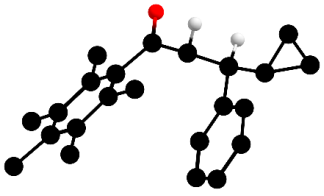
7	-1.424399000	0.419376000	1.883765000
6	-1.399317000	1.805327000	2.422382000
6	-2.381745000	-0.397097000	2.670372000
15	-0.827326000	2.448666000	-0.137571000
15	-2.470923000	-1.769458000	0.309777000
1	-1.136461000	1.796611000	3.486966000
1	-2.098156000	-0.379116000	3.733837000
1	-2.410421000	2.222099000	2.332469000
1	-3.379552000	0.048552000	2.579506000
6	-1.541865000	0.045226000	-1.924470000
8	-1.517368000	-0.138954000	-3.082513000
6	-2.105799000	3.726022000	-0.481946000
6	-2.624937000	3.785131000	-1.786688000
6	-2.618852000	4.591205000	0.492921000
1	-2.249723000	3.104083000	-2.546631000
1	-2.244470000	4.557650000	1.510850000
6	-3.624887000	4.699574000	-2.111317000
6	-3.628245000	5.504271000	0.167782000
1	-4.014734000	4.735261000	-3.124853000
1	-4.019041000	6.168385000	0.933997000
6	-4.130564000	5.562451000	-1.132655000
1	-4.914244000	6.271709000	-1.383868000
6	0.572806000	3.077949000	-1.135807000
6	0.954662000	2.404173000	-2.301510000
6	1.263633000	4.236266000	-0.751131000
1	0.432271000	1.504737000	-2.602267000
1	0.982056000	4.760236000	0.158173000
6	2.018155000	2.877828000	-3.073170000
6	2.329112000	4.705364000	-1.519248000
1	2.311710000	2.341487000	-3.971212000
1	2.867602000	5.596765000	-1.209235000
6	2.708497000	4.025904000	-2.681860000
1	3.541441000	4.390041000	-3.276948000
6	-0.390259000	2.646879000	1.643668000
1	-0.381368000	3.686379000	1.986245000
1	0.614097000	2.231392000	1.757597000
6	-2.374438000	-1.836773000	2.156506000
1	-1.412503000	-2.300564000	2.383403000
1	-3.157789000	-2.435367000	2.628939000
6	-3.293413000	0.924979000	-0.227306000
8	-4.380266000	1.346018000	-0.222274000
6	-1.735069000	-3.354565000	-0.248209000
6	-1.920715000	-4.541168000	0.476954000
6	-0.996253000	-3.385824000	-1.437119000
1	-2.490641000	-4.529378000	1.401893000
1	-0.855813000	-2.473827000	-2.004700000
6	-1.359152000	-5.736473000	0.026778000
6	-0.435280000	-4.583571000	-1.889196000
1	-1.499408000	-6.649191000	0.599293000
1	0.140430000	-4.595171000	-2.810570000
6	-0.612070000	-5.758799000	-1.155564000
1	-0.171875000	-6.689255000	-1.502733000
6	-4.235575000	-2.018641000	-0.152035000

6	-4.589333000	-1.775621000	-1.490470000
6	-5.226523000	-2.435384000	0.746417000
1	-3.838447000	-1.424581000	-2.192123000
1	-4.987256000	-2.621824000	1.787993000
6	-5.901821000	-1.962236000	-1.921822000
6	-6.545650000	-2.610319000	0.315114000
1	-6.159411000	-1.770856000	-2.959766000
1	-7.304988000	-2.927116000	1.024865000
6	-6.884882000	-2.379132000	-1.018745000
1	-7.909714000	-2.516214000	-1.352193000
1	-0.401489000	-0.069400000	2.109058000
1	0.239175000	-0.234314000	0.166111000
6	1.063542000	-0.787586000	2.158211000
6	1.833058000	0.028567000	3.153830000
6	1.181433000	0.569769000	4.275831000
6	3.233446000	0.142521000	3.114709000
6	1.879985000	1.250213000	5.276175000
6	3.940943000	0.834209000	4.097789000
6	3.265886000	1.401388000	5.182714000
1	0.107492000	0.435515000	4.364757000
1	3.768798000	-0.328277000	2.299862000
1	1.342035000	1.663927000	6.125767000
1	5.022147000	0.921011000	4.021825000
1	3.813746000	1.940659000	5.950849000
6	0.834756000	-3.470600000	1.894371000
6	0.979565000	-2.200697000	2.705123000
6	2.150704000	-3.166179000	2.568863000
1	0.216300000	-4.261970000	2.309849000
1	0.782704000	-3.418587000	0.811183000
1	0.501357000	-2.244731000	3.684330000
1	2.970292000	-2.840788000	1.931144000
1	2.452240000	-3.763591000	3.427115000
6	1.237430000	-0.654510000	0.688625000
6	2.318876000	0.300766000	0.193977000
8	2.286876000	1.479212000	0.526085000
1	1.333318000	-1.618292000	0.192789000
6	3.442458000	-0.254139000	-0.650615000
6	4.794962000	0.042348000	-0.346638000
6	3.130569000	-1.076514000	-1.757886000
6	5.818623000	-0.593393000	-1.079305000
6	4.161046000	-1.686711000	-2.494327000
6	5.506193000	-1.437380000	-2.161901000
6	3.820140000	-2.603754000	-3.652436000
1	4.533969000	-3.428913000	-3.729500000
1	2.827327000	-3.045252000	-3.540234000
1	3.832519000	-2.071906000	-4.614853000
6	6.618275000	-2.040469000	-2.996724000
1	6.966436000	-2.997173000	-2.580957000
1	6.294924000	-2.230116000	-4.023073000
1	7.484471000	-1.375444000	-3.048246000
6	7.268890000	-0.346180000	-0.712808000
1	7.386522000	-0.124208000	0.350246000
1	7.891533000	-1.217416000	-0.932748000
1	7.689213000	0.505305000	-1.267701000
6	5.207315000	1.040837000	0.716790000
1	5.904762000	1.767042000	0.281643000
1	4.362996000	1.588328000	1.122309000
1	5.739375000	0.553229000	1.543633000
6	1.705841000	-1.234413000	-2.249682000
1	1.019604000	-0.520477000	-1.798024000
1	1.663062000	-1.075569000	-3.332937000
1	1.316390000	-2.240166000	-2.057747000



5a

G = -968.619879 Eh

E = -968.986357 Eh

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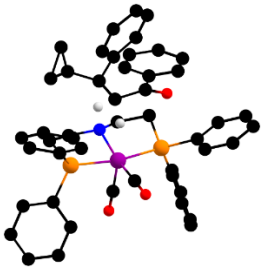
6	2.633996000	1.860199000	0.335400000

6	1.049143000	0.952195000	-1.233728000
6	2.265719000	3.155577000	-0.032347000
6	0.671955000	2.245278000	-1.601734000
6	1.278494000	3.352472000	-1.002348000
1	3.390538000	1.707458000	1.101068000
1	0.558945000	0.102751000	-1.698461000
1	2.740702000	4.009019000	0.444055000
1	-0.102128000	2.386334000	-2.351105000
1	0.982836000	4.358758000	-1.286261000
6	4.990488000	-0.746160000	-0.627344000
6	3.555740000	-1.158488000	-0.828732000
6	4.562317000	-2.170950000	-0.341930000
1	5.603195000	-0.556252000	-1.505200000
1	5.211672000	-0.104855000	0.223015000
1	3.212130000	-1.253921000	-1.857845000
1	4.493817000	-2.477753000	0.700226000
1	4.887048000	-2.954561000	-1.022382000
6	1.342256000	-1.684864000	0.233750000
6	0.325716000	-1.245926000	1.285186000
8	0.650587000	-1.219754000	2.463322000
1	1.780742000	-2.638848000	0.545658000
1	0.871397000	-1.825439000	-0.742448000
1	2.943350000	-0.591223000	1.131393000
6	-1.017499000	-0.777709000	0.793047000
6	-1.427755000	0.551319000	1.020309000
6	-1.812369000	-1.666469000	0.040776000
6	-2.636173000	0.997730000	0.449075000
6	-3.030834000	-1.219471000	-0.498527000
6	-3.454093000	0.105756000	-0.271237000
6	-3.886663000	-2.161128000	-1.321580000
1	-4.399709000	-1.629752000	-2.128625000
1	-3.289634000	-2.952851000	-1.780688000
1	-4.660608000	-2.649109000	-0.711590000
6	-4.803219000	0.562630000	-0.790494000
1	-4.736029000	0.963294000	-1.812356000
1	-5.521918000	-0.261242000	-0.813101000
1	-5.229735000	1.347607000	-0.160871000
6	-3.043672000	2.448809000	0.607747000
1	-2.169330000	3.099846000	0.684890000
1	-3.633559000	2.795560000	-0.245060000
1	-3.648458000	2.608582000	1.512075000
6	-0.586479000	1.530007000	1.810466000
1	-0.153891000	2.289225000	1.147851000
1	-1.205054000	2.053953000	2.548639000
1	0.225293000	1.042669000	2.345652000
6	-1.404835000	-3.117453000	-0.138336000
1	-2.249858000	-3.782044000	0.072557000
1	-1.079751000	-3.330678000	-1.165465000
1	-0.595237000	-3.409989000	0.534093000



$TS8_{Ph}$

G = -3971.377826 Eh

E = -3972.045042 Eh

ν = -1034.1 cm^{-1}

25	-1.219058000	0.413918000	-0.145330000
7	-0.681077000	0.280518000	1.830699000
6	-0.337250000	1.563849000	2.492324000
6	-1.609319000	-0.496573000	2.683723000
15	-0.160495000	2.452345000	-0.045310000
15	-2.129615000	-1.629412000	0.235908000
1	0.115123000	1.371375000	3.472517000
1	-1.179036000	-0.620612000	3.689873000
1	-1.260572000	2.136254000	2.652229000
1	-2.547589000	0.061871000	2.789628000
6	-1.355070000	0.352667000	-1.918556000
8	-1.460899000	0.311325000	-3.083769000
6	-1.338555000	3.863908000	0.078727000
6	-2.131096000	4.145238000	-1.046784000

6	-1.492451000	4.648742000	1.228514000	1	0.649497000	-4.106729000	-3.044815000
1	-2.034678000	3.531770000	-1.939692000	6	-0.308458000	-5.455919000	-1.658088000
1	-0.896847000	4.450142000	2.113168000	1	0.136021000	-6.347538000	-2.091388000
6	-3.043445000	5.198367000	-1.027824000	6	-3.930280000	-1.847071000	-0.065112000
6	-2.416612000	5.698409000	1.251629000	6	-4.500285000	-1.193447000	-1.168499000
1	-3.645591000	5.406581000	-1.907990000	6	-4.740182000	-2.675553000	0.726075000
1	-2.527712000	6.296666000	2.152074000	1	-3.884219000	-0.547211000	-1.785304000
6	-3.190096000	5.978059000	0.124343000	1	-4.321232000	-3.204149000	1.576423000
1	-3.906127000	6.795039000	0.142590000	6	-5.852052000	-1.362025000	-1.472337000
6	1.071615000	3.166074000	-1.198741000	6	-6.094460000	-2.837261000	0.427143000
6	1.139437000	2.726231000	-2.526091000	1	-6.279533000	-0.847592000	-2.328386000
6	1.930671000	4.185369000	-0.765704000	1	-6.711585000	-3.476923000	1.052169000
1	0.489125000	1.928876000	-2.866864000	6	-6.653042000	-2.180708000	-0.672618000
1	1.880091000	4.537541000	0.260719000	1	-7.707184000	-2.305914000	-0.903910000
6	2.056330000	3.299054000	-3.410408000	1	0.340229000	-0.371470000	1.847885000
6	2.855383000	4.747929000	-1.646023000	1	0.530858000	-0.444776000	-0.157823000
1	2.101444000	2.951459000	-4.438985000	6	1.623547000	-1.158098000	1.634147000
1	3.524448000	5.530856000	-1.299376000	6	2.646458000	-0.380457000	2.410322000
6	2.918852000	4.306281000	-2.971112000	6	2.319246000	-0.020418000	3.736343000
1	3.637020000	4.746718000	-3.657509000	6	3.948236000	-0.061375000	1.978921000
6	0.636878000	2.348119000	1.611588000	6	3.209049000	0.658213000	4.565839000
1	0.887700000	3.319461000	2.048511000	6	4.840867000	0.635381000	2.798861000
1	1.562394000	1.782993000	1.471681000	6	4.478789000	1.006776000	4.094390000
6	-1.866294000	-1.872052000	2.061032000	1	1.334578000	-0.284669000	4.113092000
1	-0.978351000	-2.498689000	2.162943000	1	4.287878000	-0.367782000	0.997935000
1	-2.699061000	-2.374881000	2.560293000	1	2.909508000	0.921691000	5.577443000
6	-2.790762000	1.169113000	0.122580000	1	5.832874000	0.872547000	2.422078000
8	-3.821610000	1.656389000	0.362382000	1	5.175762000	1.546202000	4.729968000
6	-1.438555000	-3.153532000	-0.523820000	6	1.188440000	-3.826320000	1.555347000
6	-1.734602000	-4.420908000	-0.000422000	6	1.464725000	-2.528340000	2.282343000
6	-0.588420000	-3.052061000	-1.632391000	6	2.548390000	-3.588084000	2.168376000
1	-2.402292000	-4.510260000	0.851855000	1	0.528404000	-4.542548000	2.038867000
1	-0.355031000	-2.073625000	-2.038771000	1	1.094114000	-3.834583000	0.473798000
6	-1.172556000	-5.566479000	-0.563567000	1	1.019270000	-2.481548000	3.276602000
6	-0.020974000	-4.198943000	-2.195186000	1	3.374483000	-3.366221000	1.496202000
1	-1.402196000	-6.543396000	-0.147221000	1	2.828140000	-4.156750000	3.053136000

6	1.473188000	-1.079108000	0.152099000
6	2.544895000	-0.398595000	-0.661382000
8	2.634487000	0.824358000	-0.671448000
6	3.494350000	-1.233381000	-1.464812000
6	4.358352000	-0.574333000	-2.356595000
6	3.555614000	-2.633338000	-1.359776000
1	4.299403000	0.507189000	-2.423687000
1	2.907841000	-3.159936000	-0.669054000
6	5.257156000	-1.300062000	-3.134145000
6	4.464725000	-3.357758000	-2.131923000
1	5.915701000	-0.783240000	-3.826698000
1	4.509650000	-4.439022000	-2.038018000
6	5.313283000	-2.694001000	-3.022188000
1	6.016753000	-3.260023000	-3.626694000
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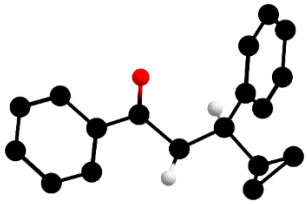

5a$_{Ph}$

G = -772.0755816 Eh

E = -772.3138906 Eh

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6	2.300432000	-1.289410000	-1.043228000
6	2.044881000	-0.936186000	1.325903000
6	2.807282000	-2.568465000	-0.799283000
6	2.549080000	-2.213484000	1.575687000
6	2.933993000	-3.034687000	0.511431000
1	2.183546000	-0.932872000	-2.062521000
1	1.749630000	-0.301421000	2.158056000
1	3.098810000	-3.201406000	-1.633347000
1	2.642813000	-2.567742000	2.598978000
1	3.326112000	-4.029840000	0.703062000
6	3.462691000	2.496331000	-0.248873000
6	2.213916000	2.005386000	0.433810000
6	2.245278000	3.393504000	-0.158375000
1	4.328727000	2.739815000	0.361745000
1	3.701631000	2.061301000	-1.217145000
1	2.245596000	1.934384000	1.520071000
1	1.671313000	3.560597000	-1.067940000
1	2.284250000	4.248042000	0.513211000
6	-0.097988000	1.054054000	0.190685000
6	-1.061098000	0.281964000	-0.702482000
8	-0.702238000	-0.155229000	-1.788257000
6	-2.472445000	0.097672000	-0.234043000
6	-2.951421000	0.667974000	0.956417000
6	-3.345844000	-0.665776000	-1.027040000
1	-2.294053000	1.265590000	1.578893000
1	-2.962358000	-1.097482000	-1.945726000
6	-4.278135000	0.477646000	1.345512000
6	-4.667697000	-0.860261000	-0.635801000
1	-4.641136000	0.924571000	2.266648000
1	-5.334466000	-1.455462000	-1.253314000
6	-5.136757000	-0.288060000	0.552194000
1	-6.168629000	-0.438672000	0.857527000
1	-0.407968000	2.109211000	0.172626000
1	-0.210924000	0.721037000	1.228774000
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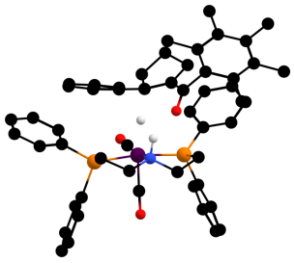

TS9

G = -4167.964649 Eh

E = -4168.767156 Eh

ν = -683.1 cm^{-1}

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7	-0.599048000	0.053964000	-1.724290000
6	-1.406730000	-0.793987000	-2.632306000

6	-0.019103000	1.212516000	-2.444685000	1	-1.444671000	6.378659000	-2.597493000
15	-3.000901000	-1.090921000	-0.456570000	6	-2.061965000	6.518865000	-0.535546000
15	-0.096035000	2.347190000	0.050740000	1	-2.545841000	7.483561000	-0.660015000
1	-0.766485000	-1.217892000	-3.418301000	1	-0.301392000	-0.343596000	0.759975000
1	0.572868000	0.867647000	-3.303058000	1	0.210633000	-0.506698000	-1.425647000
1	-2.152628000	-0.147991000	-3.108422000	1	1.702913000	1.353616000	-1.193412000
1	-0.848104000	1.827614000	-2.811409000	6	1.128368000	2.730429000	1.359590000
6	-2.180467000	0.884388000	1.753257000	6	0.829064000	2.420658000	2.692912000
8	-2.571693000	1.049993000	2.845740000	6	1.724936000	2.750004000	3.713185000
6	-4.588557000	-0.533441000	-1.222967000	1	1.484018000	2.500400000	4.742516000
6	-5.497440000	0.150216000	-0.397605000	6	2.929520000	3.387103000	3.407605000
6	-4.924517000	-0.746157000	-2.565909000	1	3.632670000	3.631535000	4.198791000
1	-5.240907000	0.345255000	0.640871000	6	3.226930000	3.715686000	2.080965000
1	-4.241456000	-1.264331000	-3.230766000	1	4.159540000	4.217913000	1.839359000
6	-6.717671000	0.597248000	-0.900102000	6	2.324546000	3.401242000	1.064049000
6	-6.145791000	-0.288311000	-3.073502000	1	2.558130000	3.666055000	0.037536000
1	-7.408953000	1.123172000	-0.247344000	1	-1.349638000	-2.573334000	-1.394222000
1	-6.390104000	-0.458052000	-4.118815000	6	-3.707686000	-2.431764000	0.583191000
6	-7.045581000	0.379915000	-2.242699000	6	-4.245885000	-3.580288000	-0.014995000
1	-7.994217000	0.733396000	-2.636814000	1	-4.190570000	-3.704915000	-1.092570000
1	-3.381318000	-1.389742000	2.442344000	6	-3.795924000	-2.274608000	1.971321000
6	-2.095110000	-1.911634000	-1.842876000	6	-4.394028000	-3.265551000	2.754982000
1	-2.735750000	-2.517296000	-2.491866000	1	-4.449457000	-3.139477000	3.832746000
6	0.875905000	1.997357000	-1.484239000	6	-4.915166000	-4.414731000	2.155022000
1	1.286384000	2.895498000	-1.955191000	6	-4.842794000	-4.569203000	0.766249000
6	-2.753538000	1.759647000	-0.642259000	1	-5.249688000	-5.459467000	0.294465000
8	-3.489160000	2.522096000	-1.128680000	1	-5.379414000	-5.184769000	2.764881000
1	-0.103630000	1.925235000	2.934215000	6	3.007516000	-0.208310000	1.931803000
6	-0.810457000	4.024214000	-0.213665000	6	0.337742000	-2.576313000	0.689584000
6	-1.443138000	4.650286000	0.872712000	6	-0.751595000	-3.111334000	1.396849000
6	-0.820950000	4.657053000	-1.463161000	6	0.839977000	-3.338452000	-0.382148000
1	-1.453708000	4.163705000	1.844715000	6	-1.284280000	-4.363623000	1.097396000
1	-0.359263000	4.183330000	-2.323604000	6	0.304156000	-4.590273000	-0.692023000
6	-2.061293000	5.889753000	0.713941000	6	-0.753655000	-5.119106000	0.051393000
6	-1.443168000	5.899399000	-1.622209000	1	-1.209000000	-2.526366000	2.183069000
1	-2.544060000	6.364134000	1.563936000	1	1.642092000	-2.960260000	-0.992249000

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1	0.725198000	-5.153034000	-1.521150000
1	-1.164505000	-6.096161000	-0.187923000
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6	2.314975000	-0.785920000	3.172897000
6	0.956891000	-1.294662000	1.187655000
1	0.423604000	-1.880138000	3.254962000
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1	2.786131000	-1.738858000	3.442204000
6	2.228663000	-0.813403000	0.772859000
6	2.815268000	-0.883545000	-0.528264000
8	2.159612000	-0.941852000	-1.599309000
6	4.335001000	-0.923960000	-0.658365000
6	5.049822000	0.250012000	-0.949467000
6	4.996036000	-2.164893000	-0.594428000
6	6.427639000	0.183261000	-1.224010000
6	6.373999000	-2.231977000	-0.881857000
6	7.094916000	-1.056013000	-1.167787000
1	2.366903000	-0.121707000	4.042219000
6	7.081647000	-3.573548000	-0.894617000
1	7.859588000	-3.602047000	-1.663396000
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1	6.389571000	-4.392461000	-1.104710000
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1	9.089439000	-0.211335000	-1.039168000
1	9.043892000	-1.961362000	-0.858466000
6	7.183477000	1.444723000	-1.593498000
1	6.537486000	2.159937000	-2.110385000
1	7.591019000	1.955523000	-0.708620000
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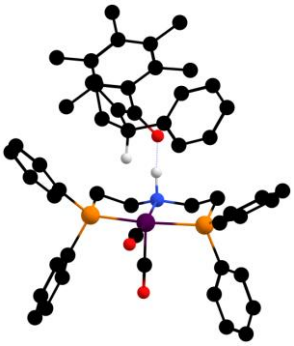

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E = -4168.793467 Eh

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6	0.257373000	1.196271000	-2.203013000
15	-2.728441000	-1.449885000	-0.657938000
15	-0.444156000	2.472425000	0.095302000
1	0.069539000	-1.313549000	-3.059418000
1	1.052158000	0.822346000	-2.858999000
1	-1.538420000	-0.547885000	-3.185486000
1	-0.491774000	1.724061000	-2.806017000
6	-2.771515000	0.898699000	1.397772000
8	-3.443614000	1.120690000	2.324875000
6	-4.185624000	-1.238799000	-1.760385000
6	-5.334417000	-0.644116000	-1.212971000
6	-4.196035000	-1.632393000	-3.104946000
1	-5.331926000	-0.318690000	-0.175842000
1	-3.321153000	-2.090515000	-3.553669000
6	-6.475660000	-0.459878000	-1.991096000
6	-5.338763000	-1.436344000	-3.887647000
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1	-5.333575000	-1.742466000	-4.930064000

6	-6.479618000	-0.854828000	-3.332925000	6	-3.180195000	-4.119672000	0.136069000
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8	-3.574166000	2.026408000	-1.819559000	1	-4.858791000	-5.506631000	2.753548000
1	-1.360974000	2.771328000	2.845174000	6	3.698862000	0.024327000	2.102704000
6	-1.287512000	4.008444000	-0.445682000	6	0.806718000	-1.943372000	1.886289000
6	-2.403714000	4.434185000	0.293923000	6	-0.522161000	-2.205252000	2.246354000
6	-0.894994000	4.739162000	-1.574598000	6	1.686392000	-3.026630000	1.766792000
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1	-3.253084000	7.198137000	-1.499736000	1	-0.409887000	-5.594422000	2.566374000
1	0.471134000	0.079247000	1.301049000	6	1.561986000	0.051597000	3.204389000
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1	1.623994000	1.516223000	-0.592313000	6	1.289514000	-0.499684000	1.775365000
6	0.413529000	2.982601000	1.626834000	1	0.873400000	-0.357342000	3.952106000
6	-0.311758000	3.048529000	2.826568000	1	1.459071000	1.137629000	3.198412000
6	0.317086000	3.451776000	4.005625000	1	3.118673000	-1.385898000	3.654761000
1	-0.250199000	3.496240000	4.930845000	6	2.630769000	-0.328443000	1.081470000
6	1.677380000	3.774066000	3.999935000	6	2.825762000	-0.675131000	-0.229411000
1	2.169271000	4.072446000	4.921234000	8	1.868583000	-1.039000000	-1.043695000
6	2.406170000	3.699832000	2.810448000	6	4.225443000	-0.732156000	-0.809279000
1	3.465734000	3.938079000	2.801249000	6	5.041346000	0.414649000	-0.917905000
6	1.776526000	3.311108000	1.625644000	6	4.704465000	-1.974676000	-1.286451000
1	2.353936000	3.254409000	0.710261000	6	6.338573000	0.314184000	-1.463501000
1	-0.639939000	-2.585767000	-1.064766000	6	5.999226000	-2.068509000	-1.830697000
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6	6.508479000	-3.399234000	-2.350803000
1	7.181703000	-3.266136000	-3.203171000
1	7.065613000	-3.954782000	-1.581667000
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1	8.919065000	-0.332612000	-1.889791000
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1	7.819910000	1.707378000	-0.682099000
1	7.888169000	1.492253000	-2.433268000
6	4.547882000	1.775627000	-0.471001000
1	3.580137000	1.691831000	0.015716000
1	5.244590000	2.241754000	0.236564000
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6	3.862209000	-3.232828000	-1.191153000
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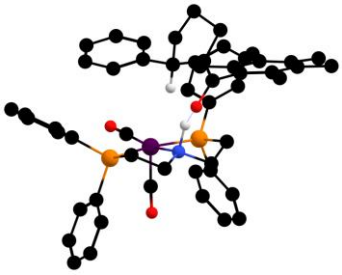

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E = -4168.790285 Eh

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6	0.302239000	1.221730000	-2.167319000
15	-2.658848000	-1.446642000	-0.681104000
15	-0.437358000	2.490576000	0.113030000
1	0.182949000	-1.272986000	-3.008666000
1	1.112962000	0.852026000	-2.809698000
1	-1.432916000	-0.543228000	-3.185623000
1	-0.431336000	1.745718000	-2.796618000
6	-2.693736000	0.852208000	1.425792000
8	-3.344566000	1.048340000	2.375569000
6	-4.094865000	-1.252647000	-1.815933000
6	-5.263163000	-0.671745000	-1.295912000
6	-4.071037000	-1.647188000	-3.160264000
1	-5.287123000	-0.343025000	-0.260178000
1	-3.180410000	-2.093284000	-3.589020000
6	-6.389359000	-0.503277000	-2.099236000
6	-5.198406000	-1.466830000	-3.968548000
1	-7.286658000	-0.054933000	-1.682148000
1	-5.165641000	-1.773747000	-5.010290000
6	-6.358919000	-0.899805000	-3.440181000
1	-7.234141000	-0.762561000	-4.068859000
1	-4.158466000	-1.368693000	1.820452000
6	-1.311764000	-2.150870000	-1.717535000
1	-1.642719000	-2.942768000	-2.396599000
6	0.894930000	2.149057000	-1.105641000
1	1.354813000	3.048078000	-1.526099000
6	-2.871105000	1.461977000	-1.043843000
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6	-1.028680000	4.578807000	-1.713502000
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1	3.413806000	4.018173000	2.871897000	6	4.976551000	0.407754000	-0.911717000
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1	2.335001000	3.333537000	0.762970000	6	6.230789000	0.302870000	-1.549928000
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6	-3.282356000	-2.766585000	0.422134000	6	6.669306000	-0.936981000	-2.046471000
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6	3.674030000	0.029826000	2.155552000	6	7.101726000	1.533871000	-1.708740000
6	0.788001000	-1.936370000	1.981113000	1	6.889529000	2.069383000	-2.646312000
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6	1.669232000	-3.017330000	1.851472000	1	8.164917000	1.278256000	-1.716502000
6	-0.974870000	-3.507856000	2.578105000	6	4.526387000	1.769140000	-0.426083000
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6	-0.085532000	-4.577211000	2.446690000	1	5.200897000	2.160864000	0.346257000
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1	2.693819000	-2.818849000	1.558943000	6	3.807672000	-3.251647000	-1.021127000
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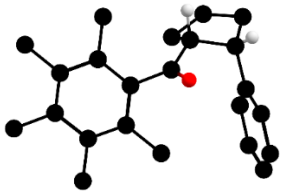

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E = -969.01377 Eh

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6	-3.288941000	1.841117000	-1.320187000
6	-3.669904000	1.977367000	1.058416000
6	-3.656148000	2.588103000	-0.198565000
1	-2.660998000	-0.071656000	-2.068963000
1	-3.295484000	0.167289000	2.167977000
1	-3.283121000	2.302912000	-2.304122000
1	-3.957126000	2.546522000	1.938487000
1	-3.934882000	3.633073000	-0.303585000
6	-2.902340000	-2.501021000	-0.909464000
6	-1.698879000	-2.513300000	-1.899927000
6	-2.506400000	-1.569165000	0.262584000
1	-3.833427000	-2.175708000	-1.382778000
1	-3.068359000	-3.509495000	-0.516160000
1	-1.953187000	-2.040028000	-2.854197000
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6	-0.212007000	-0.786422000	1.213903000
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1	5.650973000	0.869129000	-0.373364000
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1	1.447140000	3.499582000	-0.897254000
1	2.820827000	3.756867000	0.178509000
1	3.086872000	3.234024000	-1.486946000
6	-0.048763000	2.066995000	0.495875000
1	-0.861336000	1.600804000	1.048937000
1	0.229129000	2.986271000	1.024856000
1	-0.445516000	2.368747000	-0.481294000
6	2.123233000	-2.506495000	0.986538000
1	3.024777000	-2.798883000	1.535034000
1	1.273633000	-2.697731000	1.646379000
1	2.037440000	-3.183173000	0.125473000
1	-0.485885000	-0.723071000	-1.547534000
1	0.428495000	-2.214848000	-1.351702000
1	-0.773490000	-2.754956000	0.703666000
1	-2.930029000	-1.920655000	1.206698000

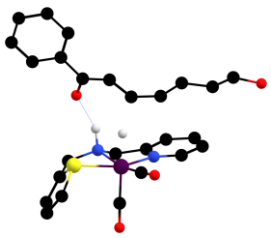
MnV

G = -2312.612736 Eh

E = -2312.779066 Eh

25	-0.038565000	0.612028000	-0.382036000
16	-2.398579000	0.365622000	-0.982560000
8	-0.620905000	0.358265000	2.516642000

8	0.172939000	3.538884000	-0.303745000
7	1.932586000	0.189304000	-0.099986000
6	2.220286000	-1.124108000	0.072648000
6	2.945704000	1.075977000	-0.065168000
1	2.672688000	2.114808000	-0.211719000
6	4.566234000	-0.654633000	0.313023000
1	5.588913000	-0.984201000	0.469635000
6	4.268655000	0.697617000	0.142421000
1	5.044384000	1.456051000	0.161702000
6	1.030292000	-2.049124000	0.047977000
1	1.332796000	-3.066606000	-0.232509000
1	0.569934000	-2.084486000	1.043453000
6	-1.278081000	-2.191371000	-0.914341000
1	-1.487323000	-2.470202000	-1.952835000
1	-1.240401000	-3.112720000	-0.323508000
6	-3.879586000	-0.236913000	1.045503000
1	-4.589027000	-0.172202000	1.864206000
6	-0.397071000	0.409146000	1.368831000
6	-2.343914000	-1.292503000	-0.368534000
6	0.069998000	2.371597000	-0.302157000
6	-3.541921000	0.824611000	0.264668000
1	-3.913293000	1.841123000	0.307774000
6	3.521548000	-1.578124000	0.270539000
1	3.702496000	-2.641816000	0.388896000
7	0.034892000	-1.479113000	-0.879068000
1	0.432365000	-1.497180000	-1.813962000
6	-3.174341000	-1.444613000	0.697203000
1	-3.252872000	-2.371882000	1.255761000
1	0.245279000	0.844773000	-1.970505000



TSMnV1

G = -2968.157354 Eh

E = -2968.549997 Eh

ν = -291.1 cm^{-1}

25	-0.501500000	-1.683385000	-0.454385000
16	1.830762000	-2.114029000	-1.004392000
8	-1.221131000	-4.514468000	0.042091000
8	-1.609609000	-1.606853000	-3.171094000
7	-2.105380000	-0.909098000	0.509143000
6	-1.938775000	-0.697269000	1.838066000
6	-3.268309000	-0.524473000	-0.055746000
1	-3.367209000	-0.715876000	-1.117307000
6	-4.106484000	0.332609000	2.022630000
1	-4.877242000	0.821993000	2.610095000
6	-4.290775000	0.088643000	0.661298000
1	-5.199629000	0.384566000	0.149182000
6	-0.676513000	-1.263057000	2.433797000
1	-0.400482000	-0.721164000	3.347548000
1	-0.869273000	-2.309981000	2.703406000
6	1.577344000	-2.085639000	1.790026000
1	2.366233000	-1.434855000	2.185620000
1	1.302115000	-2.800738000	2.571072000
6	2.519982000	-4.598247000	-0.899839000
1	2.805441000	-5.606131000	-1.184050000
6	-0.920577000	-3.393134000	-0.107394000
6	2.036679000	-2.856652000	0.587100000
6	-1.174665000	-1.677310000	-2.084700000
6	2.204012000	-3.629364000	-1.801774000
1	2.210988000	-3.680930000	-2.883639000
6	-2.908075000	-0.065521000	2.614522000
1	-2.717480000	0.098540000	3.670290000
7	0.395699000	-1.250420000	1.425025000
1	0.759781000	-0.292909000	1.339836000
6	2.400394000	-4.161991000	0.467712000
1	2.522209000	-4.820549000	1.321797000
1	-0.109685000	-0.144080000	-0.861308000
6	1.045005000	2.171086000	-0.541531000
1	1.237031000	2.754269000	-1.436192000

6	-1.393625000	2.001772000	-1.181041000
1	-1.082138000	2.578868000	-2.060119000
1	-1.891194000	1.098080000	-1.544186000
6	-2.399219000	2.800809000	-0.334577000
1	-2.575229000	2.257989000	0.602692000
1	-1.970718000	3.774477000	-0.063172000
6	-3.736049000	2.988124000	-1.054066000
1	-3.610168000	3.613361000	-1.947391000
1	-4.103791000	2.010705000	-1.390872000
6	-4.784273000	3.608964000	-0.144875000
1	-4.880444000	2.998697000	0.768310000
1	-4.464611000	4.616962000	0.165452000
8	-6.023756000	3.661441000	-0.852795000
1	-6.666137000	4.099521000	-0.278507000
6	2.132800000	1.897173000	0.361985000
6	3.421061000	2.644001000	0.197286000
6	3.501510000	3.861568000	-0.499791000
6	4.586163000	2.115774000	0.779130000
6	4.721015000	4.529604000	-0.617718000
1	2.608058000	4.301148000	-0.931131000
6	5.805816000	2.777961000	0.652643000
1	4.516507000	1.179988000	1.324441000
6	5.876358000	3.987503000	-0.047088000
1	4.769103000	5.474333000	-1.152230000
1	6.701564000	2.353497000	1.097948000
1	6.826332000	4.506121000	-0.144722000
8	2.053857000	1.035487000	1.273426000
6	-0.196706000	1.618841000	-0.356285000
1	-0.426311000	1.194312000	0.616221000

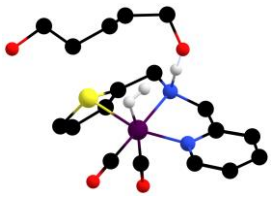
MnVI

G = -2968.183101 Eh

E = -2968.576608 Eh

25	-0.219648000	-1.758757000	-0.406678000
16	2.141204000	-1.491387000	-0.959738000
8	-0.229037000	-4.652484000	0.068924000
8	-1.278950000	-2.152175000	-3.136902000
7	-1.959928000	-1.425678000	0.556945000
6	-1.836175000	-1.137858000	1.876044000
6	-3.170445000	-1.299156000	-0.023672000
1	-3.225561000	-1.555641000	-1.074447000
6	-4.157830000	-0.521321000	2.016961000
1	-5.007900000	-0.154188000	2.583877000
6	-4.290256000	-0.851295000	0.667231000
1	-5.237978000	-0.757489000	0.148609000
6	-0.482407000	-1.401947000	2.482297000
1	-0.308900000	-0.745914000	3.343900000
1	-0.472888000	-2.439864000	2.842237000
6	1.846603000	-1.922491000	1.799192000
1	2.474680000	-1.230464000	2.372601000
1	1.651807000	-2.808455000	2.412058000
6	3.417586000	-3.718335000	-1.160028000
1	3.952575000	-4.571871000	-1.563859000
6	-0.208526000	-3.504802000	-0.120335000
6	2.513368000	-2.372204000	0.529722000
6	-0.870041000	-1.992195000	-2.059767000
6	2.866000000	-2.749093000	-1.940144000
1	2.897730000	-2.642507000	-3.017380000
6	-2.913580000	-0.671612000	2.626962000
1	-2.765893000	-0.430685000	3.674549000
7	0.561176000	-1.252564000	1.454464000
1	0.835020000	-0.227244000	1.366861000
6	3.191592000	-3.517104000	0.248530000
1	3.473641000	-4.236398000	1.010554000
1	-0.161657000	0.063430000	-0.972620000
6	0.623394000	2.023339000	-0.599060000
1	0.652750000	2.711374000	-1.437703000
6	-1.775372000	1.450500000	-1.280782000
1	-1.511169000	1.985930000	-2.202520000

1	-2.319711000	0.550412000	-1.586848000
6	-2.697482000	2.312781000	-0.415111000
1	-2.888300000	1.777667000	0.525844000
1	-2.183306000	3.246207000	-0.149086000
6	-4.033239000	2.618614000	-1.093533000
1	-3.870189000	3.171174000	-2.028293000
1	-4.534449000	1.677013000	-1.357334000
6	-4.955451000	3.425626000	-0.193703000
1	-5.114027000	2.881466000	0.752611000
1	-4.481317000	4.387811000	0.058225000
8	-6.194197000	3.630150000	-0.875067000
1	-6.748318000	4.181677000	-0.306617000
6	1.645752000	1.984873000	0.320558000
6	2.759127000	2.993320000	0.241436000
6	2.624177000	4.229351000	-0.416618000
6	3.985672000	2.706180000	0.864511000
6	3.685380000	5.133598000	-0.470916000
1	1.673103000	4.492215000	-0.869779000
6	5.049916000	3.608304000	0.809983000
1	4.086566000	1.763441000	1.392977000
6	4.906510000	4.826362000	0.139330000
1	3.556251000	6.084975000	-0.981370000
1	5.992215000	3.361388000	1.293481000
1	5.731809000	5.532704000	0.099640000
8	1.737705000	1.099984000	1.275141000
6	-0.500463000	1.056460000	-0.526056000
1	-0.750418000	0.847459000	0.517763000



TSMnV2$_{5\text{-ass}}$

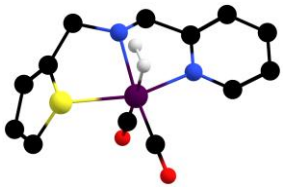
G = -2660.797044 Eh

E = -2661.144114 Eh

ν = -463.8 cm^{-1}

25	-0.509680000	0.480151000	0.574452000
16	1.714073000	1.180364000	-0.119734000
8	-1.605051000	3.201072000	0.327310000
8	-0.190931000	0.935246000	3.478168000
7	-2.367836000	-0.327315000	0.586662000
6	-2.957134000	-0.402072000	-0.630759000
6	-3.025257000	-0.800400000	1.663004000
1	-2.508800000	-0.720236000	2.612782000
6	-4.904112000	-1.446218000	0.320515000
1	-5.891262000	-1.885976000	0.214198000
6	-4.292438000	-1.364811000	1.573209000
1	-4.780188000	-1.734282000	2.468864000
6	-2.152659000	0.165284000	-1.770676000
1	-2.419966000	-0.345367000	-2.706371000
1	-2.398242000	1.231824000	-1.890792000
6	0.192963000	0.656758000	-2.398560000
1	0.829130000	-0.111613000	-2.857010000
1	-0.352282000	1.160051000	-3.205226000
6	1.802895000	3.677583000	-0.735654000
1	2.002663000	4.744071000	-0.708377000
6	-1.158750000	2.131305000	0.405641000
6	1.021481000	1.677151000	-1.674658000
6	-0.315976000	0.740607000	2.336633000
6	2.115315000	2.837945000	0.288014000
1	2.615463000	3.058625000	1.223162000
6	-4.223091000	-0.961419000	-0.794383000
1	-4.655147000	-1.015585000	-1.788196000
7	-0.731498000	-0.000023000	-1.438362000
1	-0.009796000	-1.376898000	0.378268000
6	1.152812000	3.019526000	-1.843499000
1	0.752732000	3.545412000	-2.704405000
1	0.200259000	-1.104808000	1.076015000
8	-0.443727000	-2.479743000	-1.279799000
6	0.711967000	-2.930451000	-1.923685000
1	0.738306000	-4.040024000	-1.953031000
1	0.749571000	-2.605696000	-2.986302000
6	2.000727000	-2.444732000	-1.240159000

1	2.872410000	-2.660684000	-1.873884000
1	1.937662000	-1.352242000	-1.161225000
6	2.199278000	-3.056192000	0.158993000
1	2.718813000	-4.019696000	0.064068000
1	1.214216000	-3.271323000	0.590131000
6	2.961220000	-2.148398000	1.134547000
1	3.122255000	-2.666760000	2.089080000
1	2.353627000	-1.261365000	1.351219000
6	4.304108000	-1.675948000	0.599518000
1	4.974827000	-2.535754000	0.441097000
1	4.169194000	-1.173980000	-0.368619000
8	4.867353000	-0.766671000	1.555152000
1	5.705880000	-0.450243000	1.191688000
1	-0.550398000	-1.178007000	-1.435679000



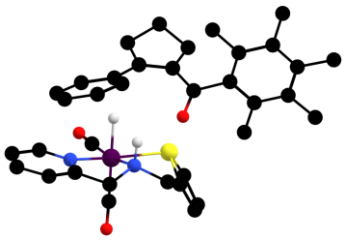
TSMnV2$_{self}$

G = -2312.579979 Eh

E = -2312.739094 Eh

ν = -1125.6 cm^{-1}

25	-0.054145000	0.569631000	-0.389272000
16	-2.412252000	0.341545000	-0.964372000
8	-0.559962000	0.395740000	2.515578000
8	0.085000000	3.517152000	-0.395472000
7	1.924145000	0.186396000	-0.086653000
6	2.228122000	-1.127569000	0.034289000
6	2.913727000	1.096940000	-0.001551000
1	2.620717000	2.135239000	-0.107784000
6	4.561350000	-0.613413000	0.329212000
1	5.588776000	-0.927409000	0.488063000
6	4.240971000	0.740391000	0.207769000
1	5.000972000	1.512233000	0.268197000
6	1.055743000	-2.071592000	-0.038669000
1	1.400018000	-3.047488000	-0.420126000
1	0.702600000	-2.246214000	0.999949000
6	-1.247021000	-2.187693000	-0.920275000
1	-1.487721000	-2.474736000	-1.957115000
1	-1.211427000	-3.115676000	-0.334133000
6	-3.824828000	-0.243292000	1.106732000
1	-4.512786000	-0.175514000	1.943757000
6	-0.377501000	0.469110000	1.367829000
6	-2.339497000	-1.322568000	-0.353199000
6	0.026795000	2.350535000	-0.381906000
6	-3.510361000	0.819317000	0.318273000
1	-3.885821000	1.834201000	0.362715000
6	3.539797000	-1.556488000	0.236724000
1	3.743587000	-2.619402000	0.317406000
7	0.027950000	-1.466681000	-0.857883000
1	0.266328000	-0.401283000	-1.816201000
6	-3.136776000	-1.458286000	0.739950000
1	-3.206503000	-2.382021000	1.305404000
1	0.282804000	0.489062000	-2.108539000



RCMnV

G = -3280.041018 Eh

E = -3280.582009 Eh

25	-2.673762000	1.112047000	0.502747000
7	-1.519798000	0.528036000	-1.212924000
6	-2.488689000	-0.016847000	-2.184377000
6	-0.648997000	1.596542000	-1.793866000
16	-0.727319000	2.523551000	0.856663000
1	-2.006732000	-0.642173000	-2.946683000
1	0.350751000	1.188756000	-1.965296000
1	-2.958598000	0.838182000	-2.687596000
1	-1.049944000	1.916761000	-2.760419000
6	-3.477430000	1.330082000	2.053933000

8	-3.985113000	1.424678000	3.108106000	1	7.857575000	-1.525751000	0.556717000
6	-0.619217000	2.790313000	-0.886265000	1	6.618079000	-2.752013000	0.809720000
6	-3.622054000	2.383724000	-0.344023000	6	7.694068000	0.750431000	-0.667325000
8	-4.278143000	3.233946000	-0.813465000	1	7.811339000	1.560363000	-1.392154000
1	-1.832159000	0.006945000	1.321757000	1	8.144792000	1.093731000	0.275211000
1	-0.909465000	-0.231587000	-0.910870000	1	8.287550000	-0.096371000	-1.021897000
6	2.153288000	-0.652664000	2.384202000	6	5.655498000	2.781749000	-0.957923000
6	-0.398603000	-2.696786000	0.395754000	1	6.103346000	2.854077000	-1.958451000
6	-1.738256000	-2.957982000	0.742300000	1	4.818576000	3.480640000	-0.926554000
6	0.109031000	-3.269072000	-0.786116000	1	6.413357000	3.135080000	-0.248276000
6	-2.546396000	-3.747992000	-0.072411000	6	2.806620000	2.071274000	-0.644480000
6	-0.700877000	-4.058505000	-1.600026000	1	1.825089000	1.689725000	-0.372206000
6	-2.033514000	-4.299374000	-1.248634000	1	3.019099000	2.918246000	0.018213000
1	-2.149681000	-2.518688000	1.643824000	1	2.737188000	2.469739000	-1.664623000
1	1.143171000	-3.103116000	-1.061986000	6	4.165800000	-2.749885000	0.253011000
1	-3.580249000	-3.920609000	0.206294000	1	4.746148000	-3.437195000	-0.372971000
1	-0.287441000	-4.496198000	-2.504845000	1	4.385633000	-3.007139000	1.298133000
1	-2.664461000	-4.914523000	-1.884591000	1	3.108811000	-2.961301000	0.081321000
6	0.138965000	-1.953883000	2.811302000	1	3.244127000	-0.741667000	2.399638000
6	1.459385000	-1.505671000	3.466349000	1	1.920488000	0.415997000	2.504246000
6	0.441702000	-1.926836000	1.323888000	6	-3.568237000	-0.785505000	-1.471159000
1	-0.206551000	-2.936852000	3.149682000	7	-3.830017000	-0.395086000	-0.203339000
1	-0.674237000	-1.237354000	2.999694000	6	-4.827086000	-1.013476000	0.460609000
1	2.073985000	-2.388682000	3.678363000	6	-5.617128000	-2.002172000	-0.116588000
6	1.545236000	-1.165906000	1.088513000	6	-5.358046000	-2.391832000	-1.431599000
6	2.089451000	-0.731853000	-0.208724000	6	-4.304647000	-1.781869000	-2.108683000
8	1.400680000	-0.645395000	-1.231838000	1	-4.047213000	-2.063714000	-3.124531000
6	3.542656000	-0.330180000	-0.255084000	1	-5.952050000	-3.163574000	-1.911844000
6	3.881926000	1.010254000	-0.526938000	1	-6.415064000	-2.454625000	0.462969000
6	4.531953000	-1.309716000	-0.048046000	1	-4.993835000	-0.685575000	1.480130000
6	5.240318000	1.358246000	-0.649214000	6	-0.717741000	4.114737000	-1.180897000
6	5.888599000	-0.945890000	-0.142977000	1	-0.729401000	4.492955000	-2.198121000
6	6.238272000	0.374995000	-0.485139000	6	-0.890200000	4.945952000	-0.017287000
1	1.308808000	-0.964530000	4.405323000	1	-0.982411000	6.026588000	-0.060737000
6	6.964523000	-1.979771000	0.118022000	6	-0.963203000	4.236260000	1.141935000
1	7.276553000	-2.487154000	-0.806419000	1	-1.086312000	4.602764000	2.153751000

TSMnV3

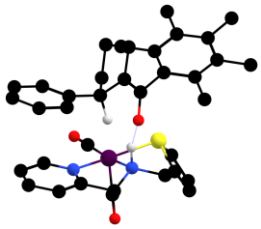
G = -3280.02507 Eh

E = -3280.569043 Eh

ν = -489.8 cm^{-1}

25	-2.218014000	1.153381000	0.515607000
7	-1.503078000	0.762711000	-1.447272000
6	-2.630686000	0.297789000	-2.274633000
6	-0.735955000	1.882396000	-2.065422000
16	-0.060373000	2.213411000	0.638044000
1	-2.300481000	-0.338468000	-3.105103000
1	0.108006000	1.479037000	-2.635776000
1	-3.118283000	1.182707000	-2.703755000
1	-1.385159000	2.430758000	-2.754259000
6	-2.603693000	1.140459000	2.235131000
8	-2.814183000	1.074845000	3.387903000
6	-0.285168000	2.836810000	-0.997330000
6	-3.138254000	2.640781000	0.133817000
8	-3.756301000	3.616615000	-0.054786000
1	-1.331257000	-0.187645000	0.915273000
1	-0.830490000	-0.004151000	-1.334538000
6	1.748895000	-0.610295000	2.219503000
6	-0.952021000	-2.367850000	0.182292000
6	-2.248972000	-2.756548000	0.566978000
6	-0.405188000	-2.959337000	-0.968784000
6	-2.975361000	-3.689993000	-0.166905000
6	-1.135266000	-3.891523000	-1.710642000
6	-2.422644000	-4.261924000	-1.316628000
1	-2.692191000	-2.305763000	1.447524000
1	0.593137000	-2.700234000	-1.291075000
1	-3.976131000	-3.962416000	0.153217000
1	-0.685815000	-4.336654000	-2.594627000
1	-2.986411000	-4.990076000	-1.893787000
6	-0.387612000	-1.655932000	2.603186000
6	1.031599000	-1.560874000	3.186872000
6	-0.188187000	-1.452794000	1.083455000
1	-0.872460000	-2.612462000	2.819785000
1	-1.025555000	-0.864902000	3.007564000
1	1.513531000	-2.545708000	3.145994000
6	1.092668000	-0.920610000	0.882081000
6	1.728918000	-0.603436000	-0.367244000
8	1.107868000	-0.452598000	-1.449019000
6	3.238146000	-0.460913000	-0.369593000
6	3.843715000	0.755029000	-0.750790000
6	4.030367000	-1.563099000	0.021270000
6	5.247181000	0.875320000	-0.701449000
6	5.432158000	-1.437908000	0.053066000
6	6.041610000	-0.229158000	-0.338369000
1	1.039461000	-1.217287000	4.227245000
6	6.280911000	-2.602973000	0.522603000
1	6.552546000	-3.274493000	-0.305069000
1	7.211621000	-2.261092000	0.982908000
1	5.753950000	-3.206189000	1.266930000
6	7.553130000	-0.120551000	-0.379912000
1	7.882336000	0.604350000	-1.128907000
1	7.967841000	0.198655000	0.587281000
1	8.015675000	-1.079225000	-0.630507000
6	5.904718000	2.199502000	-1.038206000
1	6.213221000	2.246351000	-2.092861000
1	5.232358000	3.041864000	-0.859522000
1	6.800677000	2.363613000	-0.432367000
6	3.023632000	1.948694000	-1.193895000
1	1.999388000	1.670780000	-1.419127000
1	3.006259000	2.731963000	-0.423754000
1	3.451653000	2.399931000	-2.096510000
6	3.407355000	-2.895153000	0.393776000
1	3.985178000	-3.724552000	-0.028046000
1	3.388076000	-3.037243000	1.483060000
1	2.380485000	-2.991145000	0.039443000

1	2.833182000	-0.744330000	2.205363000
1	1.557140000	0.437542000	2.505103000
6	-3.653618000	-0.414319000	-1.430529000
7	-3.687560000	-0.078194000	-0.120727000
6	-4.663264000	-0.605942000	0.647188000
6	-5.631803000	-1.469225000	0.149434000
6	-5.585991000	-1.828170000	-1.198366000
6	-4.573847000	-1.296622000	-1.993357000
1	-4.491395000	-1.548786000	-3.045602000
1	-6.317097000	-2.512515000	-1.618042000
1	-6.396009000	-1.856177000	0.815354000
1	-4.653468000	-0.317905000	1.691594000
6	-0.193967000	4.193888000	-1.015152000
1	-0.350150000	4.785226000	-1.911700000
6	0.045892000	4.763769000	0.285531000
1	0.154315000	5.829247000	0.462278000
6	0.087911000	3.834367000	1.280097000
1	0.260191000	3.983864000	2.338887000



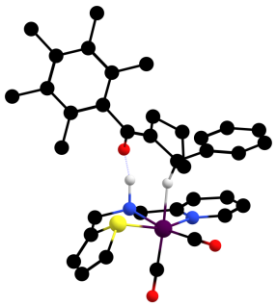
MnVH-3a

G = -3280.052927 Eh

E = -3280.600634 Eh

25	2.399753000	-0.846860000	0.183618000
7	1.208036000	-1.060042000	-1.508674000
6	1.925203000	-0.452696000	-2.643179000
6	0.668194000	-2.423833000	-1.788670000
16	1.016250000	-2.667790000	0.970075000
1	1.249568000	-0.214184000	-3.474160000
1	-0.419669000	-2.340669000	-1.895575000
1	2.677896000	-1.165096000	-3.007693000
1	1.077693000	-2.821488000	-2.722572000
6	3.263286000	-0.502624000	1.715434000
8	3.827633000	-0.288894000	2.709629000
6	1.050794000	-3.342212000	-0.667658000
6	3.723449000	-1.877752000	-0.371840000
8	4.592629000	-2.553432000	-0.746836000
1	0.865948000	0.210386000	0.646581000
1	0.337618000	-0.455842000	-1.330649000
6	-1.946278000	0.771643000	2.365977000
6	0.740254000	2.317650000	0.923138000
6	1.433237000	3.163846000	1.798912000
6	0.435146000	2.798303000	-0.363286000
6	1.799448000	4.458564000	1.410278000
6	0.809126000	4.081986000	-0.754782000
6	1.490975000	4.923491000	0.132491000
1	1.681674000	2.832555000	2.801428000
1	-0.098030000	2.146497000	-1.047817000
1	2.324195000	5.100272000	2.113876000
1	0.567132000	4.428788000	-1.756241000
1	1.776025000	5.927654000	-0.170760000
6	0.431615000	0.543878000	2.791412000
6	-0.853896000	1.123258000	3.403890000
6	0.288306000	0.908663000	1.301182000
1	1.351366000	0.895776000	3.265220000
1	0.414415000	-0.548150000	2.880180000
1	-0.752899000	2.212088000	3.486931000
6	-1.188461000	0.656775000	1.048968000
6	-1.738243000	0.325016000	-0.151920000
8	-1.104318000	0.146036000	-1.291282000
6	-3.233267000	0.113729000	-0.219371000
6	-3.734009000	-1.201498000	-0.281573000
6	-4.111348000	1.213256000	-0.275762000
6	-5.119329000	-1.420386000	-0.400497000
6	-5.498442000	0.991563000	-0.393767000
6	-6.003821000	-0.322985000	-0.423960000
1	-1.064626000	0.727498000	4.403249000
6	-6.449767000	2.168377000	-0.482505000
1	-7.287832000	1.957490000	-1.154580000

1	-6.880160000	2.420098000	0.498214000
1	-5.948616000	3.065470000	-0.853854000
6	-7.501312000	-0.556623000	-0.470902000
1	-7.878828000	-0.608197000	-1.503042000
1	-7.777163000	-1.493982000	0.020617000
1	-8.047955000	0.246641000	0.031468000
6	-5.658714000	-2.833553000	-0.498639000
1	-4.911191000	-3.522785000	-0.900360000
1	-5.966710000	-3.224549000	0.482577000
1	-6.534654000	-2.884266000	-1.153121000
6	-2.785277000	-2.380385000	-0.196007000
1	-1.798937000	-2.064510000	0.148132000
1	-3.158152000	-3.138813000	0.502998000
1	-2.660397000	-2.875967000	-1.168794000
6	-3.579752000	2.630534000	-0.207151000
1	-3.736684000	3.163286000	-1.155551000
1	-4.096084000	3.210879000	0.567631000
1	-2.510843000	2.643160000	0.013666000
1	-2.736690000	1.534033000	2.341571000
1	-2.438984000	-0.175249000	2.634063000
6	2.622822000	0.787804000	-2.155220000
7	2.999174000	0.771346000	-0.854239000
6	3.665883000	1.831842000	-0.355450000
6	3.991341000	2.937833000	-1.129909000
6	3.601412000	2.959170000	-2.469419000
6	2.901162000	1.870938000	-2.984829000
1	2.565983000	1.849361000	-4.016449000
1	3.829238000	3.814505000	-3.098235000
1	4.523352000	3.767868000	-0.679926000
1	3.934004000	1.781555000	0.692069000
6	1.663632000	-4.554974000	-0.667877000
1	1.842162000	-5.124410000	-1.574225000
6	2.120696000	-4.967749000	0.636847000
1	2.621807000	-5.912243000	0.822683000
6	1.894516000	-4.044350000	1.609066000
1	2.121699000	-4.097121000	2.666588000



TSMnV4

G = -3280.052407 Eh

E = -3280.596117 Eh

ν = -553.1 cm^{-1}

25	-2.434996000	0.889249000	0.125792000
7	-1.139477000	1.109397000	-1.451753000
6	-1.695289000	0.458093000	-2.640166000
6	-0.597474000	2.460919000	-1.735594000
16	-1.029502000	2.640194000	1.012584000
1	-0.910724000	0.194667000	-3.364159000
1	0.486623000	2.376129000	-1.890043000
1	-2.406339000	1.134347000	-3.142027000
1	-1.043651000	2.885390000	-2.644413000
6	-3.374456000	0.493344000	1.611121000
8	-3.975838000	0.218809000	2.565964000
6	-0.926325000	3.372832000	-0.589940000
6	-3.722730000	1.929020000	-0.513850000
8	-4.553914000	2.600830000	-0.966451000
1	-0.954713000	-0.210412000	0.687820000
1	-0.157992000	0.461660000	-1.205911000
6	1.850250000	-0.804886000	2.423199000
6	-0.809188000	-2.314033000	0.955059000
6	-1.583944000	-3.131531000	1.788106000
6	-0.411744000	-2.822516000	-0.294414000
6	-1.939827000	-4.427595000	1.397290000
6	-0.772255000	-4.109500000	-0.686712000
6	-1.535158000	-4.922863000	0.158759000
1	-1.904299000	-2.773711000	2.760399000
1	0.175617000	-2.190063000	-0.952344000
1	-2.527248000	-5.047838000	2.069453000

1	-0.455020000	-4.481305000	-1.657463000
1	-1.805793000	-5.930730000	-0.144775000
6	-0.531140000	-0.542833000	2.829891000
6	0.741888000	-1.143853000	3.450629000
6	-0.374864000	-0.900751000	1.340173000
1	-1.461874000	-0.881140000	3.292084000
1	-0.498354000	0.548636000	2.921004000
1	0.622689000	-2.230994000	3.527444000
6	1.104084000	-0.642181000	1.105976000
6	1.660784000	-0.295165000	-0.079849000
8	1.012256000	-0.085047000	-1.219491000
6	3.152332000	-0.120350000	-0.172681000
6	3.678530000	1.181669000	-0.274554000
6	4.004449000	-1.240571000	-0.203350000
6	5.064796000	1.367211000	-0.415964000
6	5.393444000	-1.049260000	-0.334043000
6	5.922839000	0.251410000	-0.418670000
1	0.949864000	-0.756415000	4.453246000
6	6.336950000	-2.234982000	-0.386616000
1	7.088035000	-2.107742000	-1.174418000
1	6.887285000	-2.352670000	0.558134000
1	5.810449000	-3.171399000	-0.576895000
6	7.423881000	0.443424000	-0.513116000
1	7.776393000	0.386678000	-1.553784000
1	7.734393000	1.413671000	-0.117435000
1	7.959541000	-0.328107000	0.047513000
6	5.643009000	2.761014000	-0.569796000
1	4.886060000	3.483368000	-0.882057000
1	6.080096000	3.128387000	0.370208000
1	6.441246000	2.776314000	-1.319221000
6	2.754486000	2.381317000	-0.203383000
1	1.766299000	2.092507000	0.156725000
1	3.149646000	3.145776000	0.475661000
1	2.631591000	2.857575000	-1.185930000
6	3.442129000	-2.645107000	-0.103479000
1	3.634909000	-3.215055000	-1.022144000
1	3.911355000	-3.200838000	0.718034000
1	2.365630000	-2.631884000	0.068855000
1	2.616197000	-1.589711000	2.384716000
1	2.369667000	0.122474000	2.702459000
6	-2.431545000	-0.779187000	-2.205186000
7	-2.933544000	-0.743918000	-0.948626000
6	-3.618170000	-1.812724000	-0.493580000
6	-3.844200000	-2.941580000	-1.269541000
6	-3.334903000	-2.976825000	-2.567577000
6	-2.614127000	-1.882314000	-3.036506000
1	-2.179606000	-1.874170000	-4.030590000
1	-3.481462000	-3.850076000	-3.195746000
1	-4.382726000	-3.781144000	-0.847355000
1	-3.975520000	-1.750359000	0.525523000
6	-1.385290000	4.651783000	-0.558514000
1	-1.458300000	5.274501000	-1.443785000
6	-1.833939000	5.067253000	0.747244000
1	-2.218063000	6.059399000	0.959204000
6	-1.756211000	4.084453000	1.685085000
1	-2.010300000	4.126046000	2.735637000

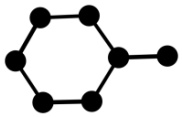
5

G = -348.2586404 Eh

E = -348.3779644 Eh

8	-3.166832000	0.512249000	-0.144300000
6	-2.431175000	-0.673713000	0.165282000
1	-2.511552000	-0.796863000	1.252274000
1	-2.899000000	-1.553460000	-0.304333000
6	-0.961607000	-0.587251000	-0.242851000
1	-0.479797000	-1.541844000	0.005833000
1	-0.900971000	-0.478883000	-1.336685000
6	-0.228485000	0.579549000	0.429136000
1	-0.207137000	0.411107000	1.515478000
1	-0.810137000	1.493766000	0.265624000
6	1.200116000	0.790049000	-0.084755000

1	1.640480000	1.674379000	0.393660000
1	1.184811000	0.981682000	-1.166414000
6	2.111603000	-0.398277000	0.188621000
1	2.097617000	-0.633456000	1.266393000
1	1.749374000	-1.289071000	-0.346807000
8	3.430471000	-0.054911000	-0.240991000
1	3.993233000	-0.826727000	-0.093261000
1	-3.108752000	0.638524000	-1.102030000

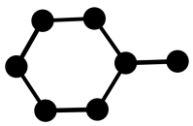


$PhCH_2^-$

G = -271.0439529 Eh

E = -271.1118819 Eh

6	1.880128000	-0.000108000	-0.000109000
6	1.140210000	1.200591000	0.000021000
6	1.140024000	-1.200702000	0.000032000
1	1.669553000	2.155813000	0.000141000
1	1.669255000	-2.156003000	0.000183000
6	-0.244538000	1.214775000	0.000019000
6	-0.244689000	-1.214623000	-0.000021000
1	-0.769382000	2.170789000	0.000137000
1	-0.769746000	-2.170505000	0.000093000
6	-1.041738000	0.000134000	-0.000139000
1	2.966960000	-0.000249000	0.000245000
6	-2.427096000	-0.000022000	0.000016000
1	-2.990338000	0.931319000	0.000028000
1	-2.990105000	-0.931428000	0.000258000

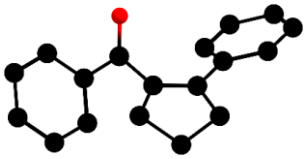


$PhCH_2^{\bullet}$

G = -270.967905 Eh

E = -271.038142 Eh

6	-1.839586000	-0.000120000	0.000012000
6	-1.133679000	1.214024000	-0.000008000
6	-1.133675000	-1.213802000	-0.000011000
1	-1.677427000	2.155063000	0.000146000
1	-1.677098000	-2.155034000	0.000019000
6	0.253106000	1.220633000	-0.000009000
6	0.253447000	-1.220590000	-0.000098000
1	0.798153000	2.161148000	0.000022000
1	0.797747000	-2.161575000	-0.000011000
6	0.994721000	-0.000308000	0.000107000
1	-2.925757000	-0.000233000	0.000025000
6	2.400278000	0.000230000	-0.000110000
1	2.958381000	0.931820000	-0.000302000
1	2.958326000	-0.931591000	0.000793000



$3a_{Ph}$

G = -772.0934662 Eh

E = -772.3382272 Eh

6	-1.294300000	1.086517000	0.022410000
6	-2.121534000	-0.121679000	-0.105383000
6	-3.523720000	-0.014960000	-0.054944000
6	-1.558175000	-1.395521000	-0.309144000
6	-4.333703000	-1.145216000	-0.169269000
6	-2.367378000	-2.523099000	-0.427647000
6	-3.759179000	-2.404986000	-0.353704000
1	-3.979125000	0.960332000	0.087834000
1	-0.482290000	-1.500363000	-0.399008000
1	-5.414034000	-1.040660000	-0.117377000
1	-1.910570000	-3.495978000	-0.587052000
1	-4.388342000	-3.285635000	-0.448190000
6	-0.572401000	3.334395000	-0.446270000
6	-1.840986000	2.463974000	-0.323992000
6	0.472954000	2.622094000	0.440830000
1	-0.228404000	3.322190000	-1.487058000
1	-0.736534000	4.376983000	-0.157610000
1	-2.448219000	2.457118000	-1.236091000
1	0.476594000	3.023617000	1.465497000

1	1.497318000	2.712764000	0.062031000
6	-0.022338000	1.186360000	0.462334000
6	0.830911000	0.114693000	1.065314000
8	0.527521000	-0.409720000	2.130786000
6	2.094962000	-0.249264000	0.352488000
6	2.337500000	0.170319000	-0.964996000
6	3.041565000	-1.052148000	1.009044000
1	1.595574000	0.775022000	-1.478137000
1	2.830180000	-1.373513000	2.023954000
6	3.513842000	-0.203889000	-1.615515000
6	4.218744000	-1.418472000	0.361907000
1	3.695076000	0.117556000	-2.637100000
1	4.952225000	-2.034402000	0.874532000
6	4.456146000	-0.994337000	-0.951325000
1	5.374182000	-1.281989000	-1.456288000
1	-2.491263000	2.816026000	0.490947000

^{t}BuO^{-}

G = -233.1540003 Eh

E = -233.2298343 Eh

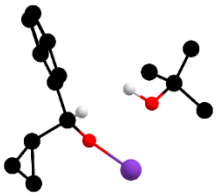
8	0.000733000	0.002708000	1.491245000
6	0.000315000	0.000128000	0.166080000
6	1.450302000	-0.119234000	-0.438899000
1	1.910825000	-1.046674000	-0.069036000
1	2.057709000	0.718868000	-0.067518000
1	1.501813000	-0.122649000	-1.542440000
6	-0.622818000	1.314039000	-0.440134000
1	-0.051435000	2.178003000	-0.070836000
1	-0.645875000	1.359257000	-1.543713000
1	-1.652364000	1.419055000	-0.068354000
6	-0.828229000	-1.197102000	-0.436692000
1	-0.404002000	-2.141502000	-0.066134000
1	-1.860704000	-1.133026000	-0.063913000
1	-0.859247000	-1.239981000	-1.540143000

^{t}BuO$^{\bullet}$

G = -233.0468185 Eh

E = -233.1239965 Eh

8	0.000443000	0.270983000	1.433834000
6	-0.000050000	-0.026841000	0.091930000
6	0.002471000	1.378967000	-0.588055000
1	0.896840000	1.940690000	-0.303678000
1	-0.889880000	1.943916000	-0.303728000
1	0.002245000	1.221624000	-1.672009000
6	-1.274867000	-0.788757000	-0.313022000
1	-2.163469000	-0.215998000	-0.027978000
1	-1.293830000	-0.963100000	-1.394902000
1	-1.308347000	-1.759965000	0.193503000
6	1.272056000	-0.793240000	-0.312969000
1	2.162677000	-0.223325000	-0.028502000
1	1.302411000	-1.764270000	0.194086000
1	1.290153000	-0.968205000	-1.394765000



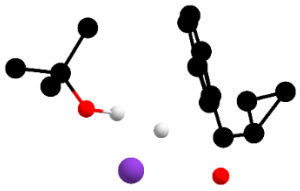
2a^{-}K^{+}

G = -1296.651351 Eh

E = -1296.89354 Eh

6	-0.819771000	0.841850000	-0.119271000
8	-0.269008000	1.211706000	1.054367000
19	1.897807000	2.107483000	0.198400000
8	2.525562000	-0.171284000	-1.069360000
1	1.737654000	-0.435761000	-1.568052000
1	-0.051434000	0.594133000	-0.929447000
6	-1.678127000	-0.435109000	-0.044968000
6	2.776002000	-1.220885000	-0.091749000
6	-2.098331000	-0.909848000	1.200527000

6	-2.047602000	-1.144716000	-1.195202000
6	-2.826041000	-2.301638000	-1.106578000
6	-2.882149000	-2.062831000	1.297590000
6	-3.248860000	-2.764304000	0.144621000
1	-1.771927000	-0.353959000	2.074126000
1	-3.202616000	-2.421293000	2.273594000
1	-3.852268000	-3.665605000	0.219141000
1	-3.099878000	-2.844552000	-2.008549000
1	-1.713226000	-0.788632000	-2.169255000
6	1.471141000	-1.572255000	0.624447000
6	3.361461000	-2.431679000	-0.821471000
6	3.797860000	-0.639086000	0.885553000
1	4.291487000	-2.162345000	-1.334948000
1	0.761087000	-2.027304000	-0.076344000
1	3.354770000	0.150271000	1.507066000
1	4.146768000	-1.418476000	1.570015000
1	4.665428000	-0.239006000	0.347879000
1	3.570044000	-3.244588000	-0.116558000
1	2.647955000	-2.804757000	-1.566164000
1	1.660227000	-2.296187000	1.425584000
1	0.994380000	-0.676132000	1.046394000
6	-1.684690000	1.957873000	-0.772868000
1	-2.094235000	1.720044000	-1.754676000
6	-1.306676000	3.400503000	-0.532205000
1	-1.439943000	4.130274000	-1.328546000
1	-3.516271000	3.125192000	-0.198626000
6	-2.531425000	2.803801000	0.132572000
1	-2.426066000	2.582178000	1.191455000
1	-0.469445000	3.580905000	0.140271000



TSH-K$_{Ph}$

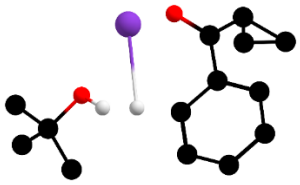
G = -1296.596412 Eh

E = -1296.836016 Eh

ν = -370.9 cm^{-1}

6	1.947873000	-0.690464000	0.686806000
8	2.138786000	-0.563324000	1.915259000
19	-0.341492000	0.267255000	2.489846000
8	-2.109227000	-0.318627000	0.651451000
1	-1.289177000	-0.901423000	0.435046000
1	0.004807000	-1.467615000	0.530290000
6	1.517241000	0.547976000	-0.083791000
6	-3.101432000	-0.488505000	-0.358471000
6	0.962827000	0.547189000	-1.373092000
6	1.699709000	1.785917000	0.556971000
6	1.318599000	2.982892000	-0.056460000
6	0.595482000	1.739668000	-1.993516000
6	0.762028000	2.964334000	-1.336600000
1	0.778956000	-0.388673000	-1.882122000
1	0.157922000	1.711288000	-2.987471000
1	0.465534000	3.890562000	-1.820974000
1	1.471444000	3.927159000	0.460298000
1	2.164152000	1.794285000	1.539089000
6	-2.536750000	-0.053111000	-1.717894000
6	-3.531302000	-1.961371000	-0.410192000
6	-4.283550000	0.399529000	0.032860000
1	-3.926625000	-2.273611000	0.563554000
1	-1.684011000	-0.684580000	-1.990962000
1	-3.968427000	1.448356000	0.087944000
1	-5.091696000	0.318086000	-0.703625000
1	-4.674543000	0.100074000	1.012389000
1	-4.305120000	-2.124199000	-1.170582000
1	-2.669565000	-2.595042000	-0.649790000
1	-3.296378000	-0.135453000	-2.505454000
1	-2.189481000	0.984160000	-1.667781000
6	2.627024000	-1.847486000	0.001363000
1	3.160447000	-2.439392000	0.740391000
6	3.294275000	-1.701373000	-1.364788000
1	4.278888000	-2.145785000	-1.492232000
1	2.282820000	-3.680220000	-1.193080000

6	2.109722000	-2.606372000	-1.196585000
1	1.138372000	-2.315837000	-1.582086000
1	3.153088000	-0.757330000	-1.883247000

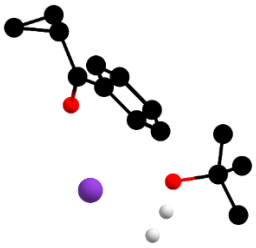


17$_{Ph}$

G = -1296.609157 Eh

E = -1296.84155 Eh

6	1.836696000	-0.731439000	0.847265000
8	1.024469000	-1.147845000	1.677943000
19	-0.705629000	-2.565869000	0.150341000
8	-2.348562000	-0.485231000	-0.044069000
1	-1.967562000	-0.655499000	-0.981621000
1	-1.177510000	-1.296072000	-2.047018000
6	1.835178000	0.701938000	0.443383000
6	-3.464394000	0.403561000	-0.110707000
6	3.029591000	1.431646000	0.337730000
6	0.602387000	1.331002000	0.201110000
6	0.577584000	2.674776000	-0.169930000
6	2.993122000	2.785005000	0.002078000
6	1.767642000	3.403624000	-0.262608000
1	3.977505000	0.944155000	0.541764000
1	3.917080000	3.352788000	-0.059734000
1	1.740332000	4.452724000	-0.544185000
1	-0.372403000	3.152208000	-0.389057000
1	-0.320349000	0.760063000	0.270491000
6	-2.986627000	1.797623000	-0.541853000
6	-4.498066000	-0.135695000	-1.108994000
6	-4.059999000	0.463809000	1.296490000
1	-4.831106000	-1.135275000	-0.805395000
1	-2.483246000	1.739293000	-1.513304000
1	-3.303890000	0.806714000	2.012449000
1	-4.910555000	1.155064000	1.329239000
1	-4.407546000	-0.529064000	1.606063000
1	-5.374532000	0.521971000	-1.161954000
1	-4.055845000	-0.210404000	-2.108517000
1	-3.829391000	2.495082000	-0.626975000
1	-2.282070000	2.195685000	0.196332000
6	2.735929000	-1.716577000	0.176462000
1	2.970543000	-2.570122000	0.808025000
6	3.672464000	-1.413886000	-0.971800000
1	4.573069000	-2.019990000	-1.024541000
1	2.340728000	-3.116683000	-1.540868000
6	2.360310000	-2.060419000	-1.281784000
1	1.588121000	-1.455878000	-1.755033000
1	3.797418000	-0.380446000	-1.274687000



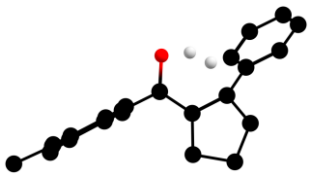
TSH2-K$_{Ph}$

G = -1296.61984 Eh

E = -1296.847829 Eh

6	-2.060427000	-0.560687000	-0.062585000
8	-1.382249000	-1.429698000	0.498197000
19	0.784875000	-1.456549000	2.058430000
8	2.429970000	-0.590344000	0.330431000
1	2.624986000	0.054914000	1.352601000
1	2.597779000	0.467655000	2.311614000
6	-1.670037000	0.874952000	0.007983000
6	3.324557000	-0.251755000	-0.701359000
6	-2.637598000	1.893977000	-0.045727000
6	-0.314271000	1.215152000	0.173608000
6	0.057180000	2.553607000	0.291810000
6	-2.259743000	3.229706000	0.088350000
6	-0.911836000	3.561342000	0.255660000
1	-3.687614000	1.642993000	-0.159354000
1	-3.015310000	4.009774000	0.062897000
1	-0.617833000	4.602750000	0.353975000

1	1.107398000	2.800052000	0.409759000
1	0.466936000	0.456703000	0.162577000
6	3.248856000	1.259052000	-0.996583000
6	4.762444000	-0.621019000	-0.291163000
6	2.927648000	-1.036022000	-1.960844000
1	4.825118000	-1.694333000	-0.072887000
1	3.498070000	1.828940000	-0.094170000
1	1.900132000	-0.784207000	-2.250232000
1	3.592874000	-0.807194000	-2.804147000
1	2.975300000	-2.114341000	-1.764566000
1	5.485456000	-0.384513000	-1.083269000
1	5.046821000	-0.071614000	0.613495000
1	3.945595000	1.551442000	-1.793448000
1	2.233874000	1.530137000	-1.308178000
6	-3.281865000	-0.936354000	-0.820556000
1	-3.797239000	-0.141167000	-1.345907000
6	-4.125068000	-2.086243000	-0.267941000
1	-5.202289000	-1.999202000	-0.380914000
1	-3.768072000	-2.389241000	-2.445658000
6	-3.285858000	-2.316814000	-1.474817000
1	-2.372265000	-2.891356000	-1.350515000
1	-3.777999000	-2.506798000	0.672116000



TS9_H2

G = -968.5562658 Eh

E = -968.9148488 Eh

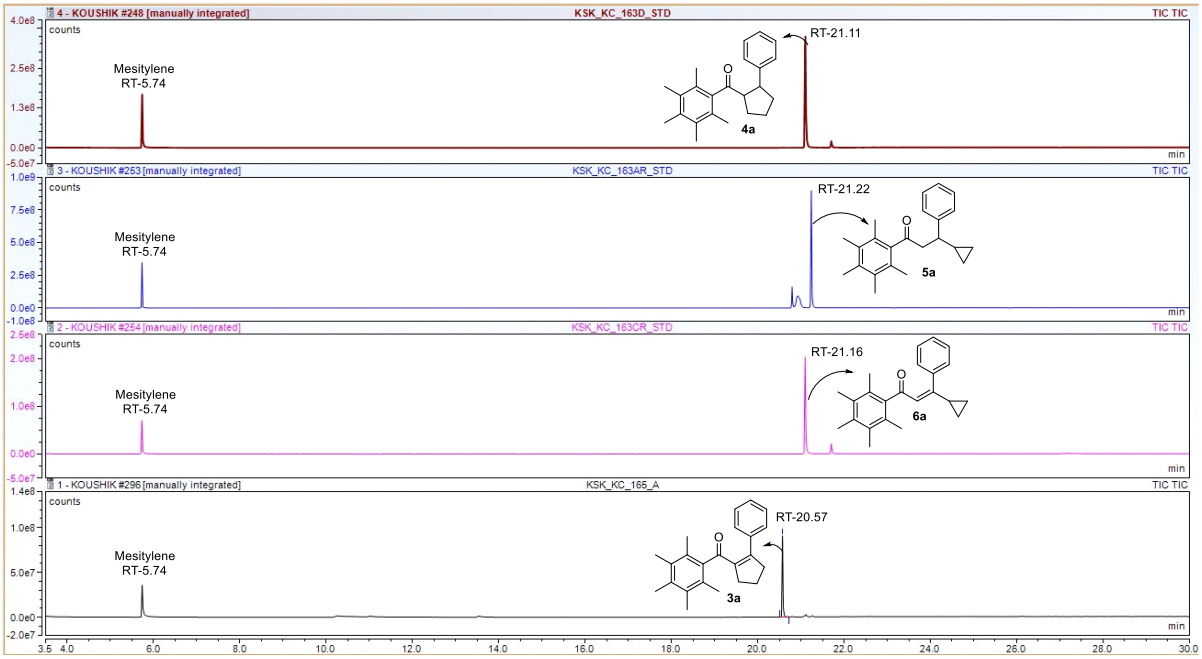
ν = -1515.1 cm^{-1}

6	0.297928000	-1.325876000	1.711698000
6	3.365173000	-0.069313000	-0.062552000
6	4.637913000	-0.596219000	-0.336671000
6	3.186853000	1.321052000	-0.102257000
6	5.704933000	0.245603000	-0.646488000
6	4.253522000	2.164160000	-0.413064000
6	5.516005000	1.630652000	-0.686358000
1	4.785498000	-1.672267000	-0.321577000
1	2.210060000	1.731663000	0.126614000
1	6.682607000	-0.178151000	-0.858753000
1	4.099131000	3.239318000	-0.437759000
1	6.347108000	2.288068000	-0.926038000
6	2.505662000	-2.210931000	1.155467000
6	1.524518000	-2.028068000	2.334282000
6	2.237868000	-0.974475000	0.293636000
1	3.548633000	-2.292302000	1.472246000
1	2.252364000	-3.113265000	0.586177000
1	1.983670000	-1.368669000	3.080111000
6	0.901923000	-0.548480000	0.553068000
6	0.154249000	0.027844000	-0.475895000
8	0.693126000	0.219823000	-1.632952000
6	-1.334320000	0.156067000	-0.339877000
6	-2.140562000	-0.925206000	-0.737139000
6	-1.893750000	1.323387000	0.204691000
6	-3.536880000	-0.830324000	-0.593595000
6	-3.291418000	1.410041000	0.353778000
6	-4.111316000	0.348221000	-0.075782000
1	1.275954000	-2.974366000	2.824771000
6	-3.912086000	2.645477000	0.974456000
1	-4.780783000	2.390217000	1.589274000
1	-3.203005000	3.175416000	1.615102000
1	-4.255504000	3.357067000	0.209584000
6	-5.619088000	0.475408000	0.014381000
1	-5.940130000	1.516028000	-0.082233000
1	-6.117104000	-0.094035000	-0.775131000
1	-6.004311000	0.104005000	0.975346000
6	-4.419464000	-1.994664000	-0.993976000
1	-3.874386000	-2.941364000	-0.968711000
1	-5.280475000	-2.094227000	-0.326013000
1	-4.812589000	-1.873715000	-2.013887000
6	-1.513664000	-2.184412000	-1.301355000
1	-0.447015000	-2.061004000	-1.499984000

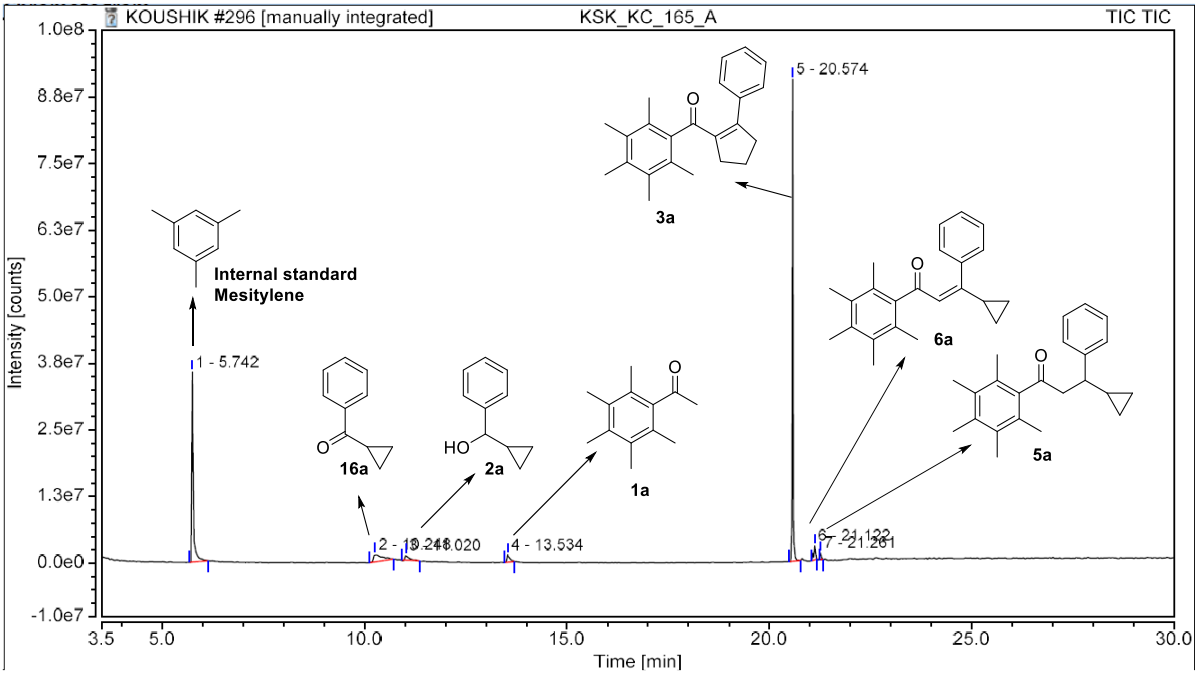
1	-1.633023000	-3.031629000	-0.612586000	1	-0.224064000	-0.679859000	2.426148000
1	-1.991041000	-2.473286000	-2.244878000	1	-0.437823000	-2.058608000	1.351590000
6	-1.008291000	2.481890000	0.615816000	1	1.542425000	-0.811638000	-1.700197000
1	0.002681000	2.378365000	0.215076000	1	2.028785000	-1.468013000	-1.279551000
1	-1.411099000	3.433968000	0.252944000				
1	-0.925820000	2.562696000	1.708350000				

9. Copies of the GCMS data of the optimise conditions

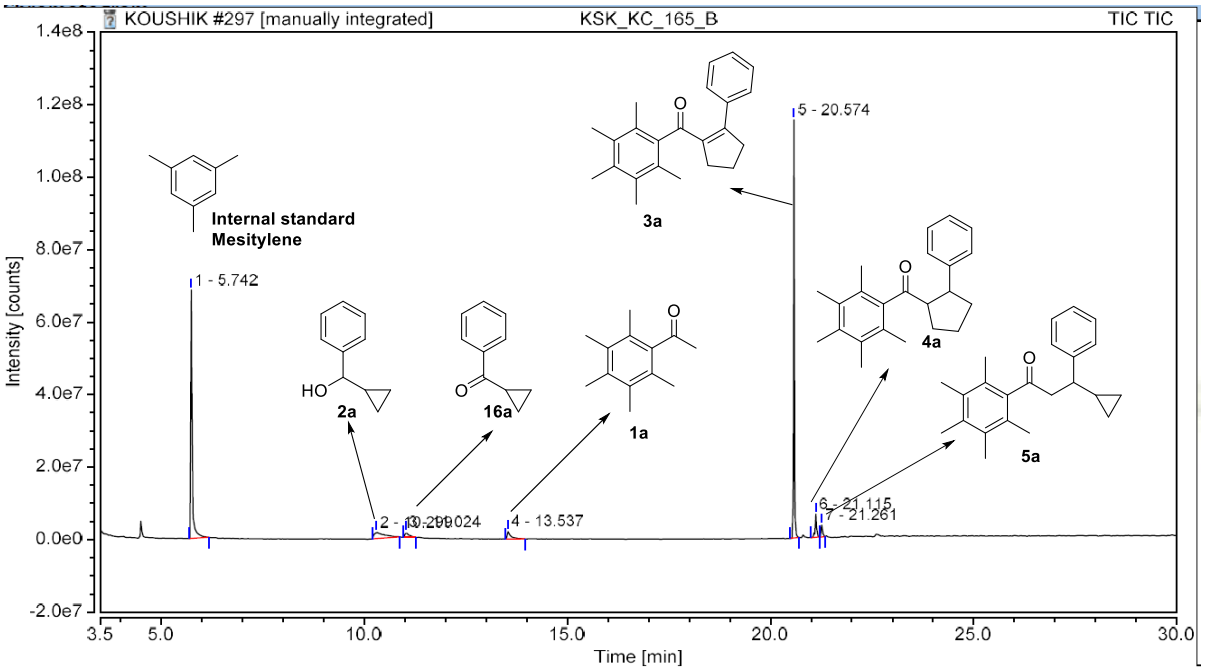
9.1 Standardization of the final product mixture of 3a, 4a, 5a, 6a.



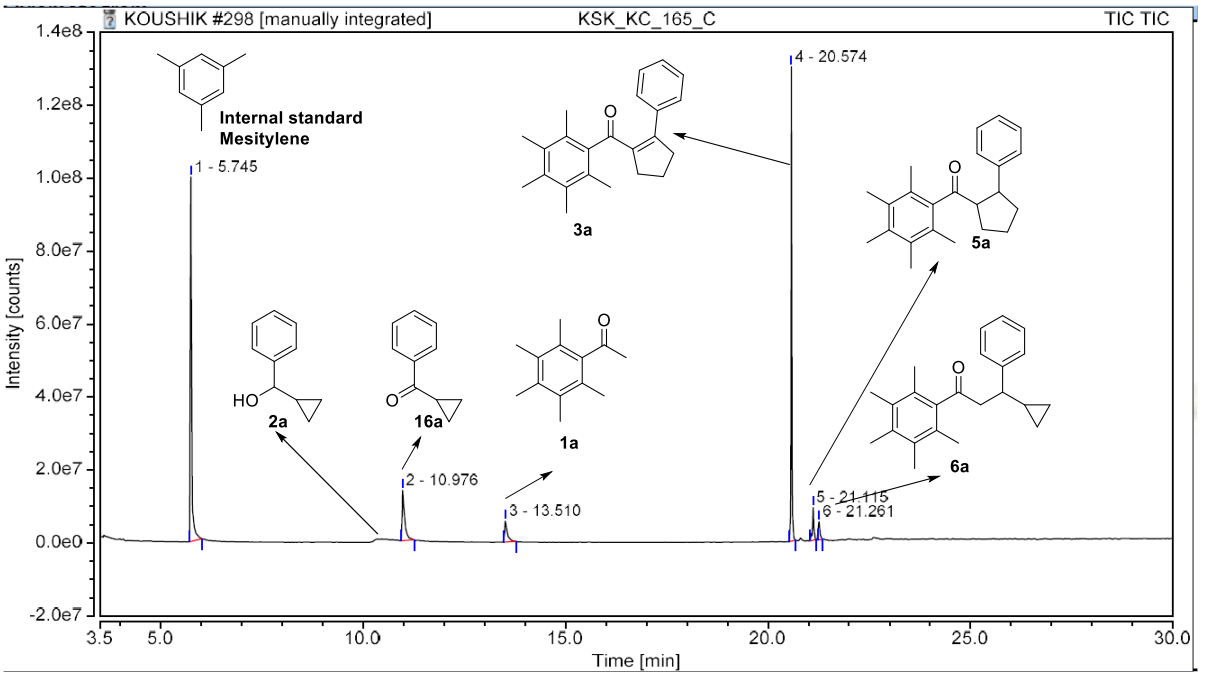
9.2 Table 1, Entry 1



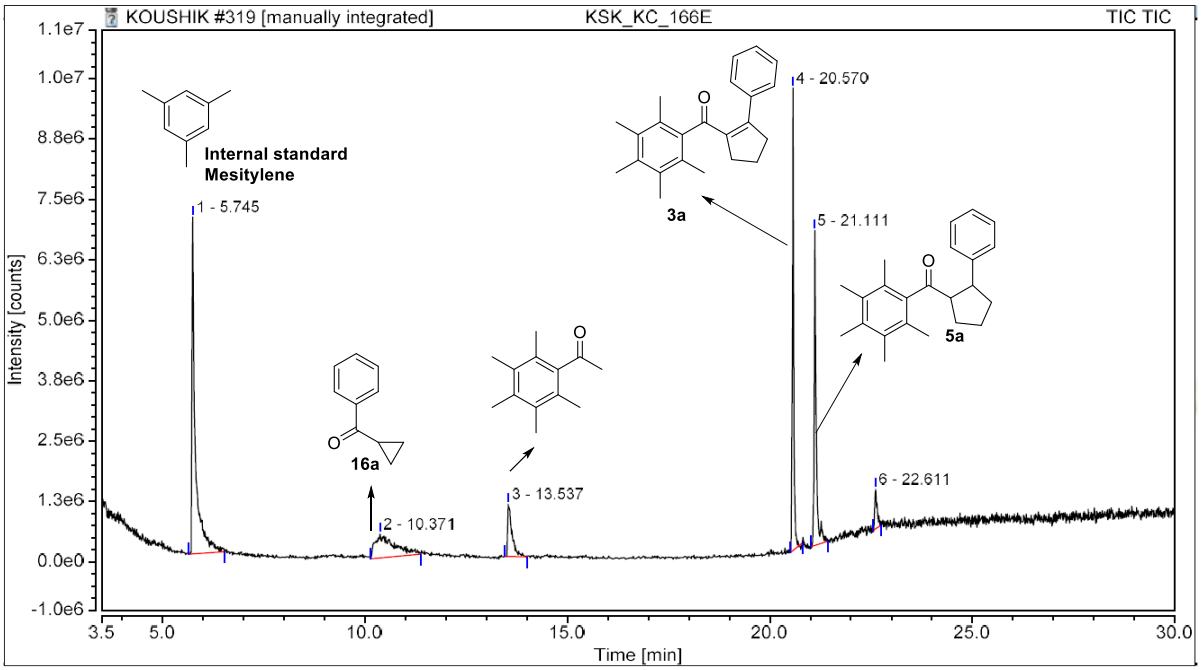
9.3 Table 1, Entry 2



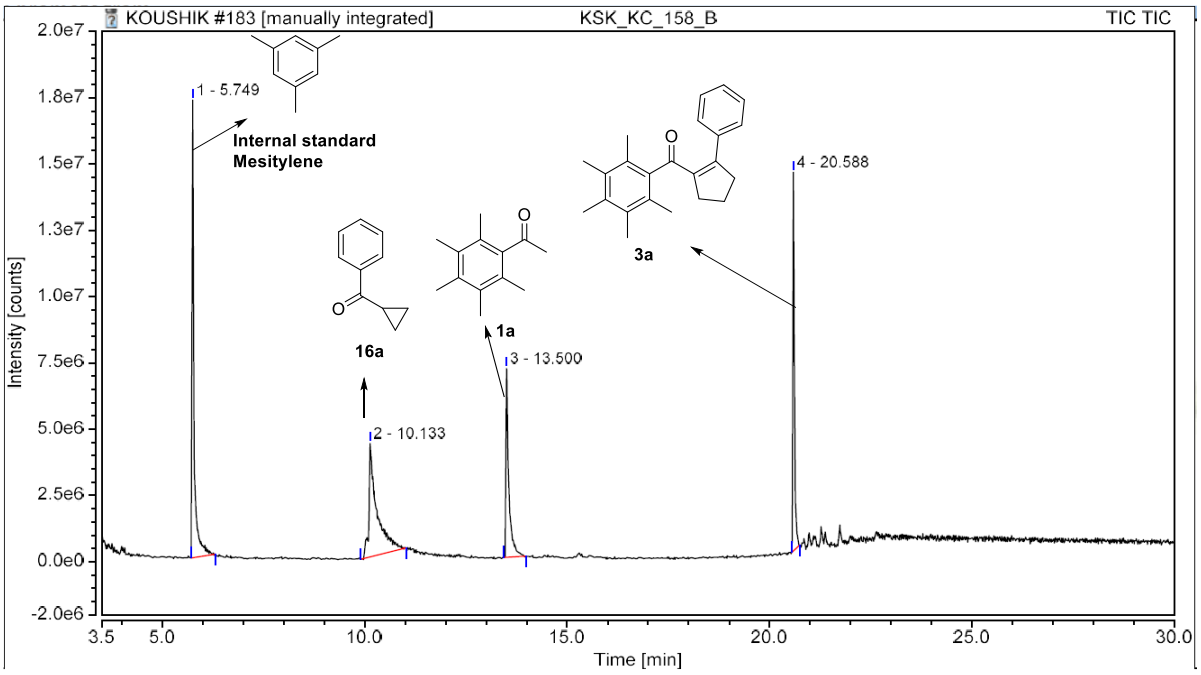
9.4 Table 1, Entry 3



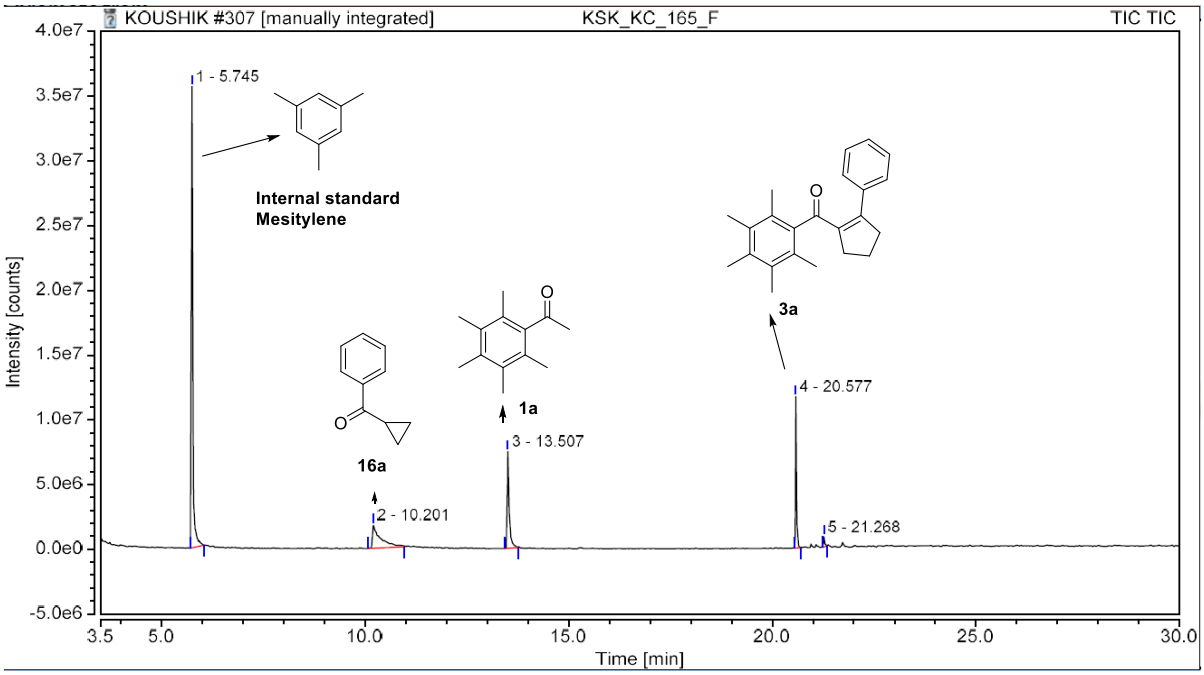
9.5 Table 1, Entry 4



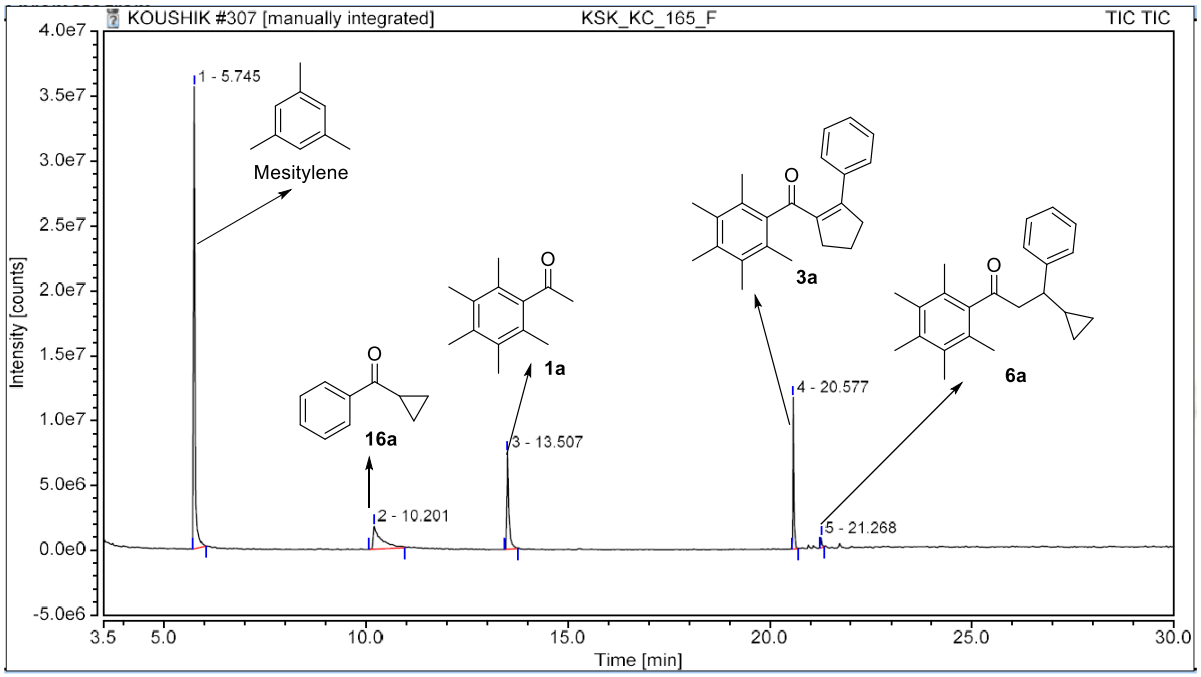
9.6 Table1, Entry 5



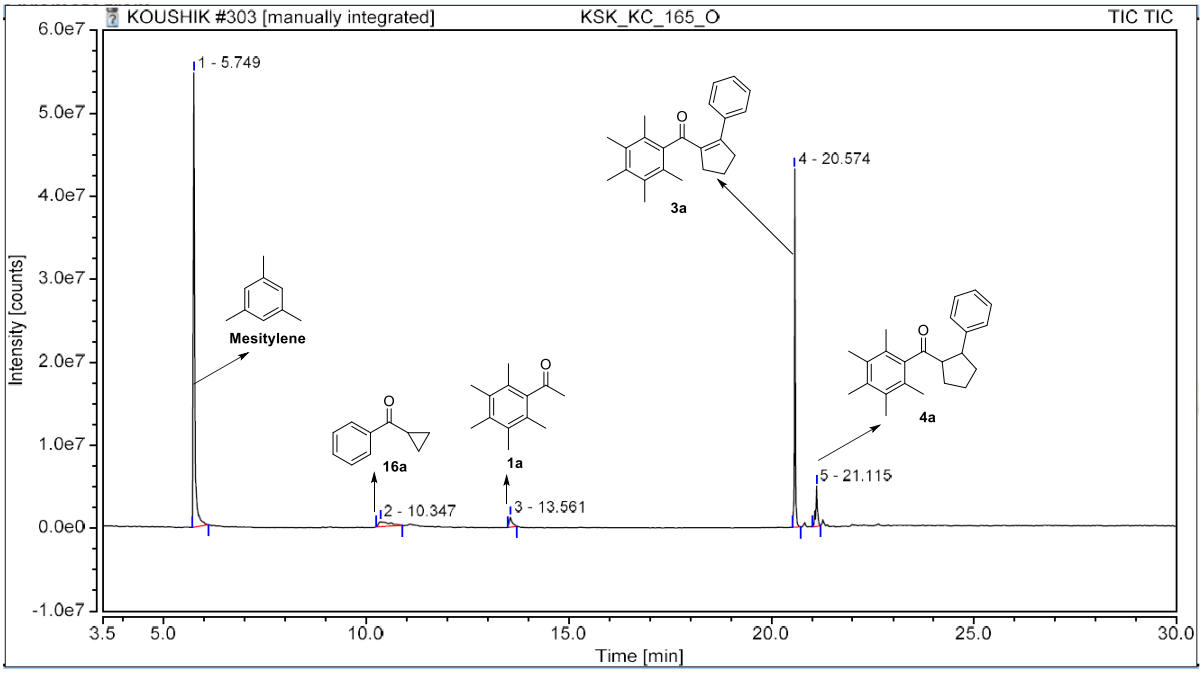
9.7 Table 1, Entry 6



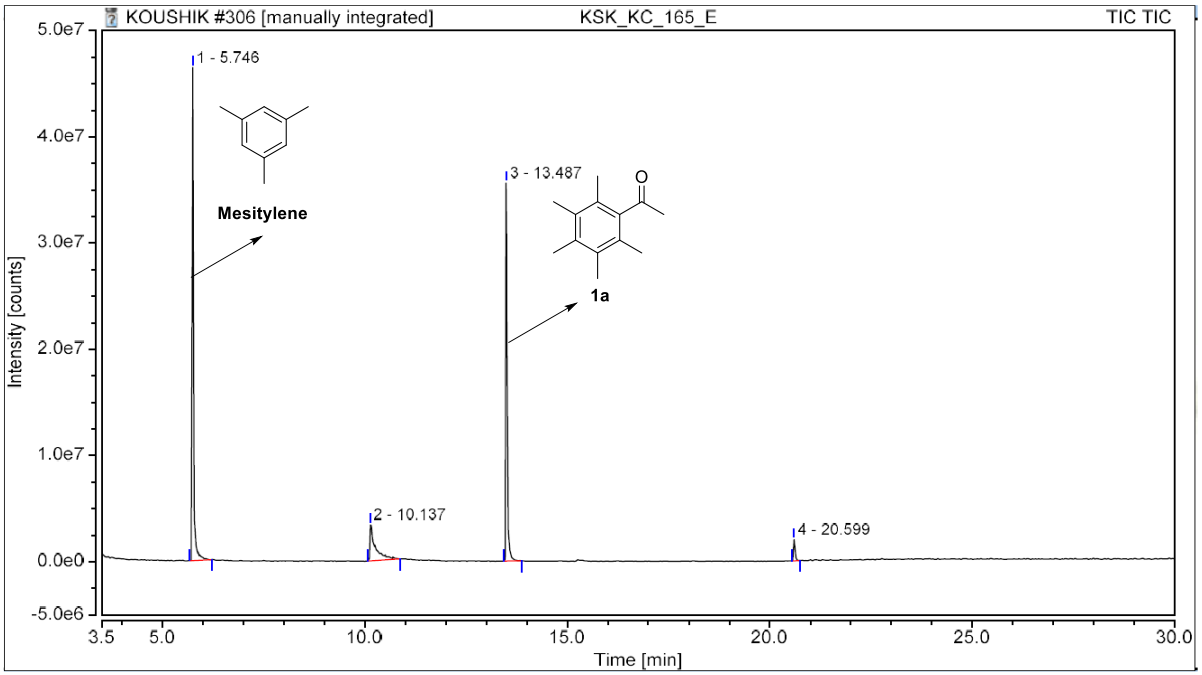
9.8 Table 1, entry 7



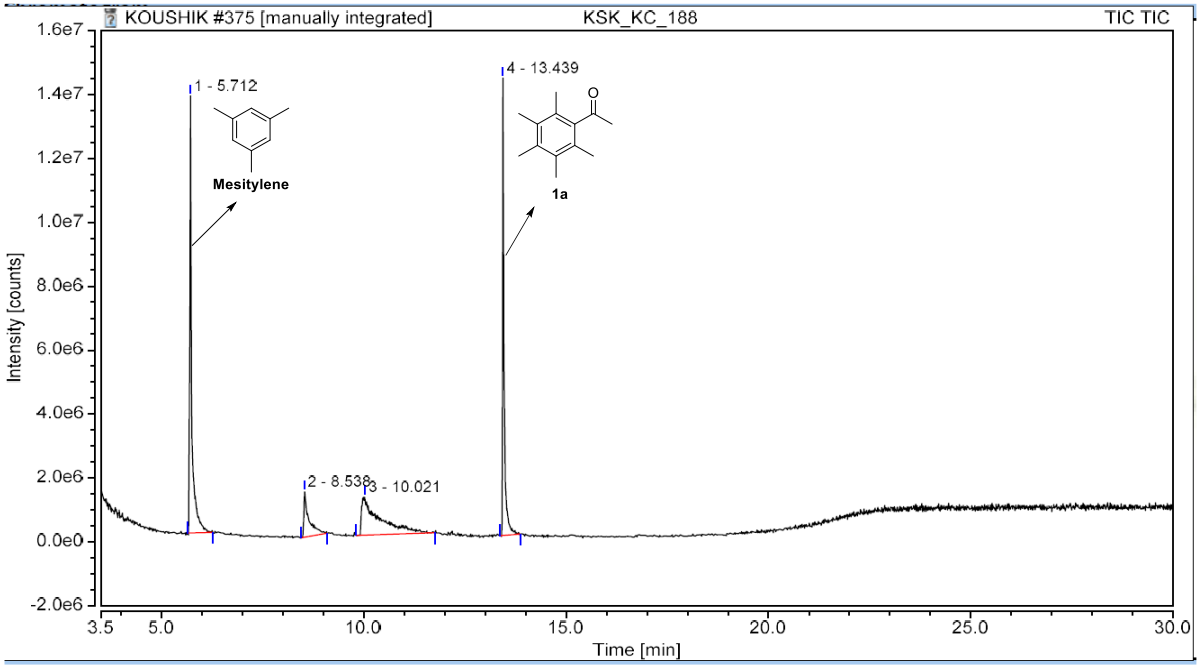
9.9 Table 1, Entry 8



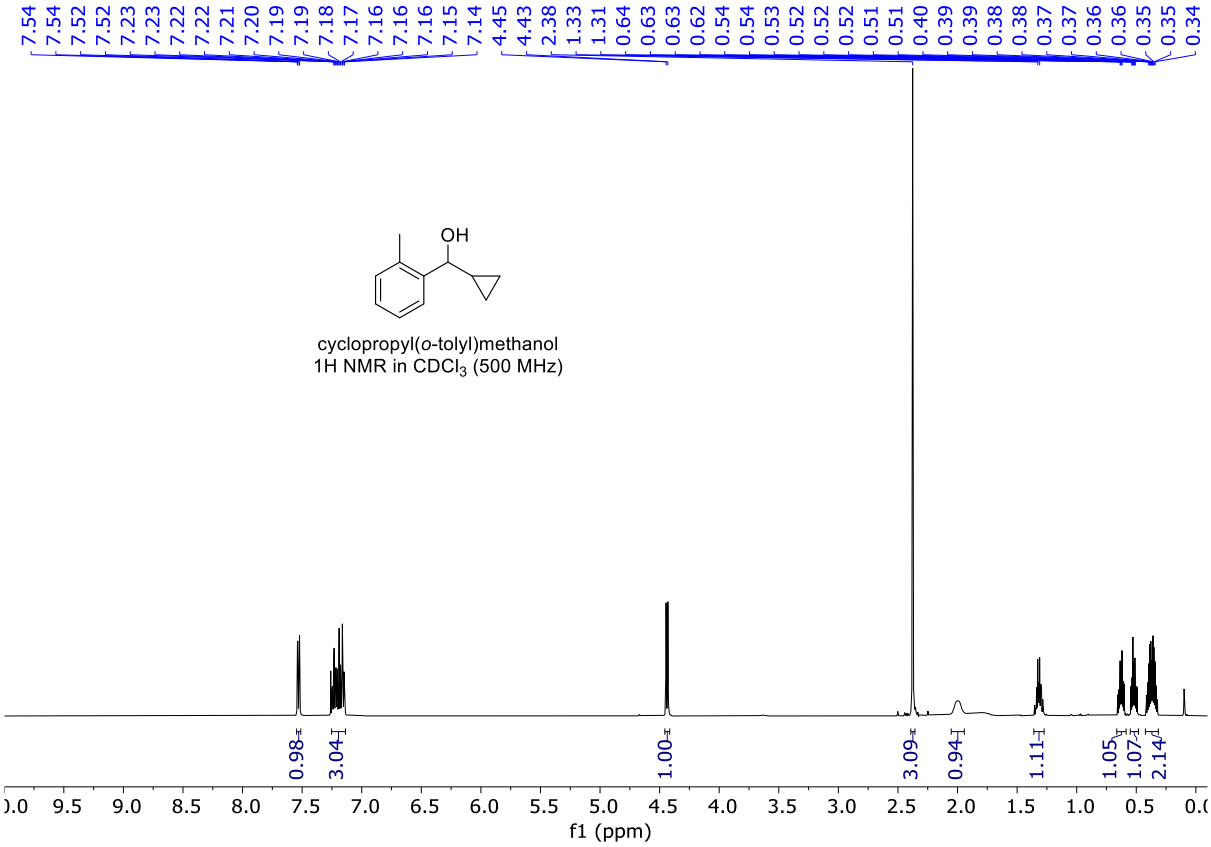
9.10 Table 1, entry 10

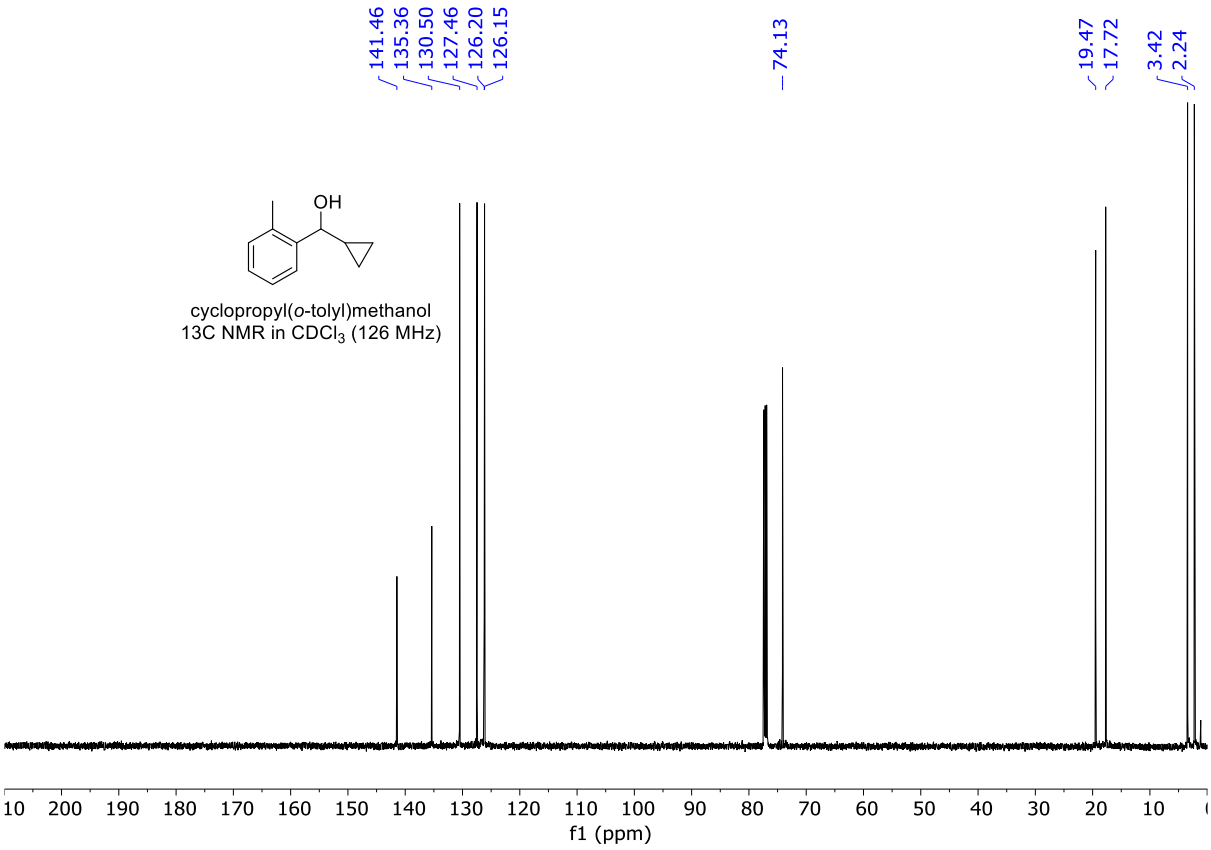


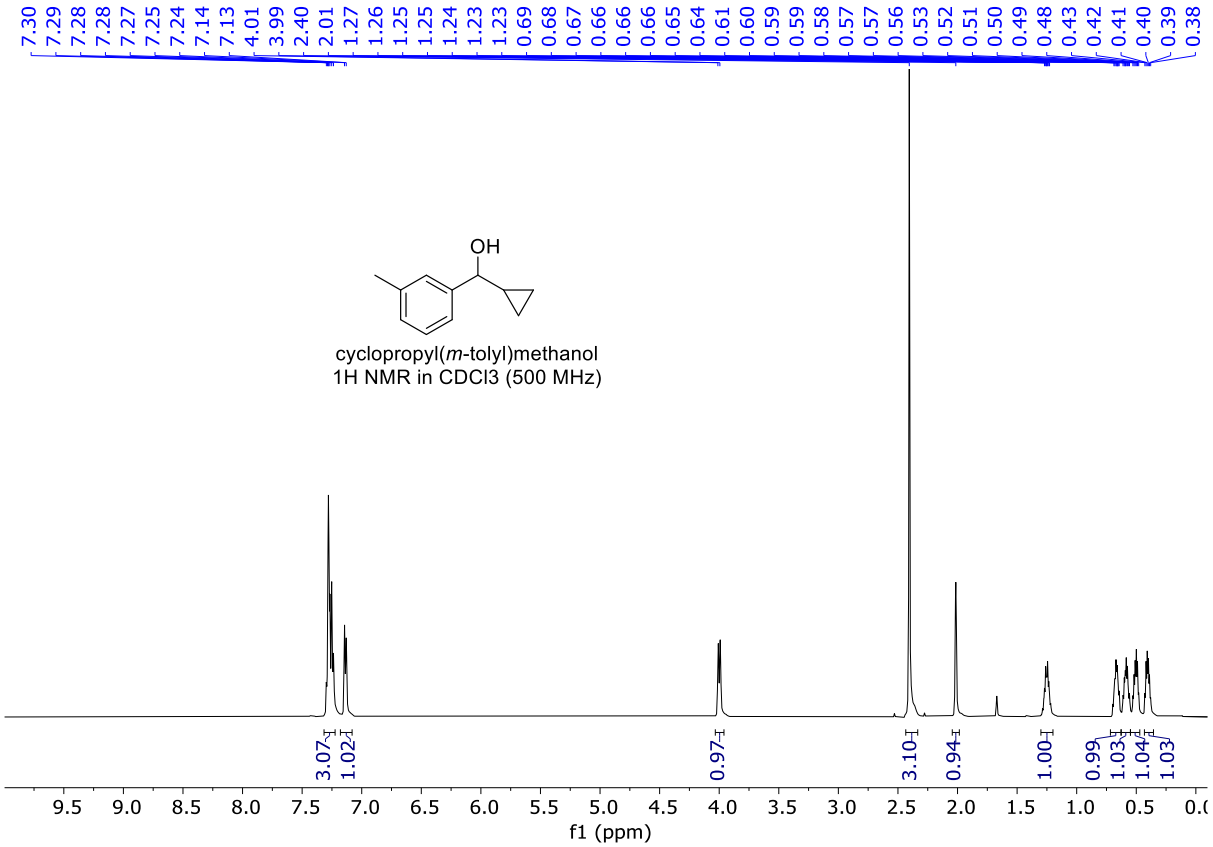
9.11 Table 1, Entry 11

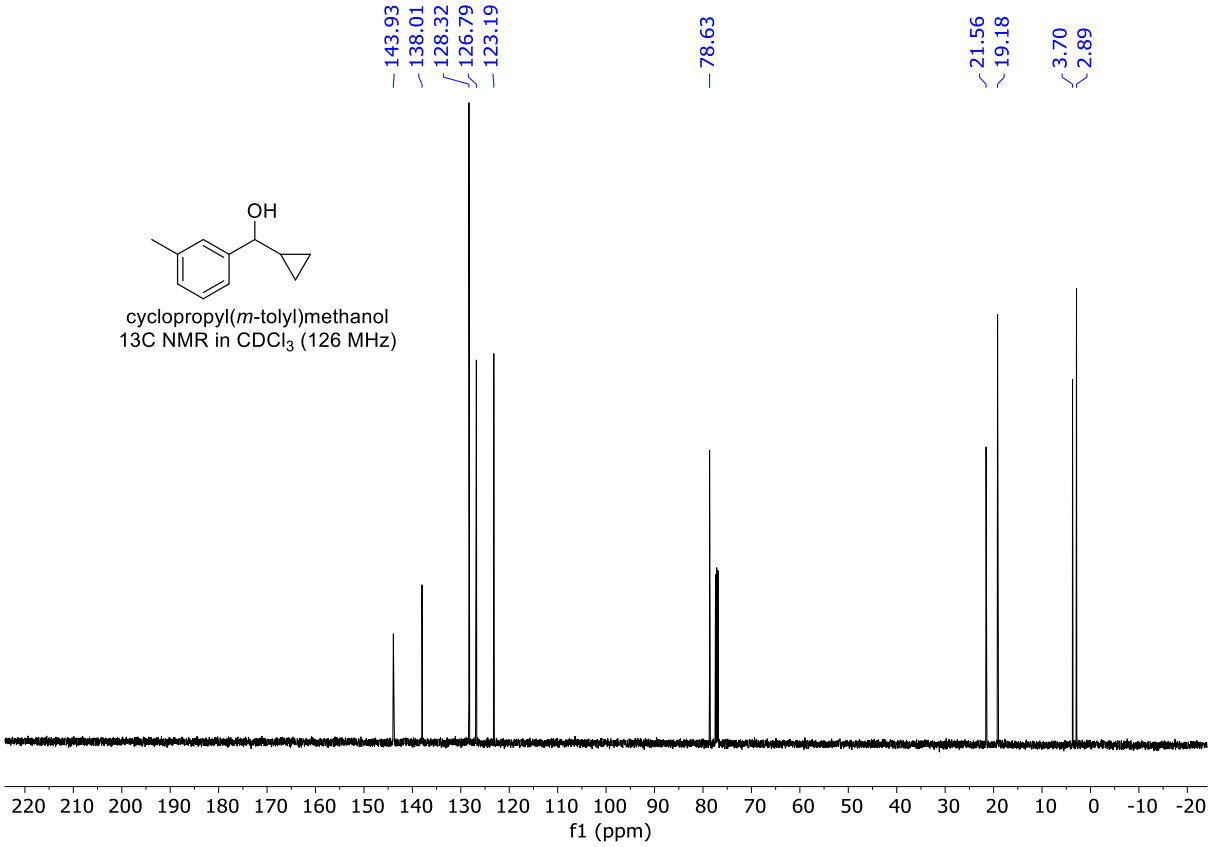


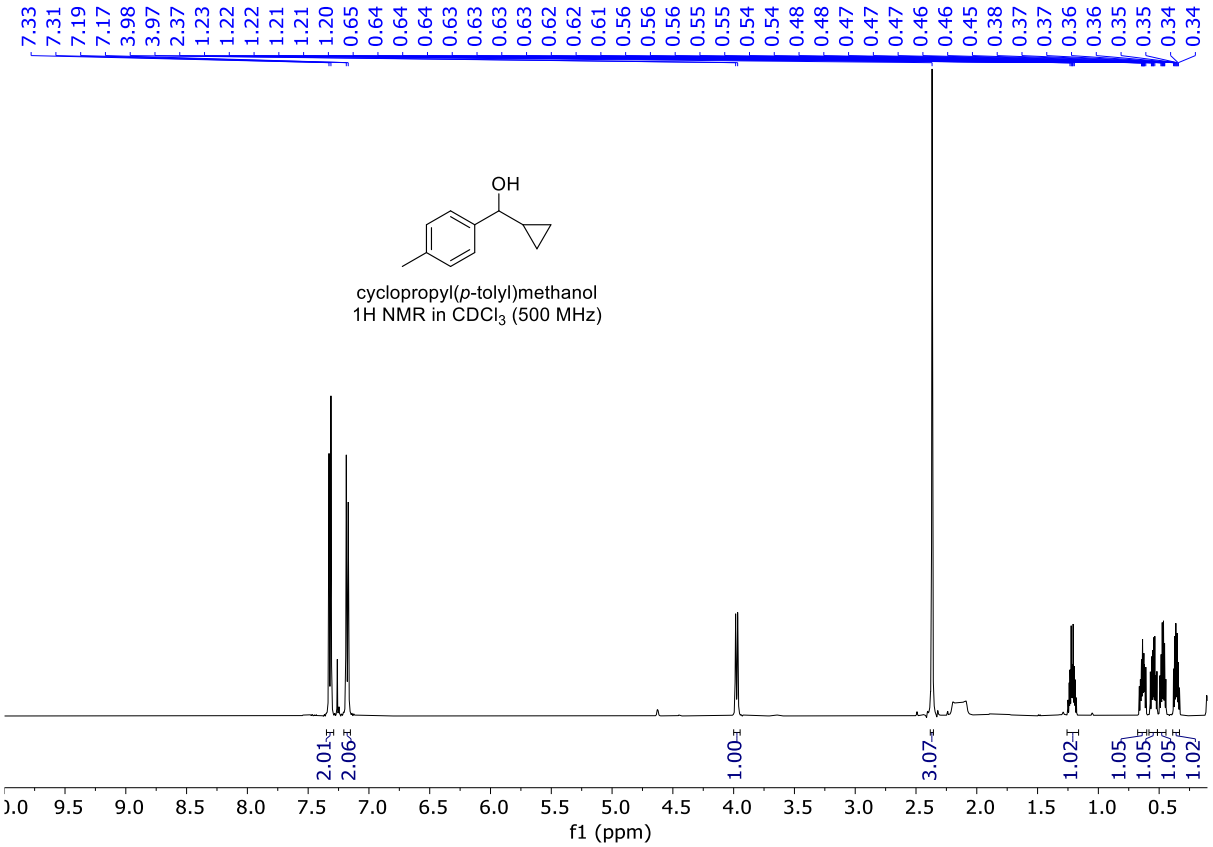
10. Copies of the ^{1}H and ^{13}C NMR data

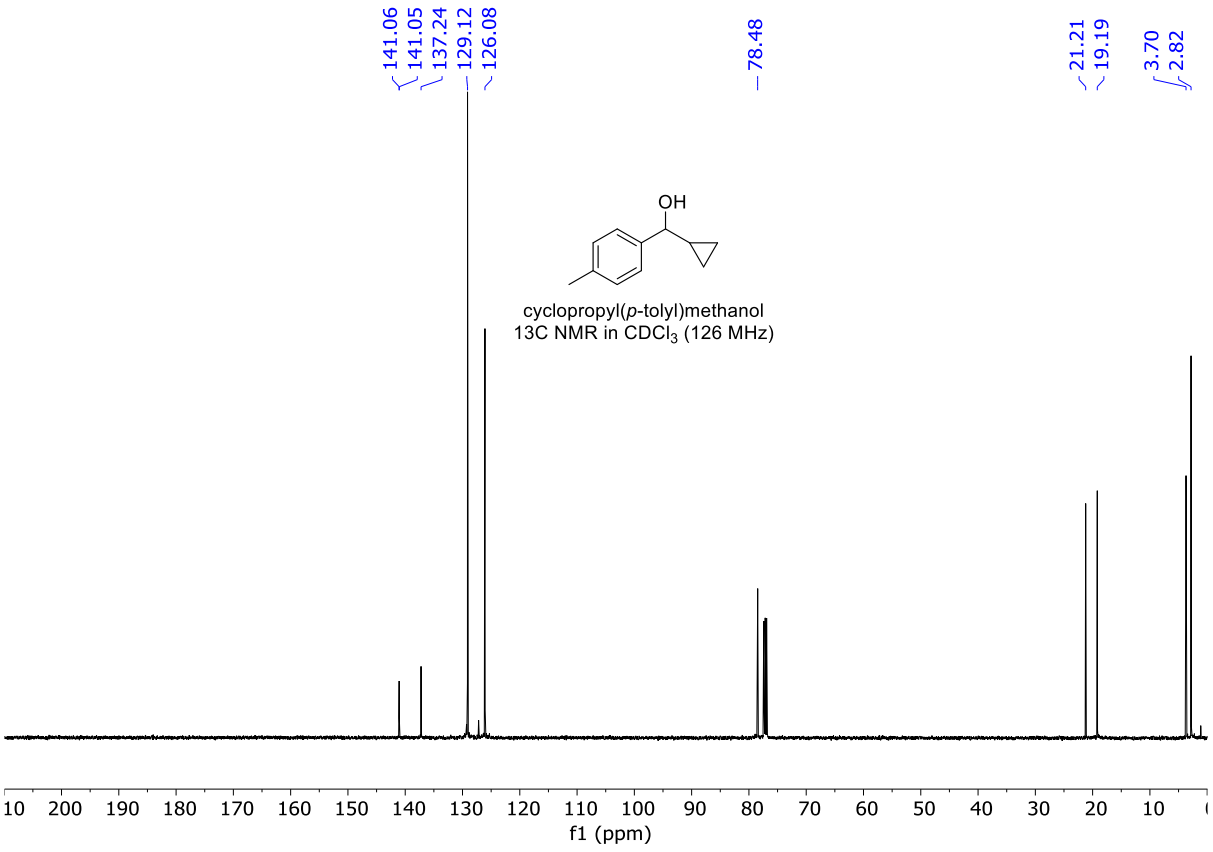


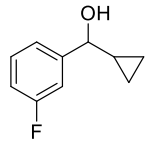



7.30 7.29 7.28 7.28 7.27 7.25 7.24 7.14 7.13 4.01 3.99 2.40 2.01 1.27 1.26 1.25 1.25 1.24 1.23 1.23 0.69 0.68 0.67 0.66 0.66 0.66 0.65 0.64 0.61 0.60 0.59 0.59 0.58 0.57 0.57 0.56 0.53 0.52 0.51 0.50 0.49 0.48 0.43 0.42 0.41 0.40 0.39 0.38
OH
cyclopropyl(m-tolyl)methanol
1H NMR in CDCl3 (500 MHz)
3.07 1.02 0.97 3.10 0.94 1.00 0.99 1.03 1.04 1.03
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)

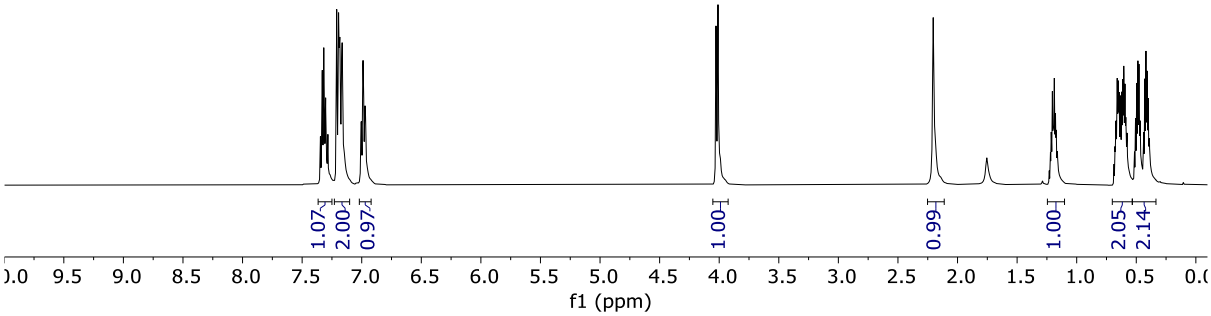

143.93 138.01 128.32 126.79 123.19 78.63 21.56 19.18 3.70 2.89
OH
cyclopropyl(m-tolyl)methanol
13C NMR in CDCl3 (126 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

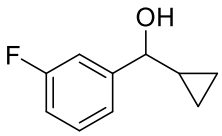

7.33 7.31 7.19 7.17 3.98 3.97 2.37 1.23 1.22 1.22 1.21 1.21 1.20 0.65 0.64 0.64 0.64 0.63 0.63 0.63 0.63 0.62 0.62 0.61 0.56 0.56 0.56 0.55 0.55 0.54 0.54 0.48 0.48 0.47 0.47 0.47 0.46 0.46 0.45 0.38 0.37 0.37 0.36 0.36 0.35 0.35 0.34 0.34
OH
cyclopropyl(p-tolyl)methanol
1H NMR in CDCl3 (500 MHz)
2.01 2.06 1.00 3.07 1.02 1.05 1.05 1.05 1.02
f1 (ppm)


141.06 141.05 137.24 129.12 126.08 78.48 21.21 19.19 3.70 2.82
OH
cyclopropyl(p-tolyl)methanol
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

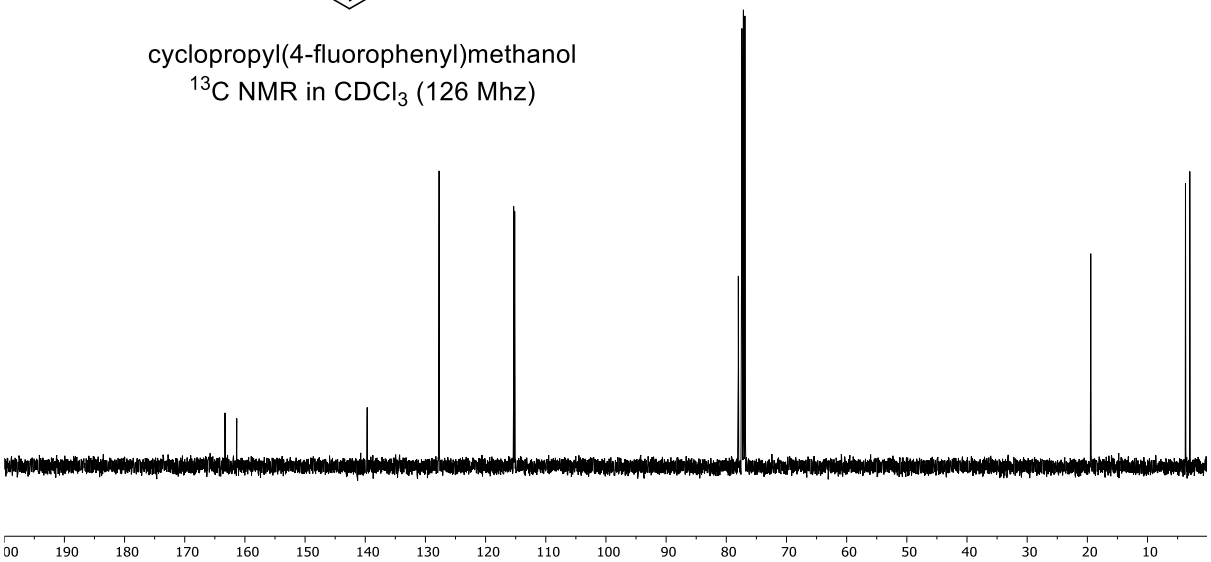


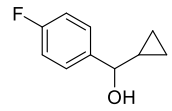
cyclopropyl(3-fluorophenyl)methanol
1H NMR in $CDCl_3$ (500 MHz)



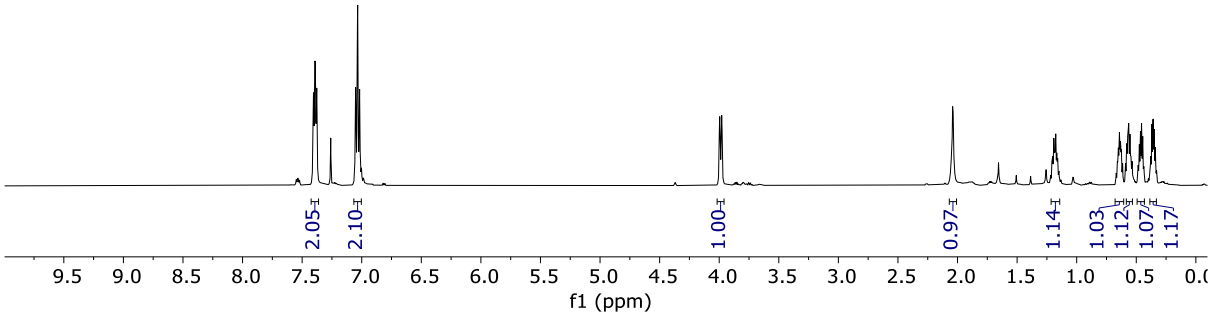


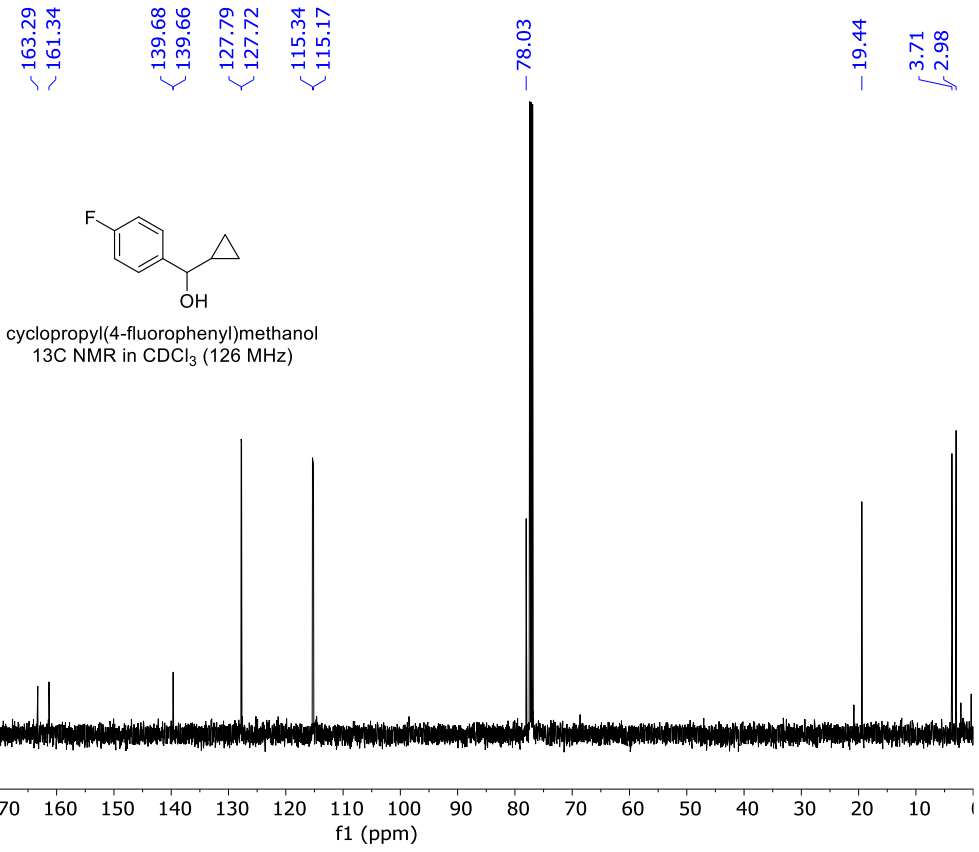
cyclopropyl(4-fluorophenyl)methanol
^{13}C NMR in $CDCl_3$ (126 Mhz)





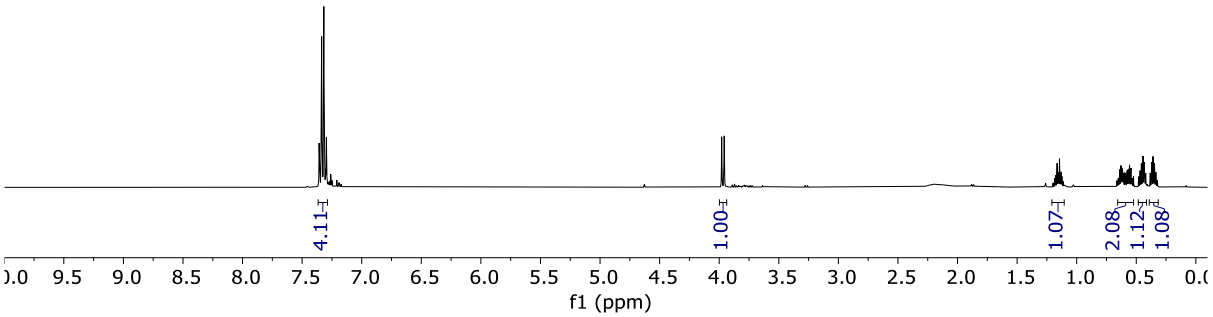
cyclopropyl(4-fluorophenyl)methanol
1H NMR in $CDCl_3$ (500 MHz)

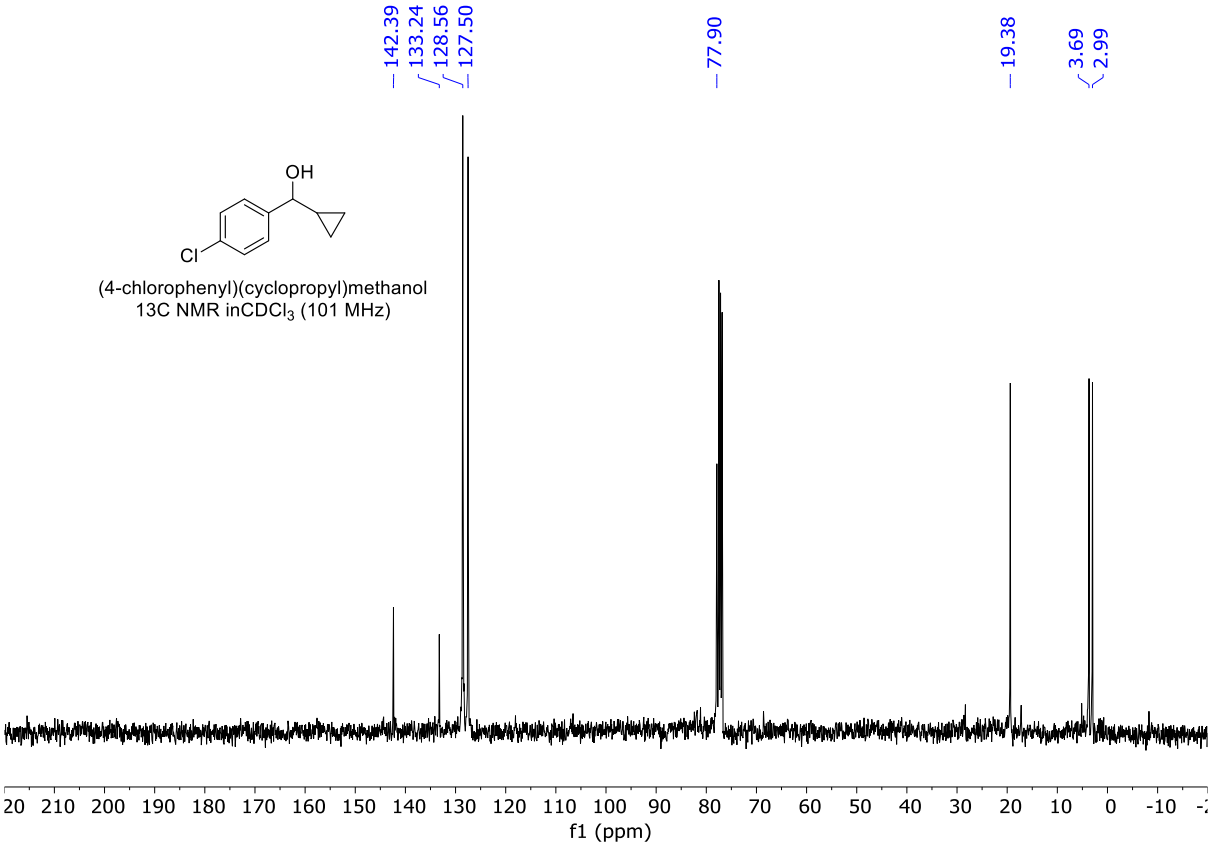




cyclopropyl(4-fluorophenyl)methanol
13C NMR in $CDCl_3$ (126 MHz)

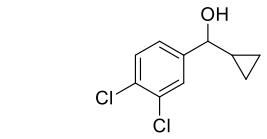
(4-chlorophenyl)(cyclopropyl)methanol
1H NMR in $CDCl_3$ (400 MHz)



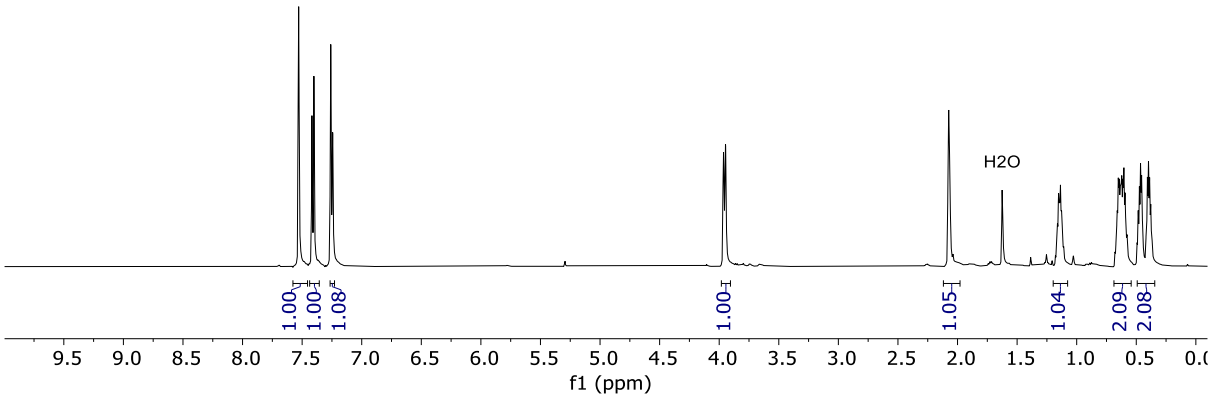


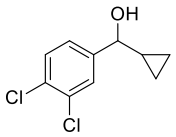
(4-chlorophenyl)(cyclopropyl)methanol
13C NMR in$CDCl_3$ (101 MHz)

temp.490.fid
GROUP BIP
BIP-KSK-KC30A 1H in CDCL3

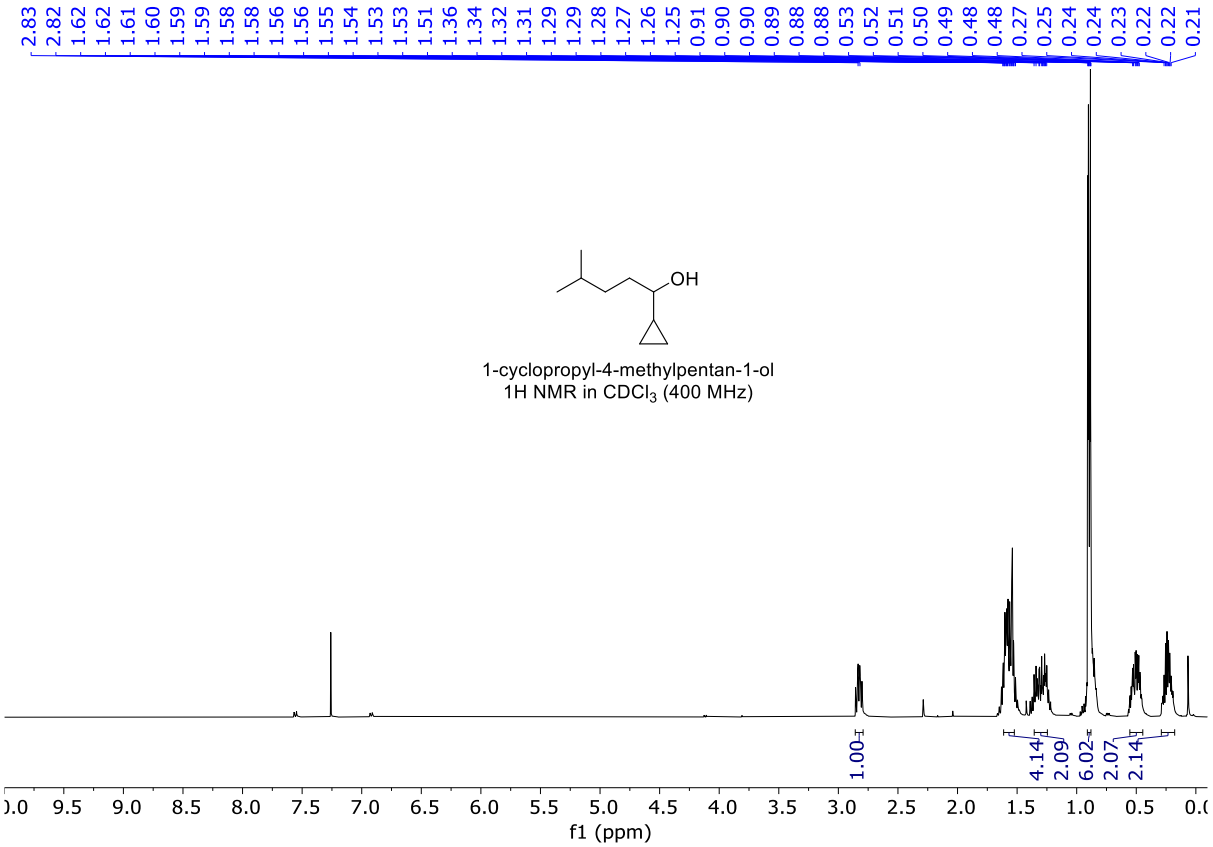


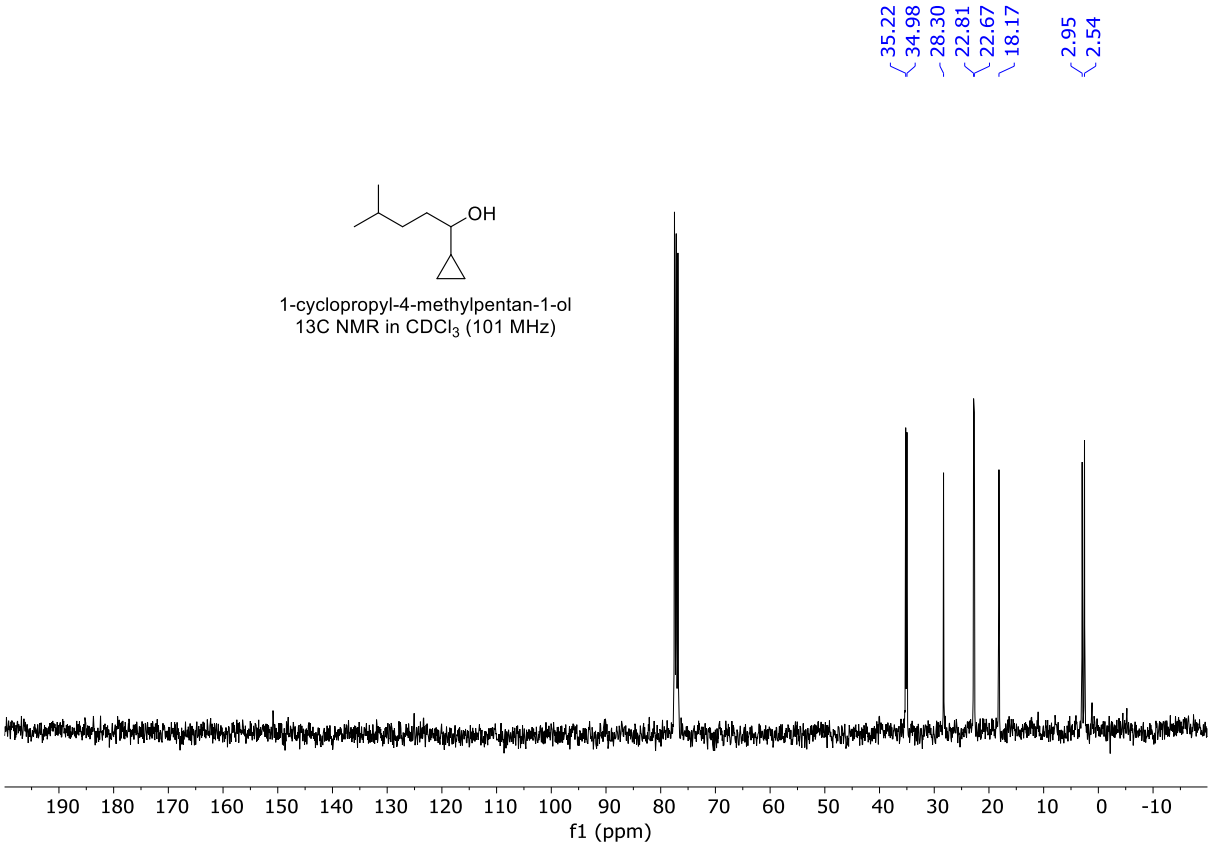
cyclopropyl(3,4-dichlorophenyl)methanol
1H NMR in $CDCl_3$ (500 MHz)

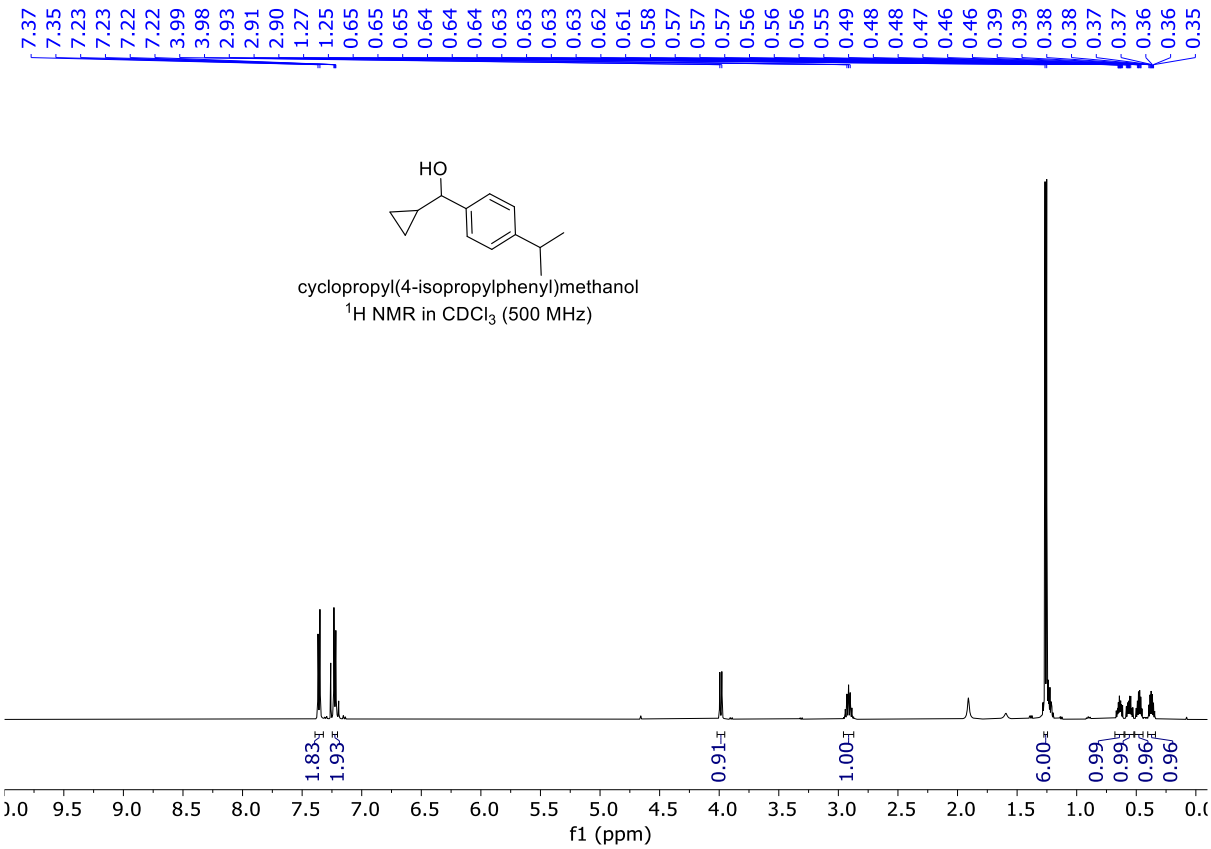


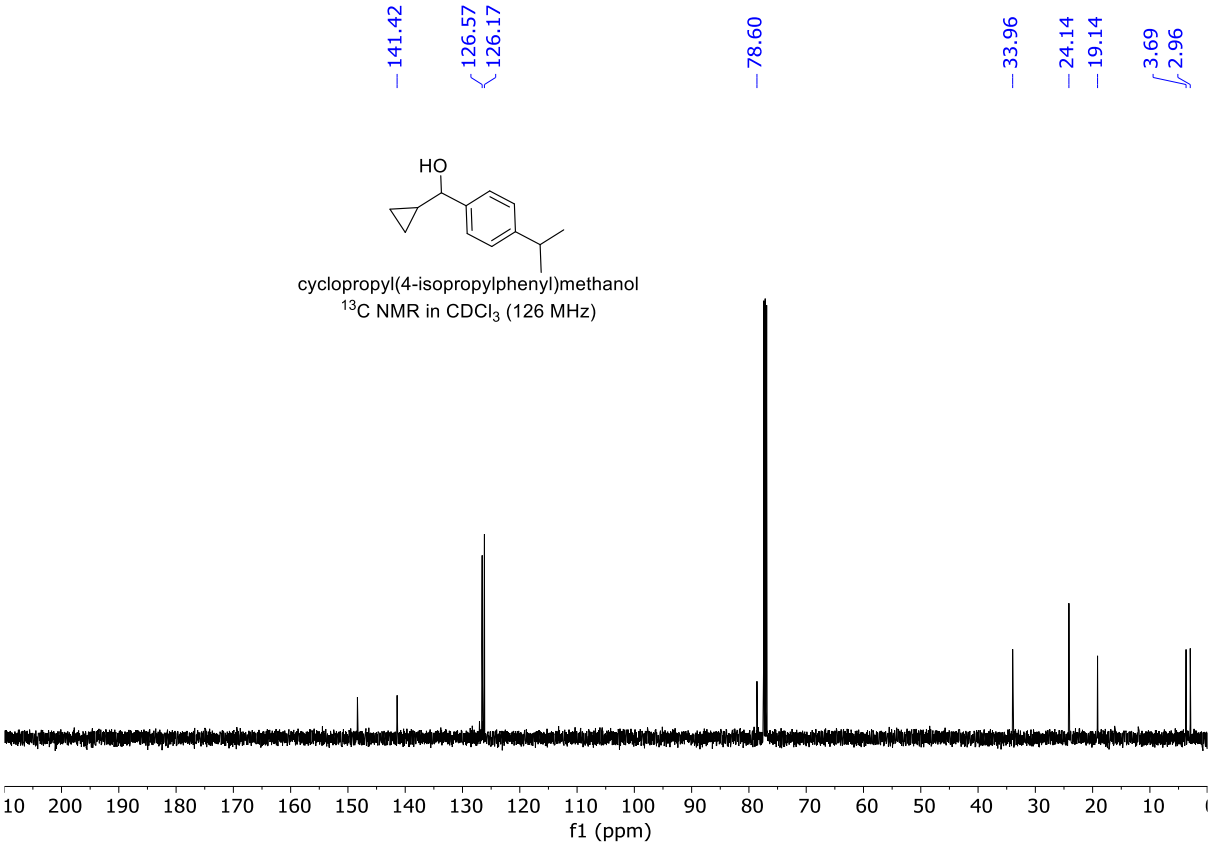


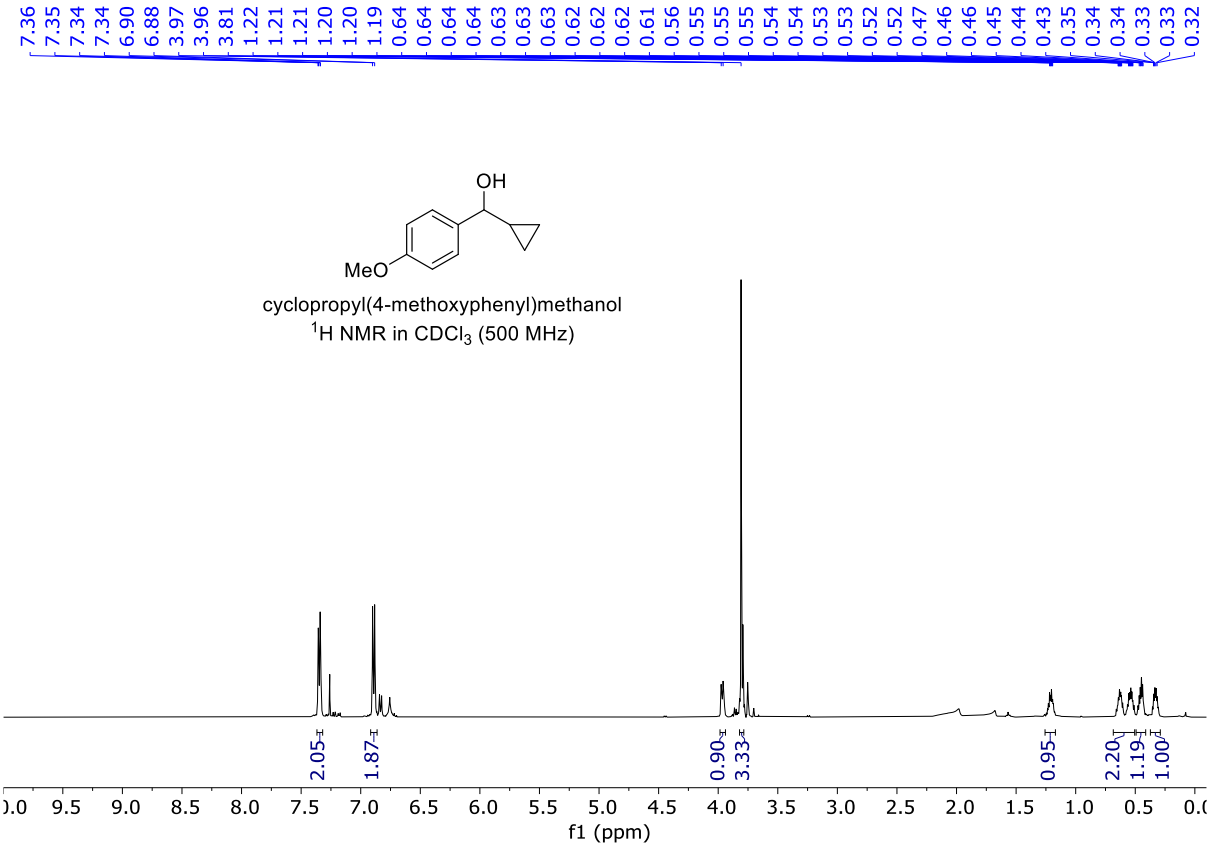
cyclopropyl(3,4-dichlorophenyl)methanol
13C NMR in $CDCl_3$ (126 MHz)

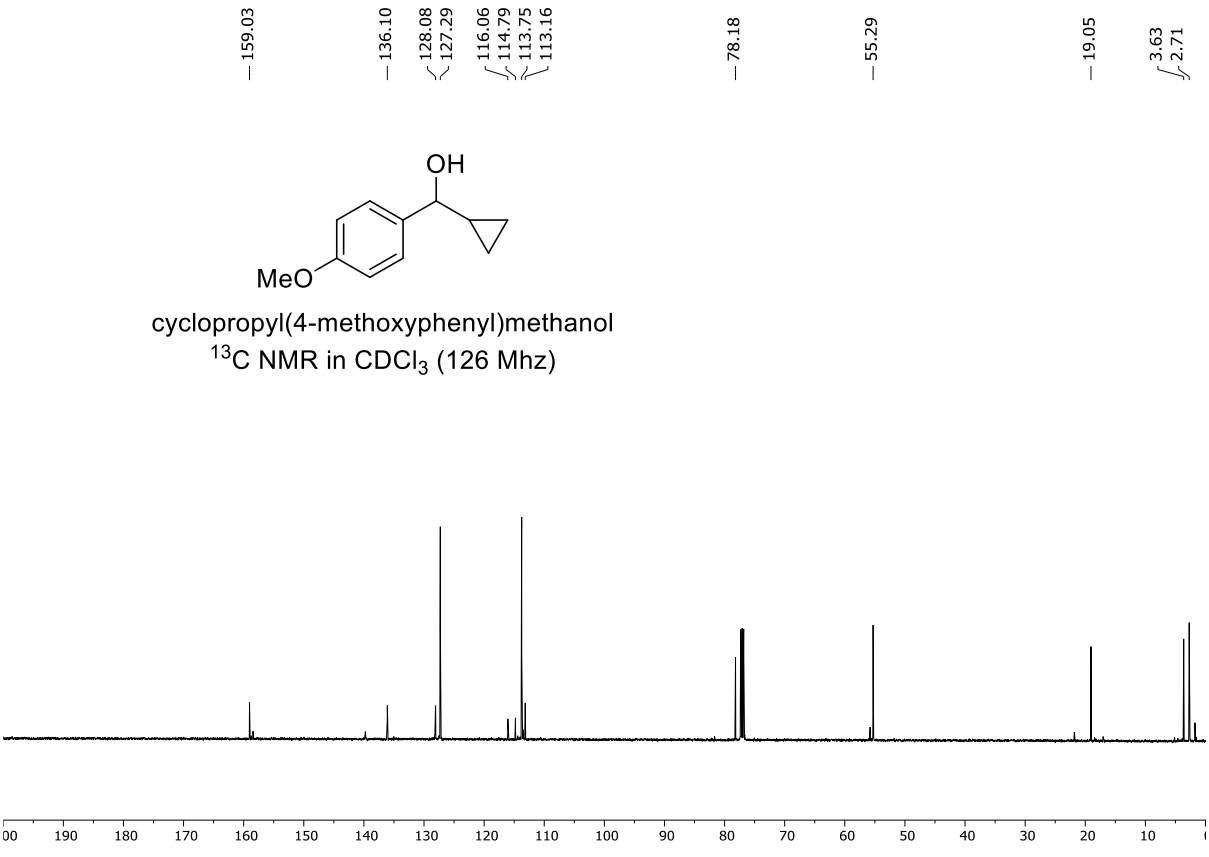

2.83 2.82 1.62 1.62 1.61 1.60 1.59 1.59 1.58 1.58 1.56 1.56 1.55 1.54 1.53 1.53 1.51 1.36 1.34 1.32 1.31 1.29 1.29 1.28 1.27 1.26 1.25 0.91 0.90 0.90 0.89 0.88 0.88 0.53 0.52 0.51 0.50 0.49 0.48 0.48 0.27 0.25 0.24 0.24 0.23 0.22 0.22 0.21
OH
1-cyclopropyl-4-methylpentan-1-ol
1H NMR in CDCl3 (400 MHz)
1.00 4.14 2.09 6.02 2.07 2.14
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
f1 (ppm)


35.22 34.98 28.30 22.81 22.67 18.17 2.95 2.54
OH
1-cyclopropyl-4-methylpentan-1-ol
13C NMR in CDCl3 (101 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.37 7.35 7.23 7.23 7.22 7.22 3.99 3.98 2.93 2.91 2.90 1.27 1.25 0.65 0.65 0.64 0.64 0.64 0.63 0.63 0.63 0.63 0.62 0.61 0.58 0.57 0.57 0.57 0.56 0.56 0.56 0.55 0.49 0.48 0.48 0.47 0.46 0.46 0.39 0.39 0.38 0.38 0.37 0.37 0.36 0.36 0.35
HO
cyclopropyl(4-isopropylphenyl)methanol
^{1}H NMR in $CDCl_3$ (500 MHz)
1.83 1.93 0.91 1.00 6.00 0.99 0.99 0.96 0.96
f1 (ppm)


141.42 126.57 126.17 78.60 33.96 24.14 19.14 3.69 2.96
HO
cyclopropyl(4-isopropylphenyl)methanol
^{13}C NMR in $CDCl_3$ (126 MHz)
f1 (ppm)


7.36 7.35 7.34 7.34 6.90 6.88 3.97 3.96 3.81 1.22 1.21 1.21 1.20 1.20 1.19 0.64 0.64 0.64 0.64 0.63 0.63 0.63 0.62 0.62 0.62 0.61 0.56 0.55 0.55 0.55 0.54 0.54 0.53 0.53 0.52 0.52 0.47 0.46 0.46 0.45 0.44 0.43 0.35 0.34 0.34 0.33 0.33 0.32
OH
MeO
cyclopropyl(4-methoxyphenyl)methanol
1H NMR in CDCl3 (500 MHz)
2.05
1.87
0.90
3.33
0.95
2.20
1.19
1.00
f1 (ppm)


159.03
136.10
128.08
127.29
116.06
114.79
113.75
113.16
78.18
55.29
19.05
3.63
2.71
OH
MeO
cyclopropyl(4-methoxyphenyl)methanol
13C NMR in CDCl3 (126 Mhz)


7.37
7.36
7.28
7.26
4.01
3.99
2.50
1.23
1.22
1.21
1.21
1.20
1.19
1.19
0.67
0.67
0.66
0.66
0.66
0.65
0.65
0.65
0.64
0.64
0.64
0.63
0.63
0.60
0.59
0.59
0.58
0.58
0.57
0.57
0.56
0.55
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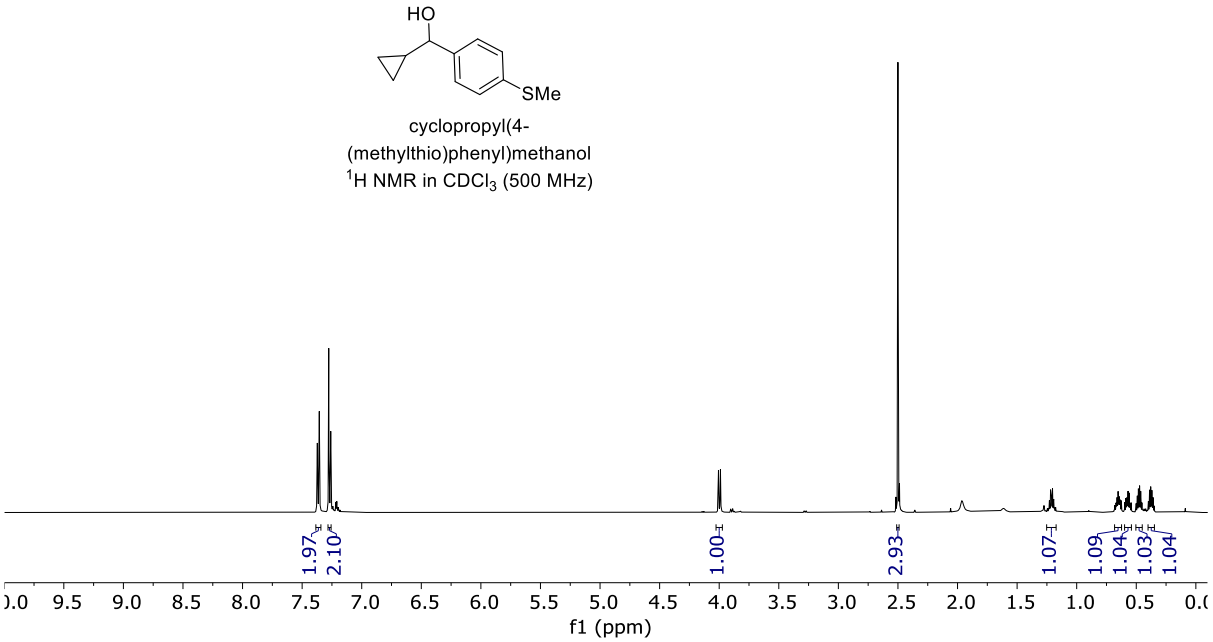
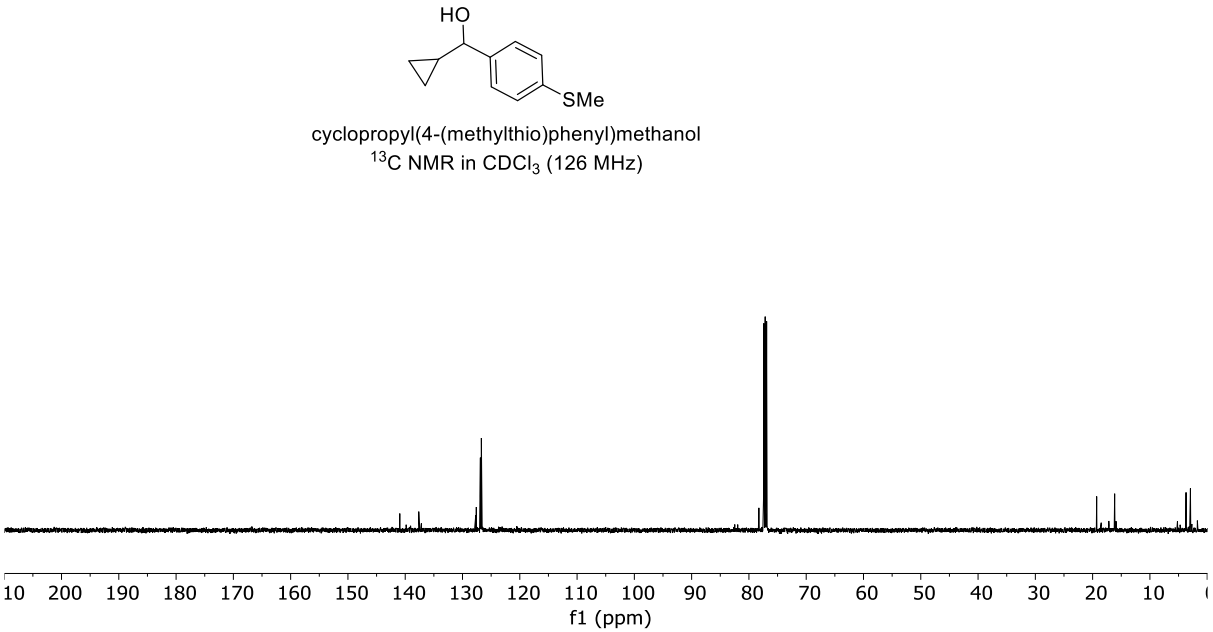
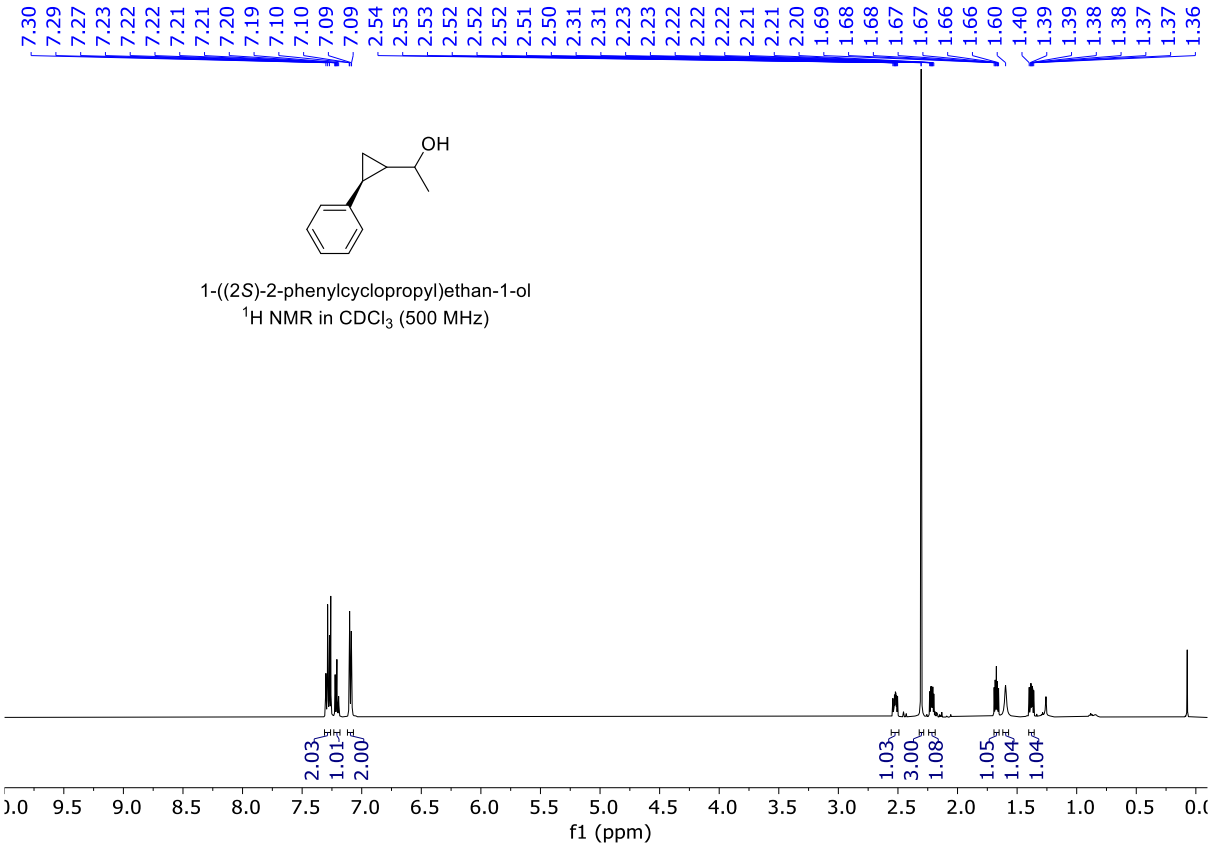
0.45
0.40
0.39
0.38
0.37
0.36

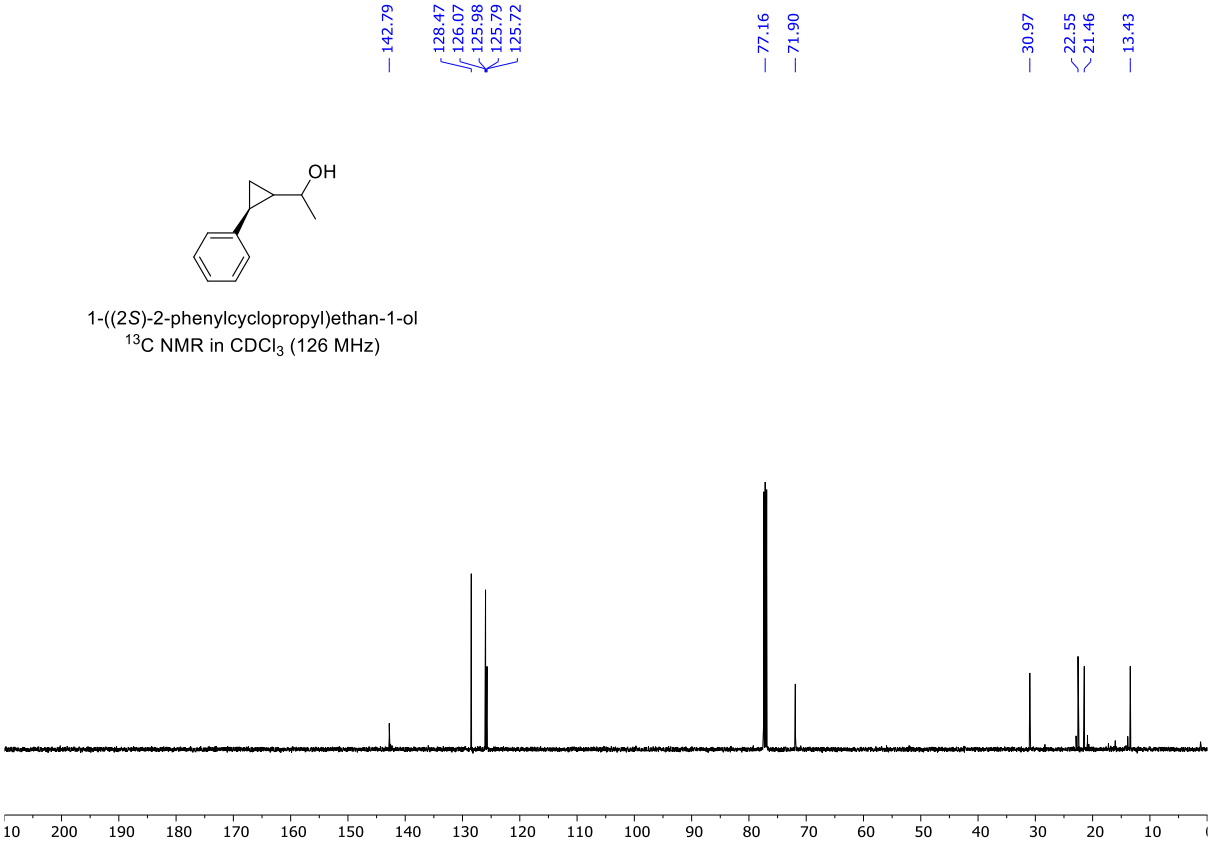

HO
SMe
cyclopropyl(4-
(methylthio)phenyl)methanol
1H NMR in CDCl3 (500 MHz)
1.97
2.10
1.00
2.93
1.07
1.09
1.04
1.03
1.04
f1 (ppm)


140.95
137.64
127.69
127.59
126.88
126.71
78.26
19.29
16.15
3.69
2.93

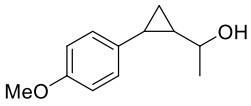

HO
SMe
cyclopropyl(4-(methylthio)phenyl)methanol
13C NMR in CDCl3 (126 MHz)
f1 (ppm)



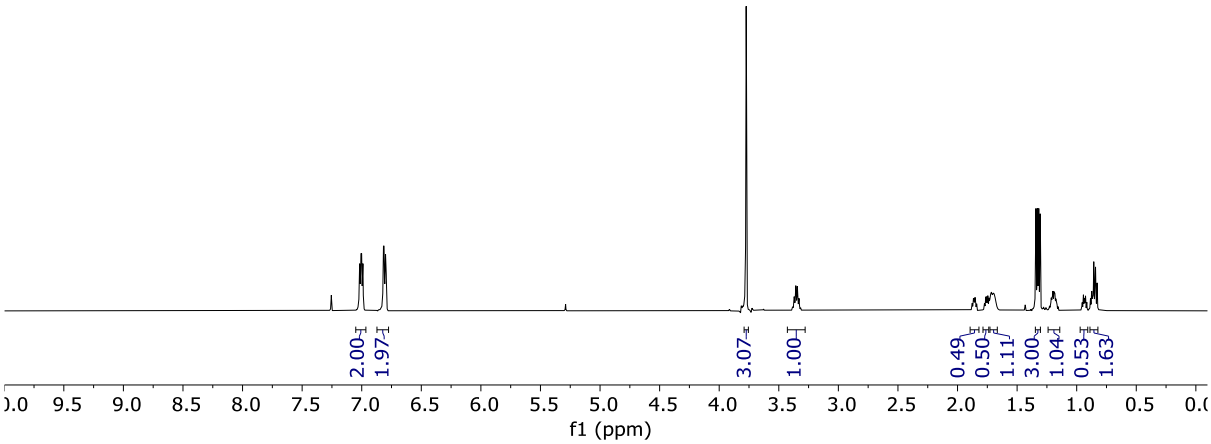
1-((2*S*)-2-phenylcyclopropyl)ethan-1-ol
^{1}H NMR in $CDCl_3$ (500 MHz)

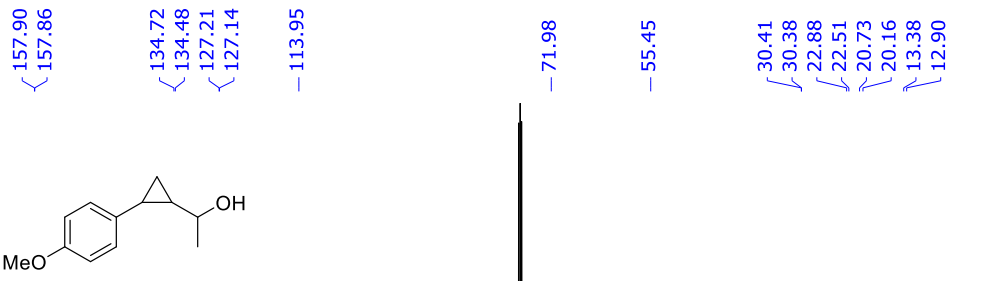


1-((2*S*)-2-phenylcyclopropyl)ethan-1-ol
^{13}C NMR in $CDCl_3$ (126 MHz)

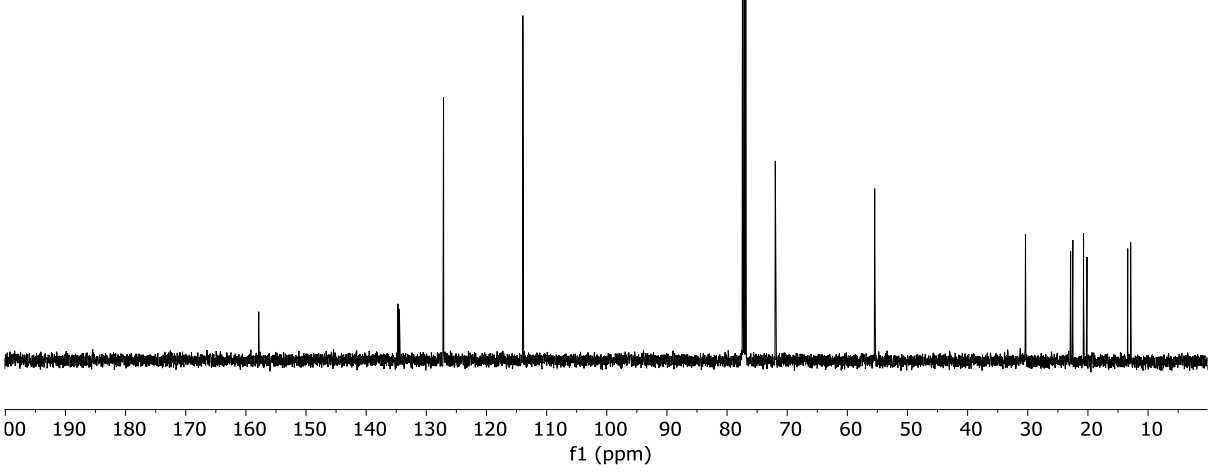


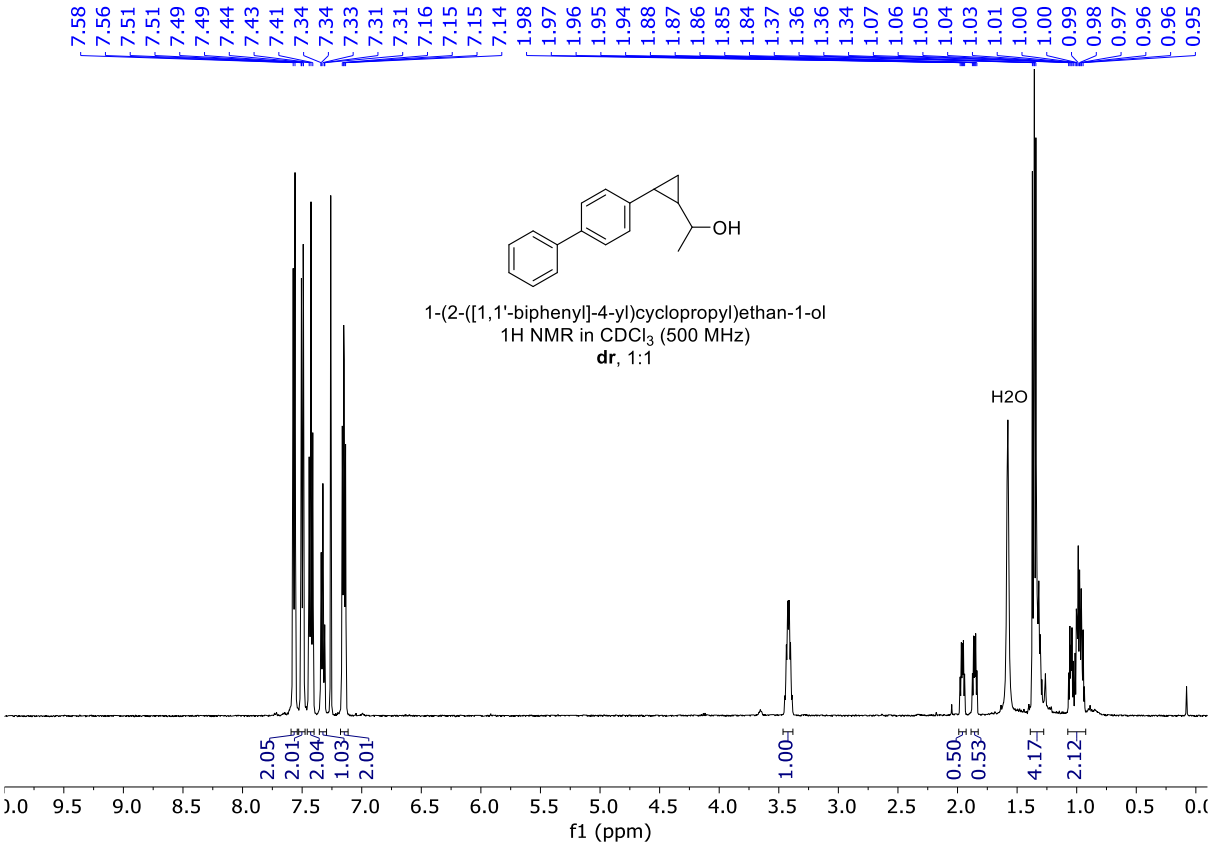
1-(2-(4-methoxyphenyl)cyclopropyl)ethan-1-ol
1H NMR in $CDCl_3$ (500 MHz)
dr, 1:1

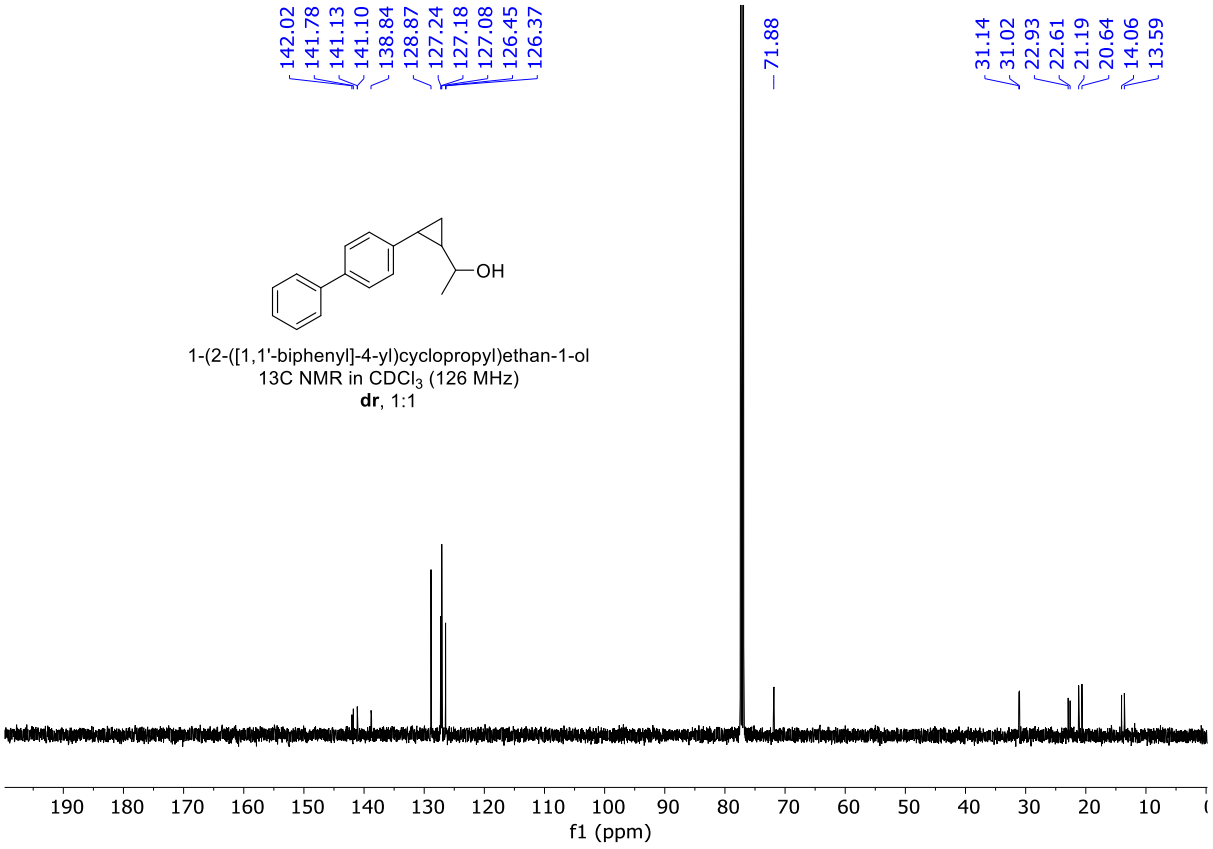


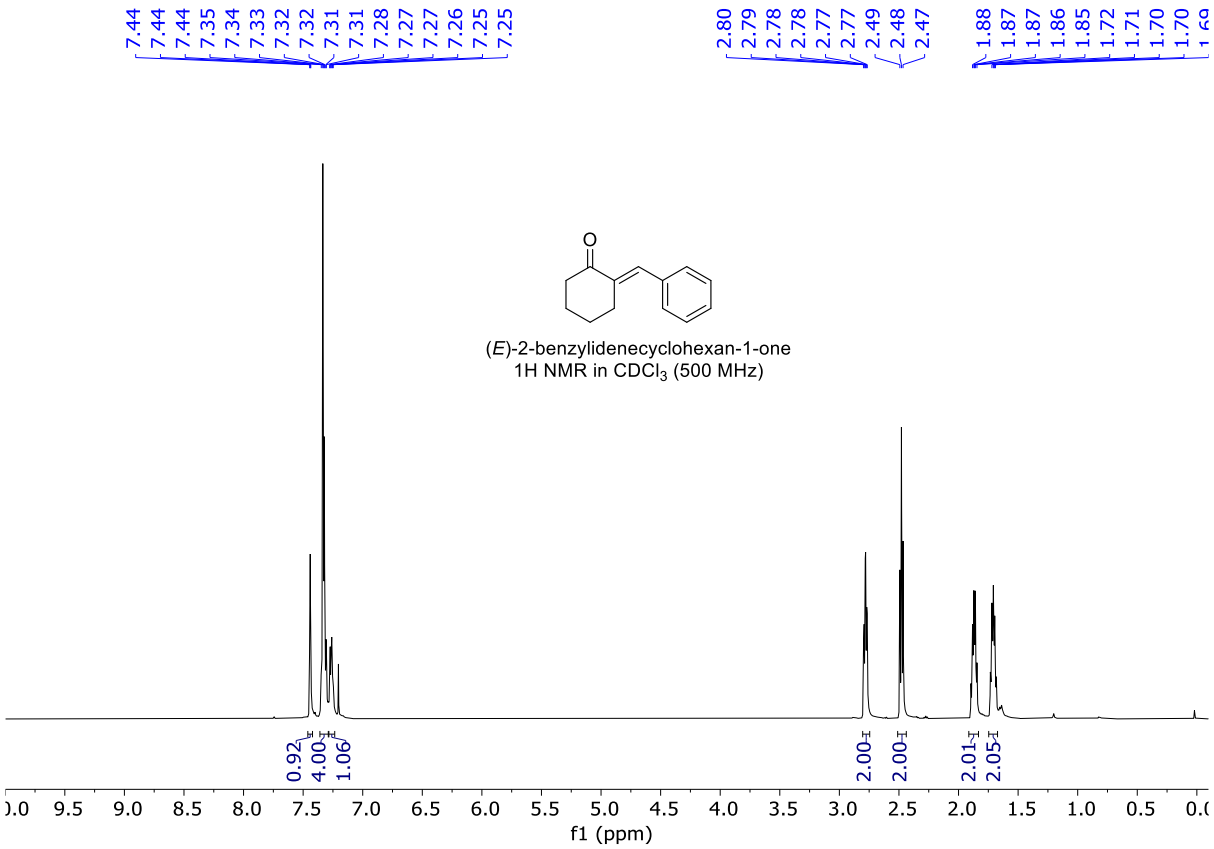


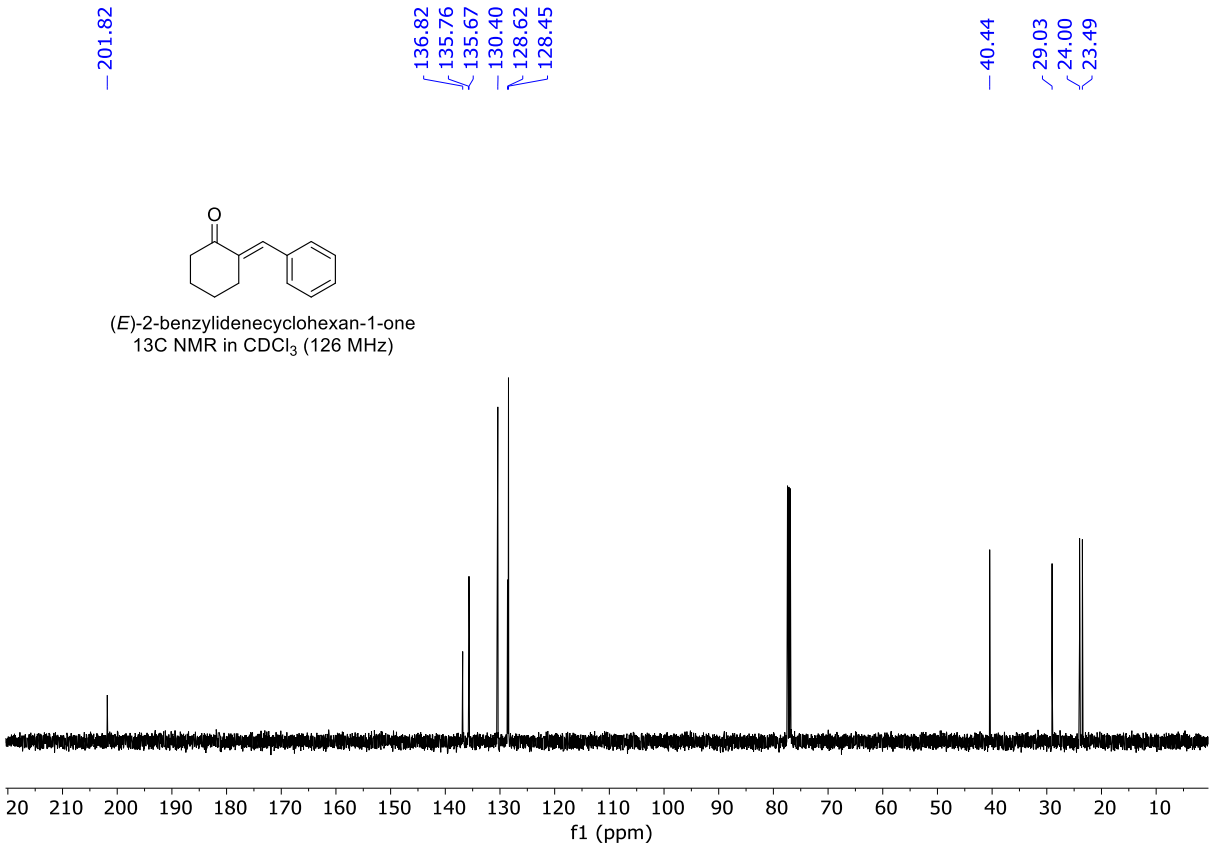
1-(2-(4-methoxyphenyl)cyclopropyl)ethan-1-ol
13C NMR in $CDCl_3$ (126 MHz)
dr, 1:1

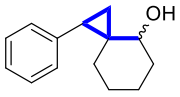



7.58 7.56 7.51 7.51 7.49 7.49 7.44 7.43 7.41 7.34 7.34 7.33 7.31 7.31 7.16 7.15 7.15 7.14
1.98 1.97 1.96 1.95 1.94 1.88 1.87 1.86 1.85 1.84 1.37 1.36 1.36 1.34 1.07 1.06 1.05 1.04 1.03 1.01 1.00 1.00 0.99 0.98 0.97 0.96 0.96 0.95
OH
1-(2-([1,1'-biphenyl]-4-yl)cyclopropyl)ethan-1-ol
1H NMR in CDCl3 (500 MHz)
dr, 1:1
H2O
2.05 2.01 2.04 1.03 2.01
1.00
0.50 0.53 4.17 2.12
f1 (ppm)

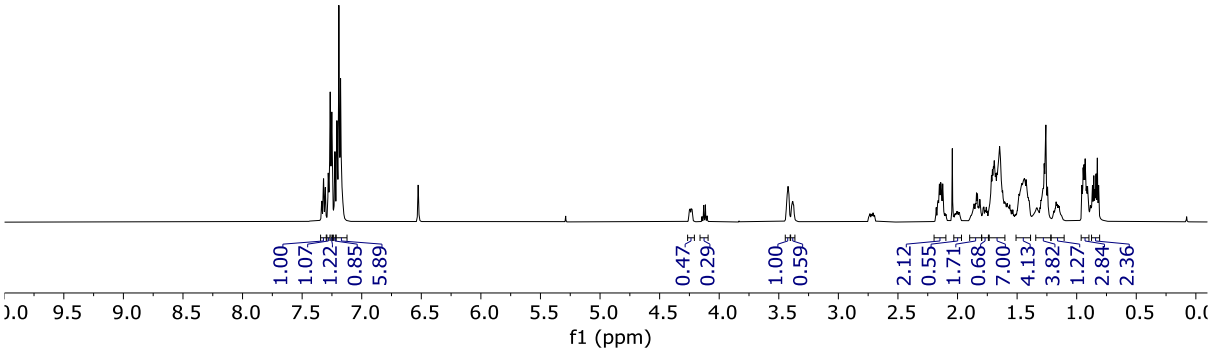

142.02 141.78 141.13 141.10 138.84 128.87 127.24 127.18 127.08 126.45 126.37
71.88
31.14 31.02 22.93 22.61 21.19 20.64 14.06 13.59
OH
1-(2-([1,1'-biphenyl]-4-yl)cyclopropyl)ethan-1-ol
13C NMR in CDCl3 (126 MHz)
dr, 1:1
f1 (ppm)

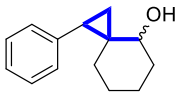

7.44
7.44
7.44
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.28
7.27
7.27
7.26
7.25
7.25
2.80
2.79
2.78
2.78
2.77
2.77
2.49
2.48
2.47
1.88
1.87
1.87
1.86
1.85
1.72
1.71
1.70
1.70
O
(E)-2-benzylidenecyclohexan-1-one
1H NMR in CDCl3 (500 MHz)
0.92
4.00
1.06
2.00
2.00
2.01
2.05
f1 (ppm)


201.82
136.82
135.76
135.67
130.40
128.62
128.45
40.44
29.03
24.00
23.49
O
(E)-2-benzylidenecyclohexan-1-one
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

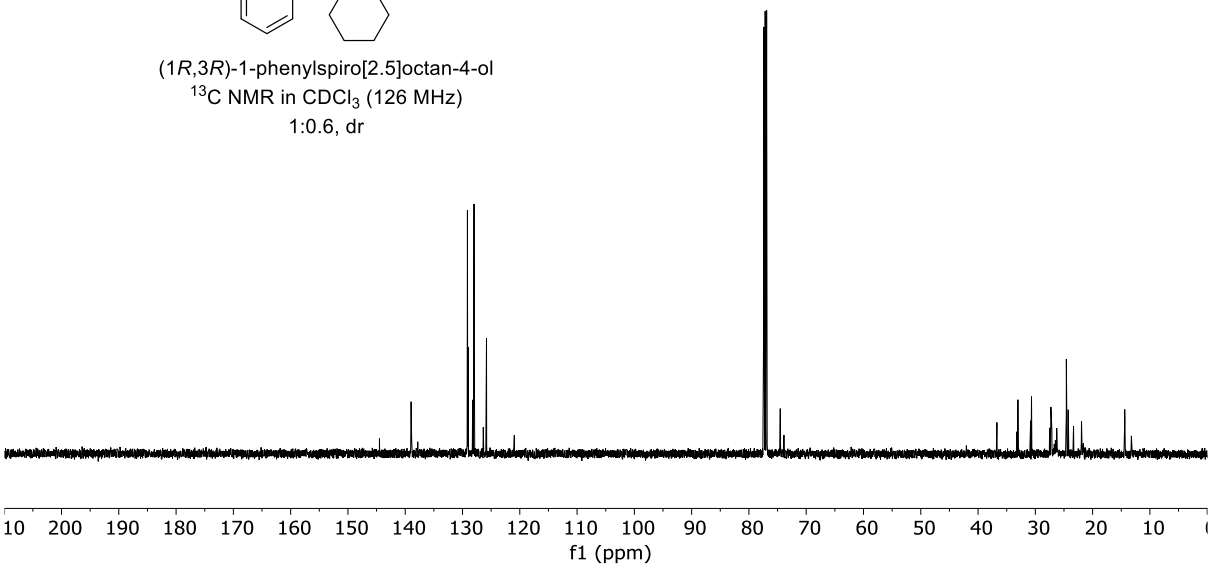


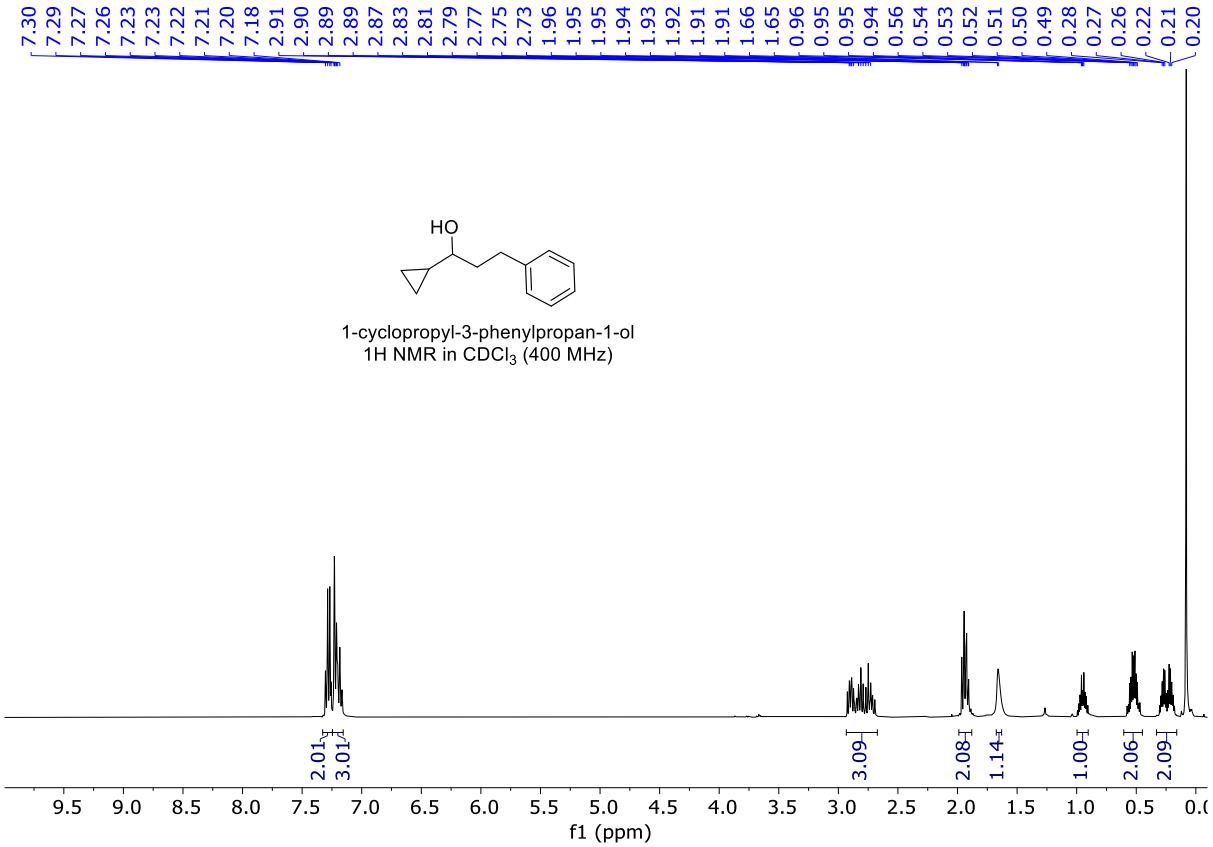
(1*R*,3*R*)-1-phenylspiro[2.5]octan-4-ol
^{1}H NMR in $CDCl_3$ (500 MHz)
1:0.6, dr



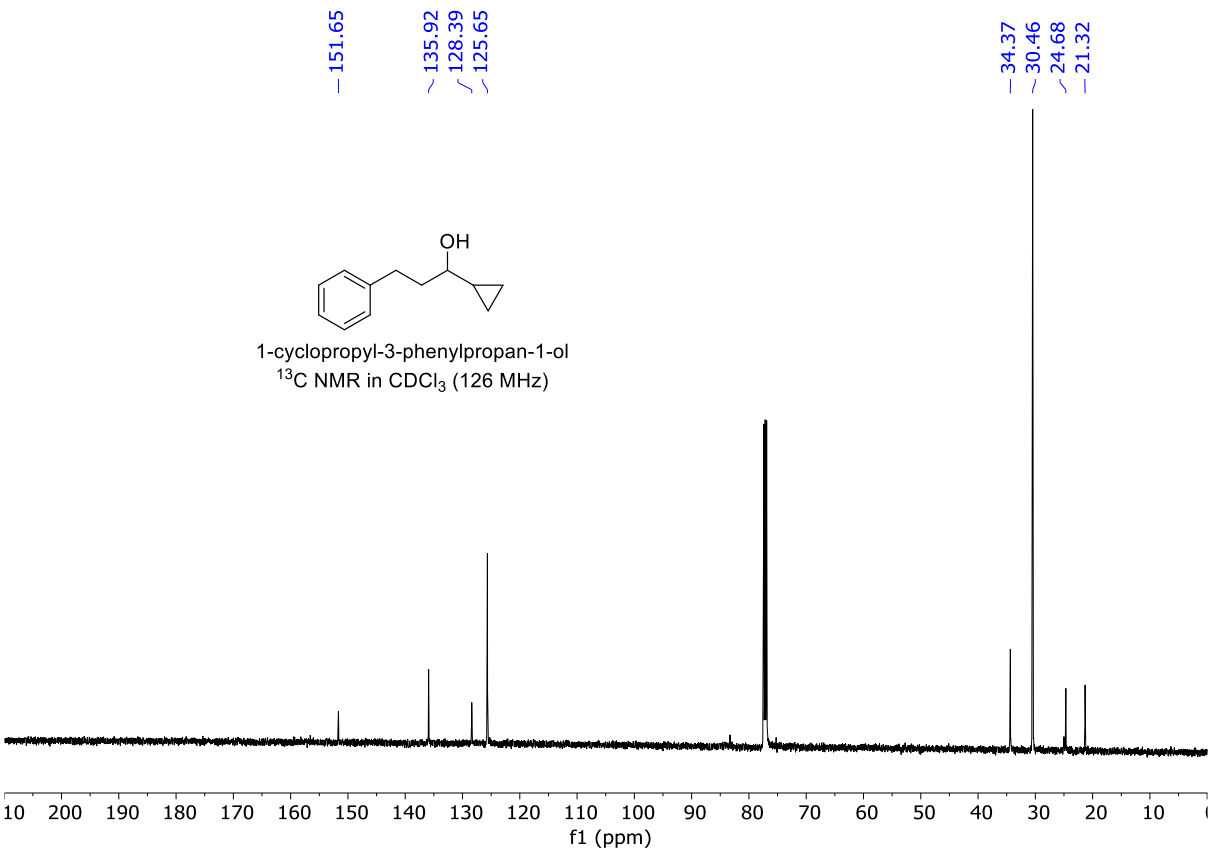


(1*R*,3*R*)-1-phenylspiro[2.5]octan-4-ol
^{13}C NMR in $CDCl_3$ (126 MHz)
1:0.6, dr

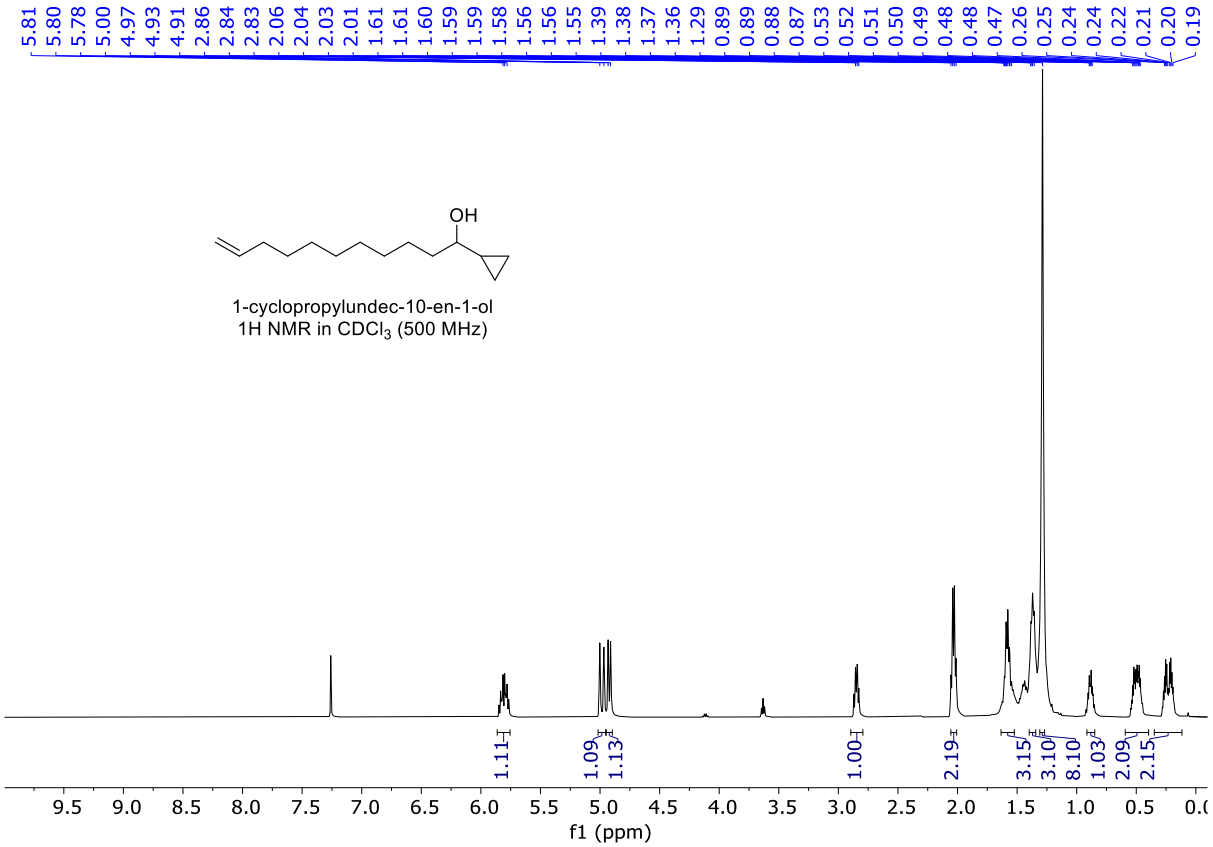


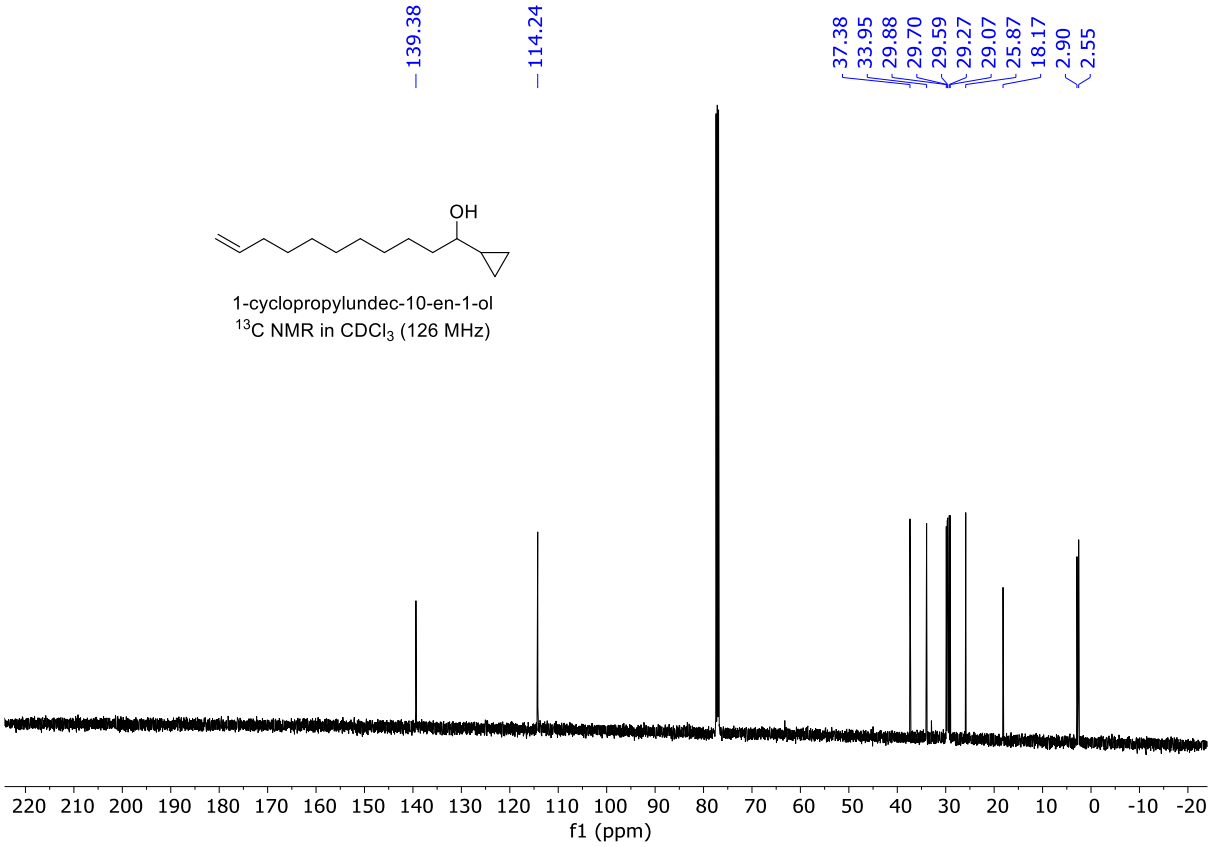


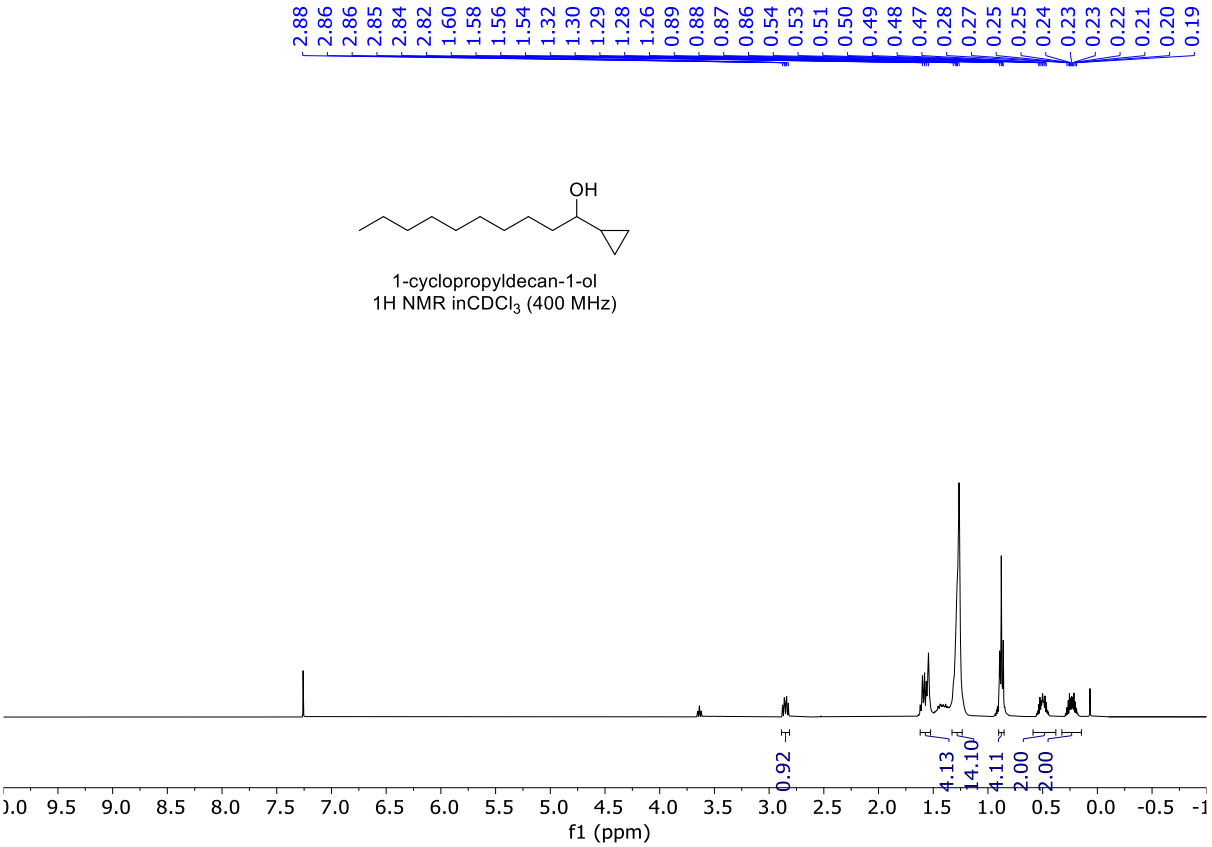
1-cyclopropyl-3-phenylpropan-1-ol
1H NMR in $CDCl_3$ (400 MHz)

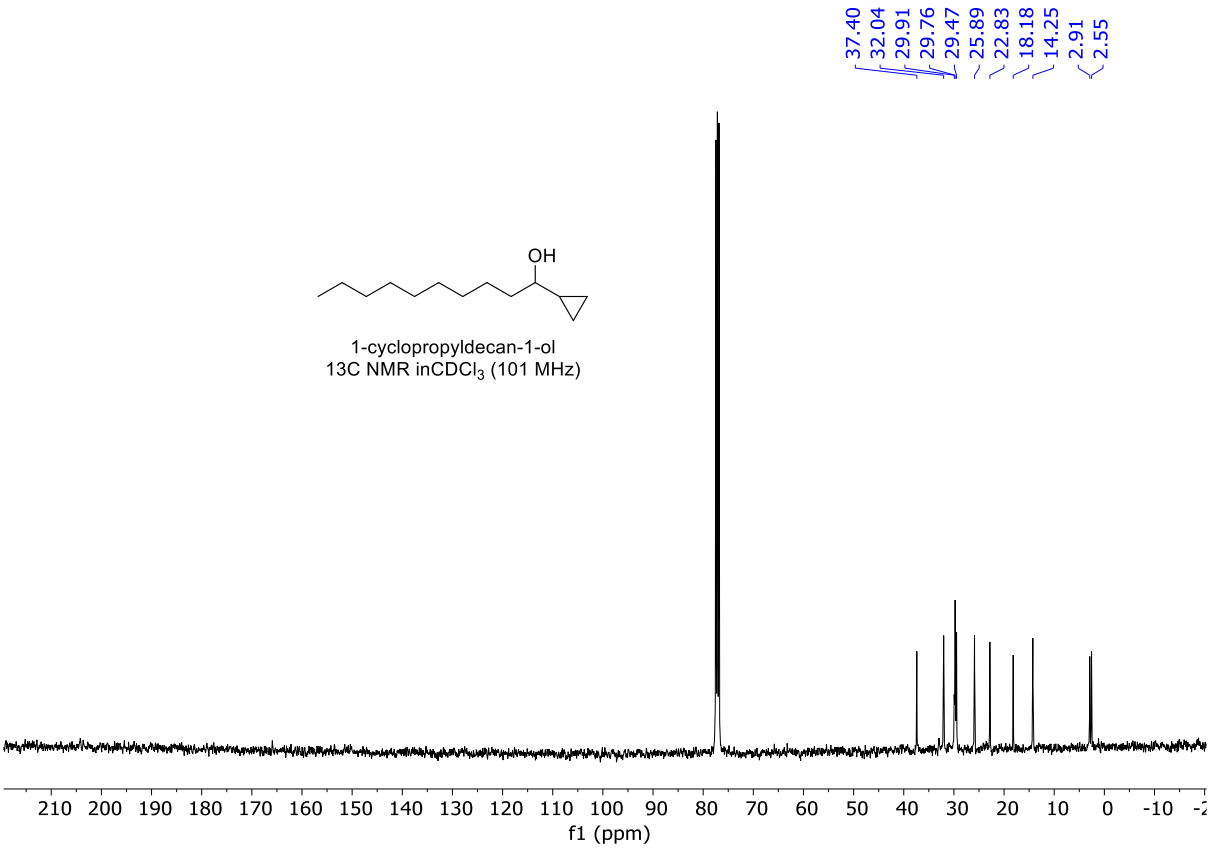


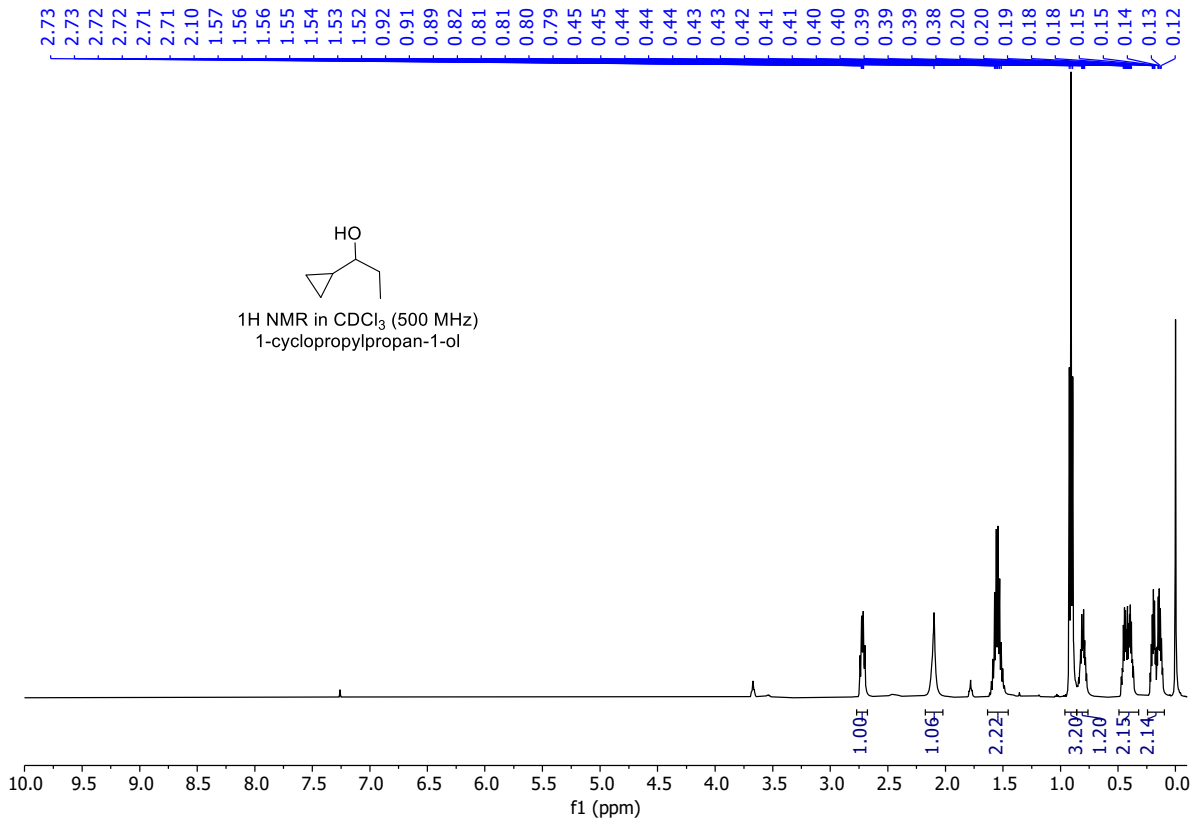
1-cyclopropyl-3-phenylpropan-1-ol
^{13}C NMR in $CDCl_3$ (126 MHz)

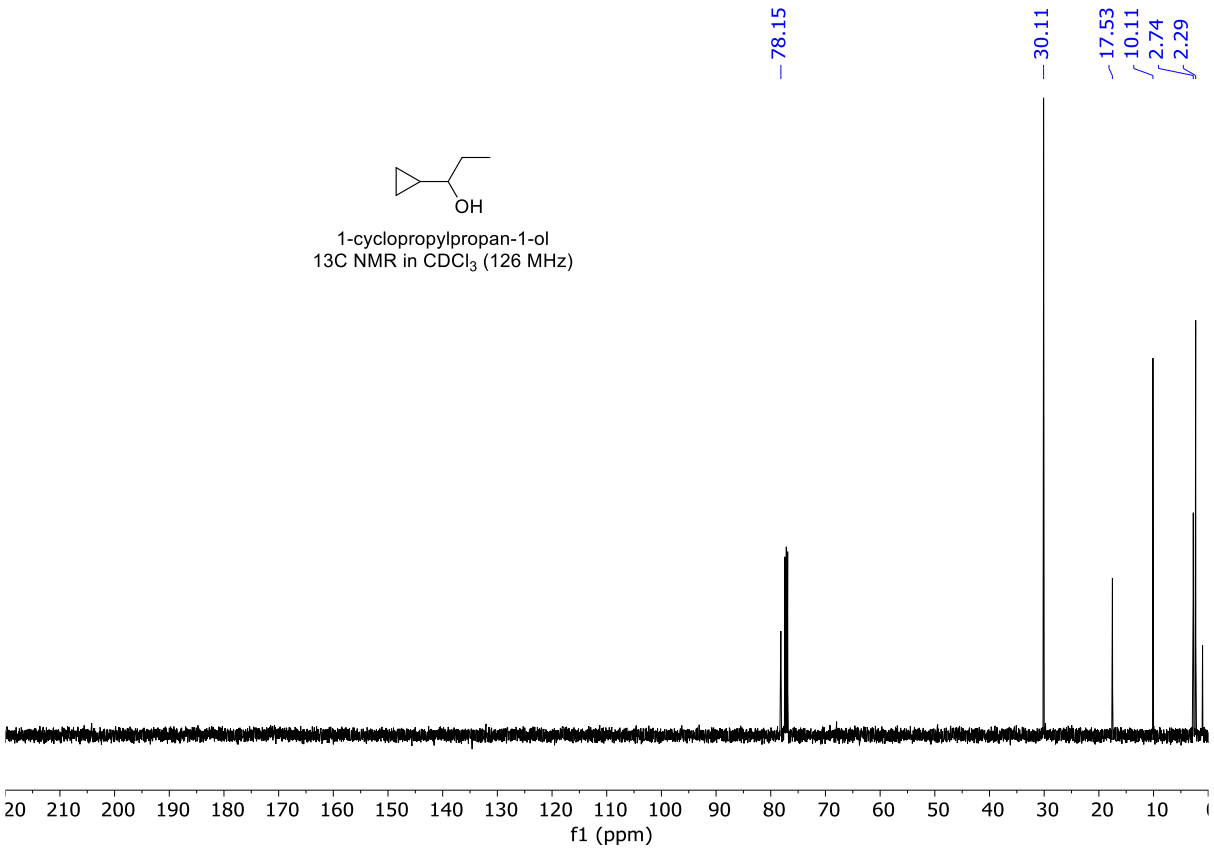

5.81 5.80 5.78 5.00 4.97 4.93 4.91 2.86 2.84 2.83 2.06 2.04 2.03 2.01 1.61 1.61 1.60 1.59 1.59 1.58 1.56 1.56 1.55 1.39 1.38 1.37 1.36 1.29 0.89 0.89 0.88 0.87 0.53 0.52 0.51 0.50 0.49 0.48 0.48 0.47 0.26 0.25 0.24 0.24 0.22 0.21 0.20 0.19
OH
1-cyclopropylundec-10-en-1-ol
1H NMR in CDCl3 (500 MHz)
1.11 1.09 1.13 1.00 2.19 3.15 3.10 8.10 1.03 2.09 2.15
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
f1 (ppm)

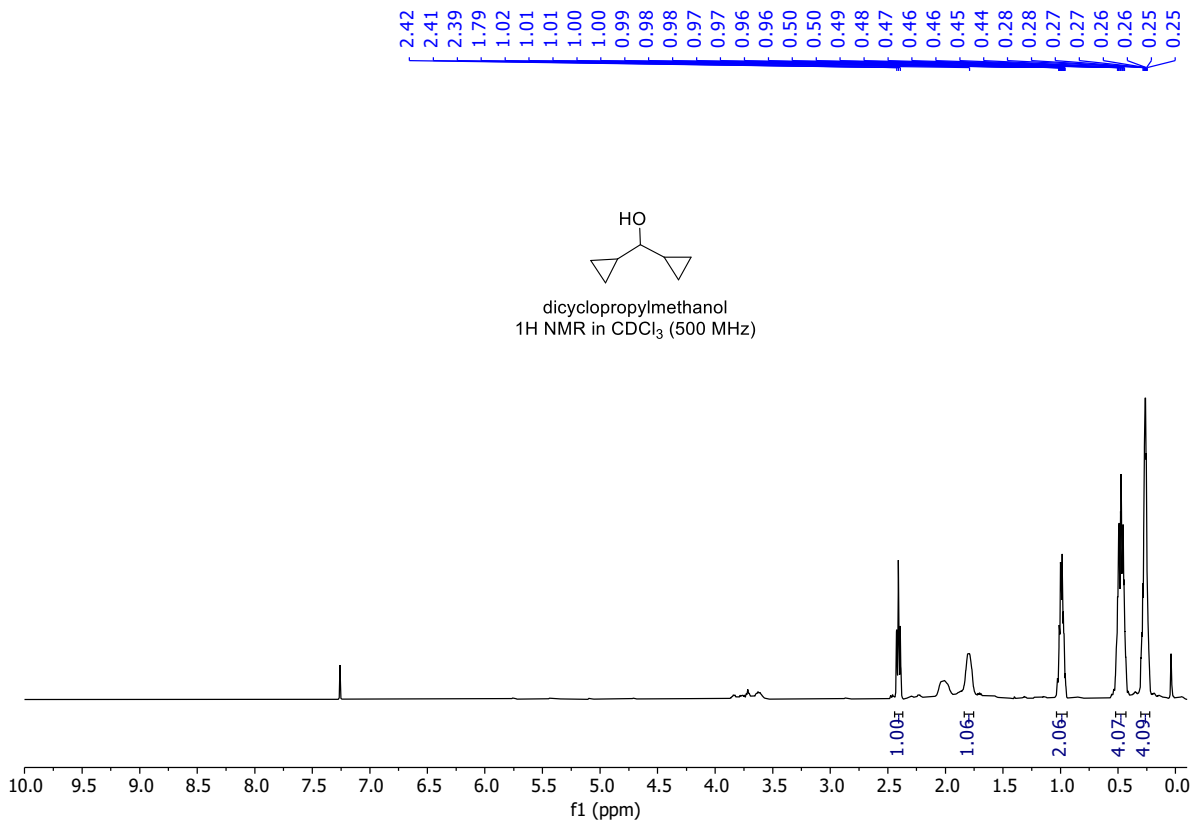

139.38 114.24
37.38 33.95 29.88 29.70 29.59 29.27 29.07 25.87 18.17 2.90 2.55
OH
1-cyclopropylundec-10-en-1-ol
13C NMR in CDCl3 (126 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

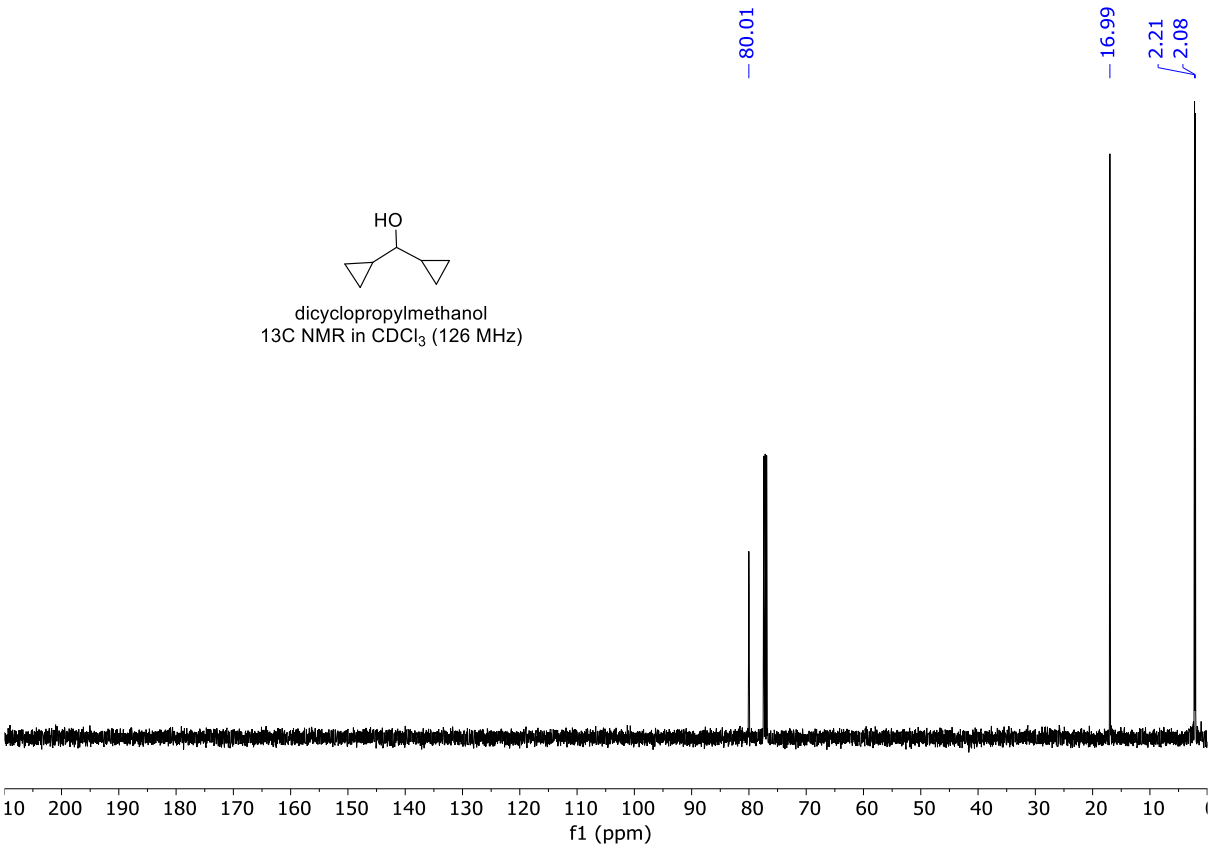

2.88
2.86
2.86
2.85
2.84
2.82
1.60
1.58
1.56
1.54
1.32
1.30
1.29
1.28
1.26
0.89
0.88
0.87
0.86
0.54
0.53
0.51
0.50
0.49
0.48
0.47
0.28
0.27
0.25
0.25
0.24
0.23
0.23
0.22
0.21
0.20
0.19
OH
1-cyclopropyldecan-1-ol
1H NMR inCDCl3 (400 MHz)
0.92
4.13
14.10
4.11
2.00
2.00
f1 (ppm)

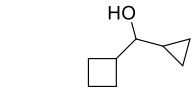

37.40
32.04
29.91
29.76
29.47
25.89
22.83
18.18
14.25
2.91
2.55
OH
1-cyclopropyldecan-1-ol
13C NMR inCDCl3 (101 MHz)
f1 (ppm)


2.73 2.73 2.72 2.72 2.71 2.71 2.10 1.57 1.56 1.56 1.55 1.54 1.53 1.52 0.92 0.91 0.89 0.82 0.81 0.81 0.80 0.79 0.45 0.45 0.44 0.44 0.44 0.43 0.43 0.42 0.41 0.41 0.40 0.40 0.39 0.39 0.39 0.38 0.20 0.20 0.19 0.18 0.18 0.15 0.15 0.14 0.13 0.12
HO
1H NMR in CDCl3 (500 MHz)
1-cyclopropylpropan-1-ol
1.00 1.06 2.22 3.20 1.20 2.15 2.14
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)

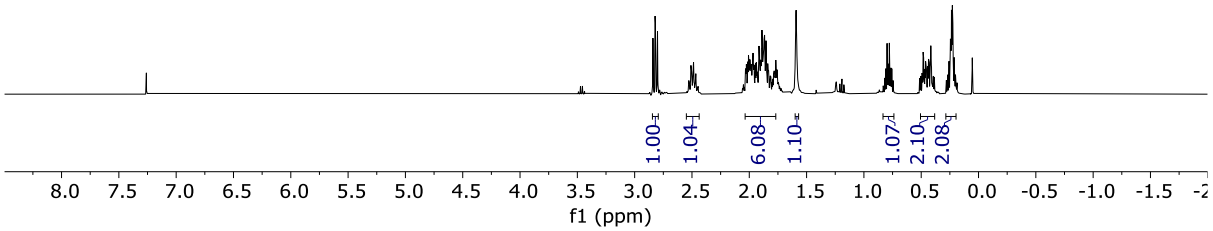

78.15
30.11
17.53
10.11
2.74
2.29
OH
1-cyclopropylpropan-1-ol
13C NMR in CDCl3 (126 MHz)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

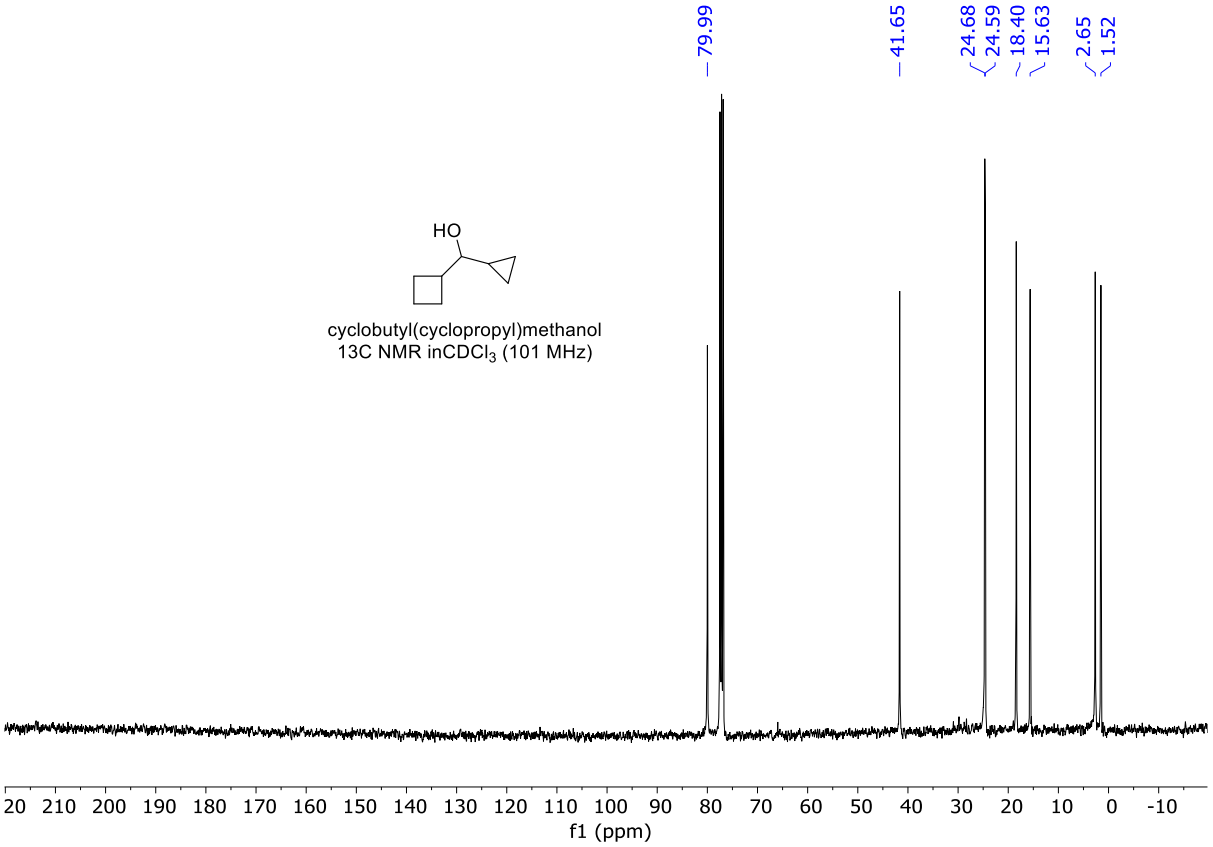

2.42 2.41 2.39 1.79 1.02 1.01 1.01 1.00 1.00 0.99 0.98 0.98 0.97 0.97 0.96 0.96 0.50 0.50 0.49 0.48 0.47 0.46 0.46 0.45 0.44 0.28 0.28 0.27 0.27 0.26 0.26 0.25 0.25
HO
dicyclopropylmethanol
1H NMR in CDCl3 (500 MHz)
1.00 1.06 2.06 4.07 4.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


80.01
16.99
2.21
2.08
HO
dicyclopropylmethanol
13C NMR in CDCl3 (126 MHz)
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

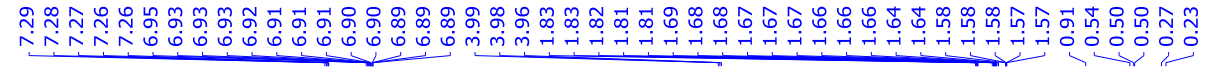


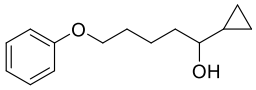
cyclobutyl(cyclopropyl)methanol
1H NMR in $CDCl_3$ (400 MHz)



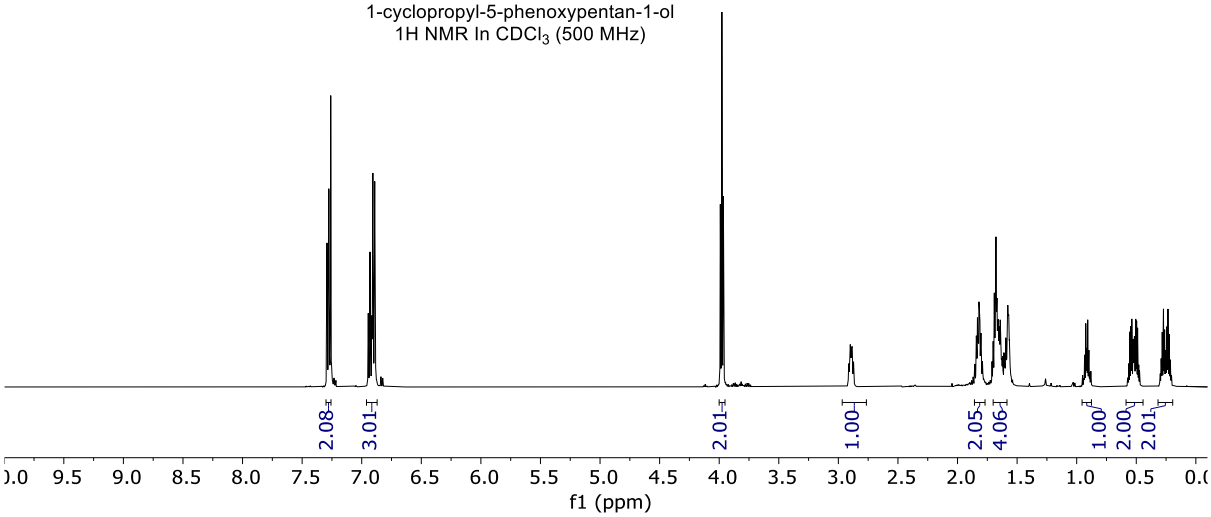


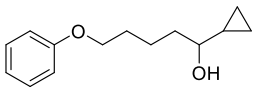
cyclobutyl(cyclopropyl)methanol
13C NMR in$CDCl_3$ (101 MHz)



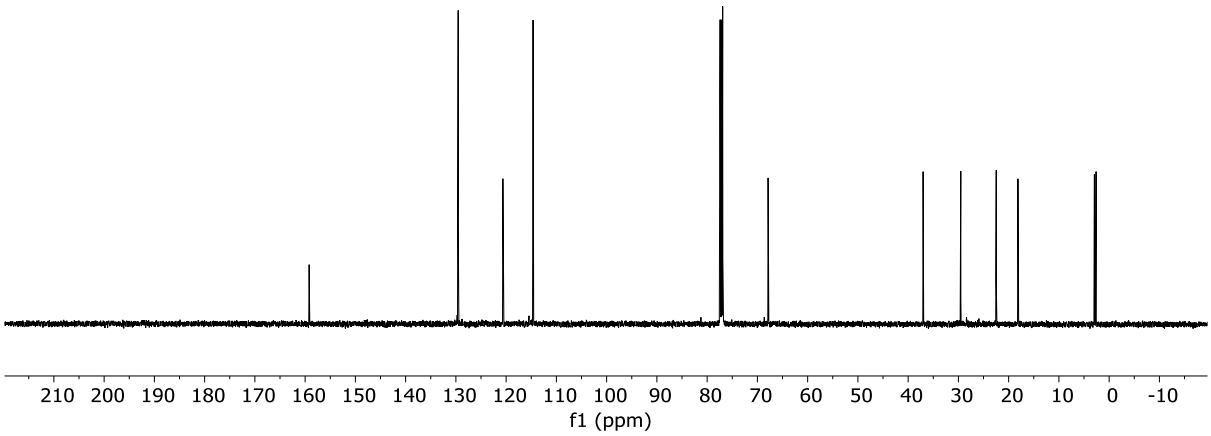


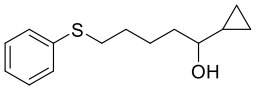
1-cyclopropyl-5-phenoxypentan-1-ol
1H NMR In $CDCl_3$ (500 MHz)



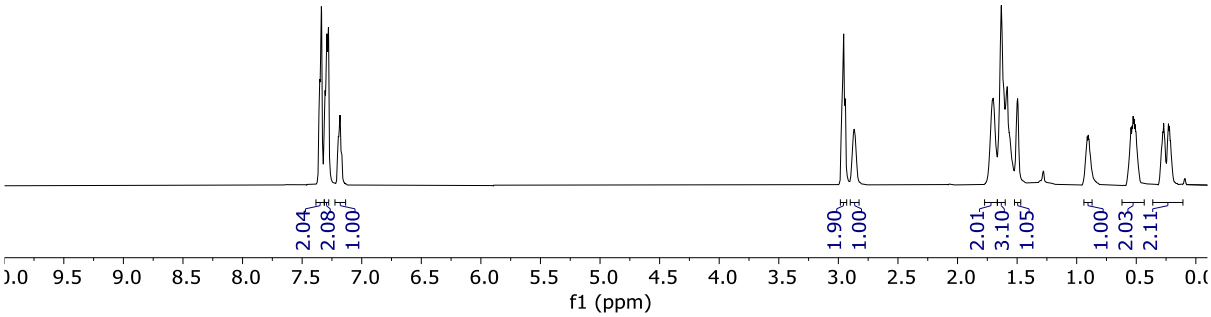


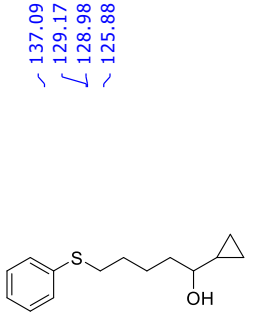
1-cyclopropyl-5-phenoxypentan-1-ol
13C NMR In $CDCl_3$ (126 MHz)



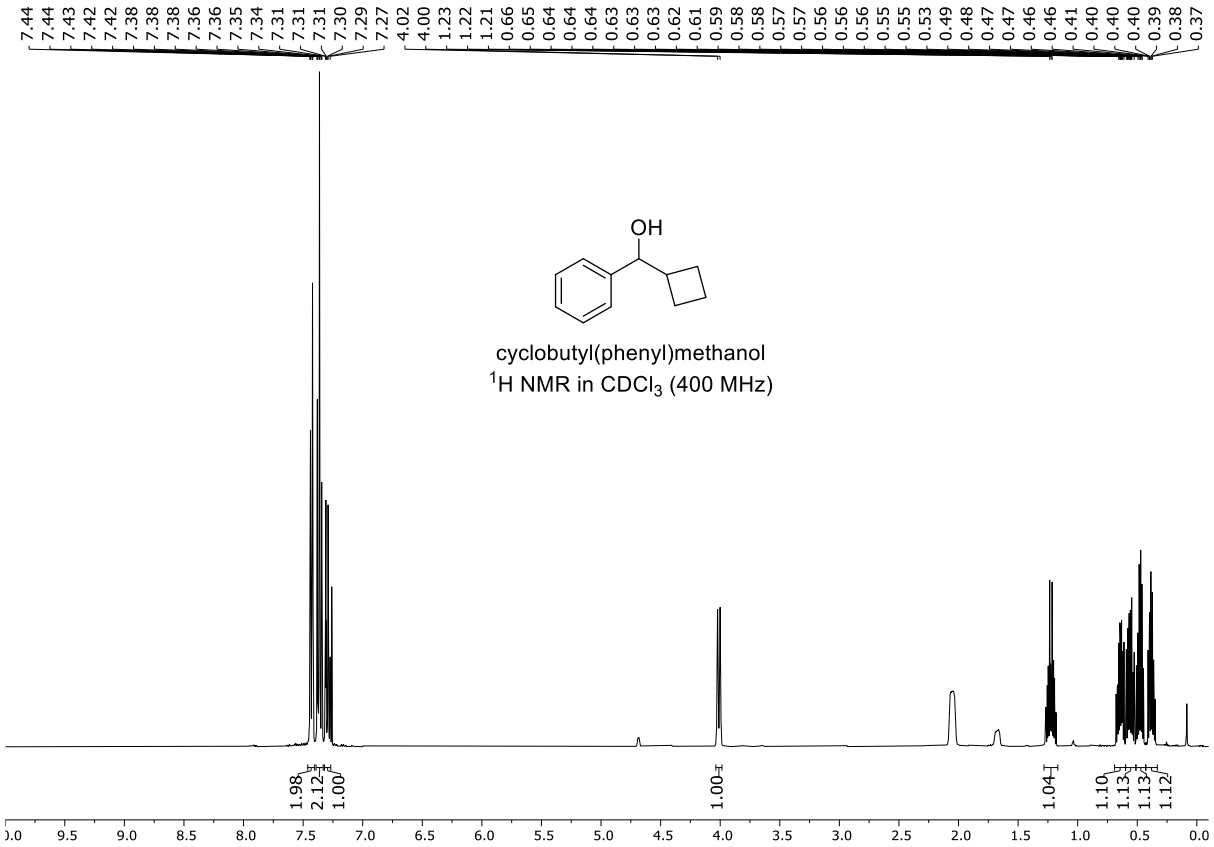


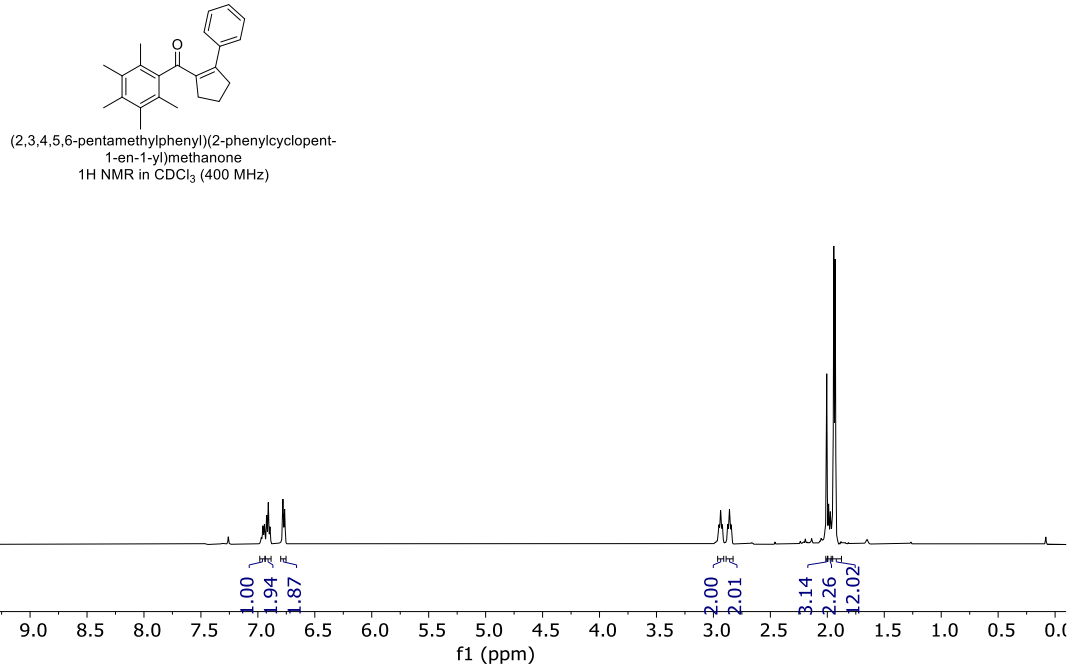
1-cyclopropyl-5-(phenylthio)pentan-1-ol
1H NMR in $CDCl_3$ (500 MHz)

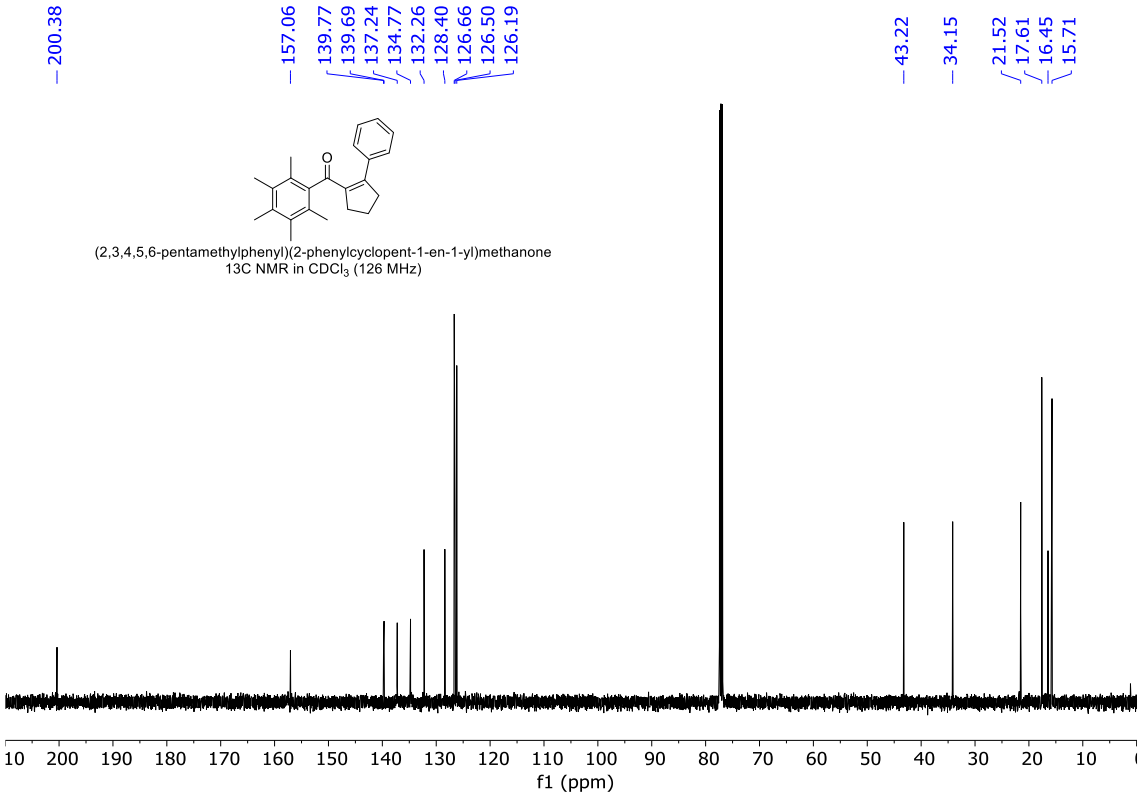


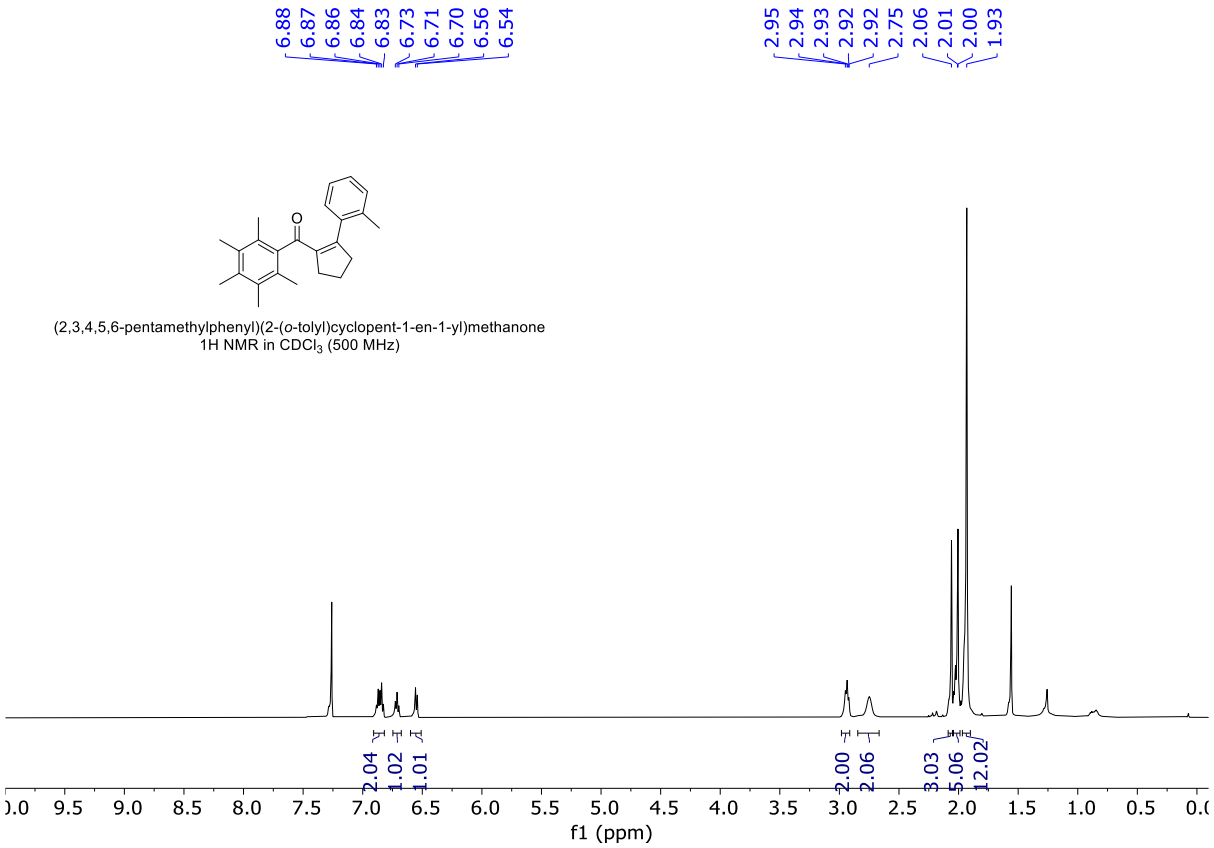


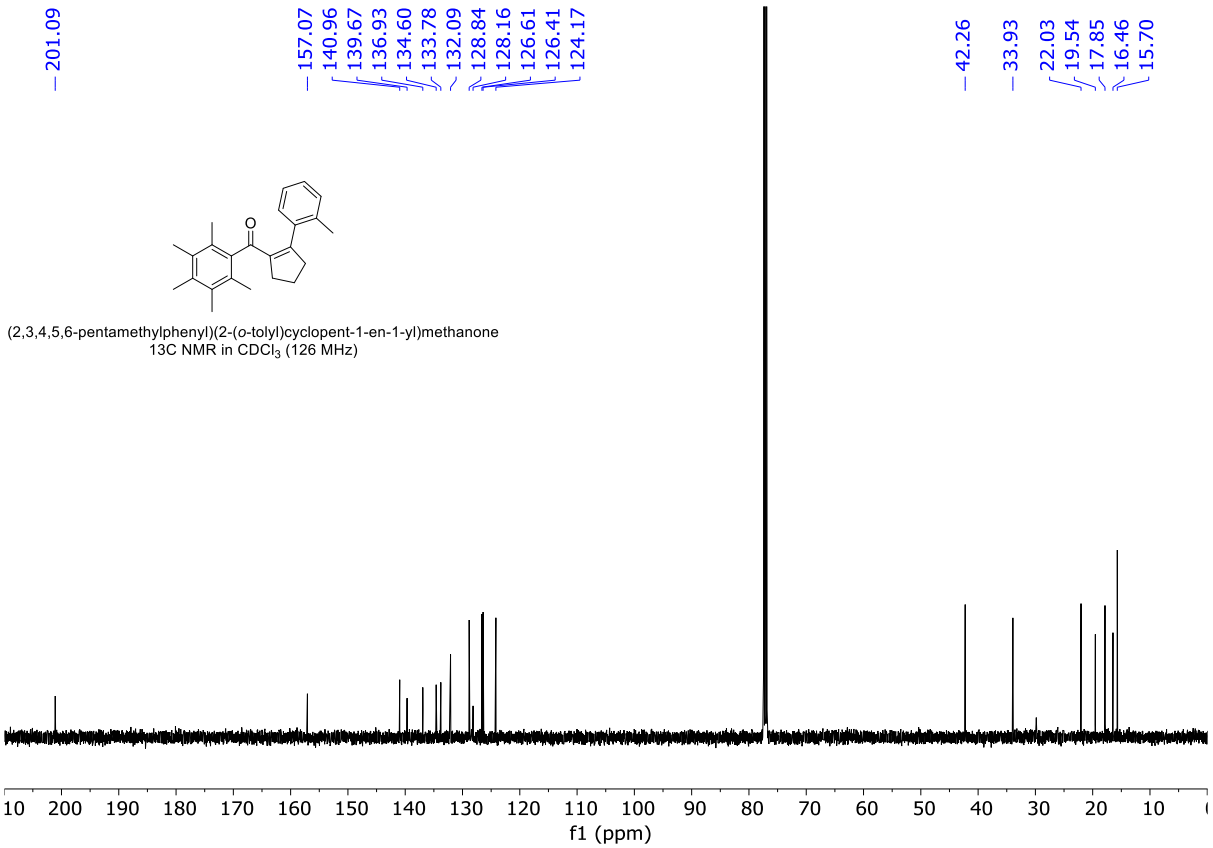
1-cyclopropyl-5-(phenylthio)pentan-1-ol
13C NMR in $CDCl_3$ (126 MHz)


OH
cyclobutyl(phenyl)methanol
1H NMR in CDCl3 (400 MHz)

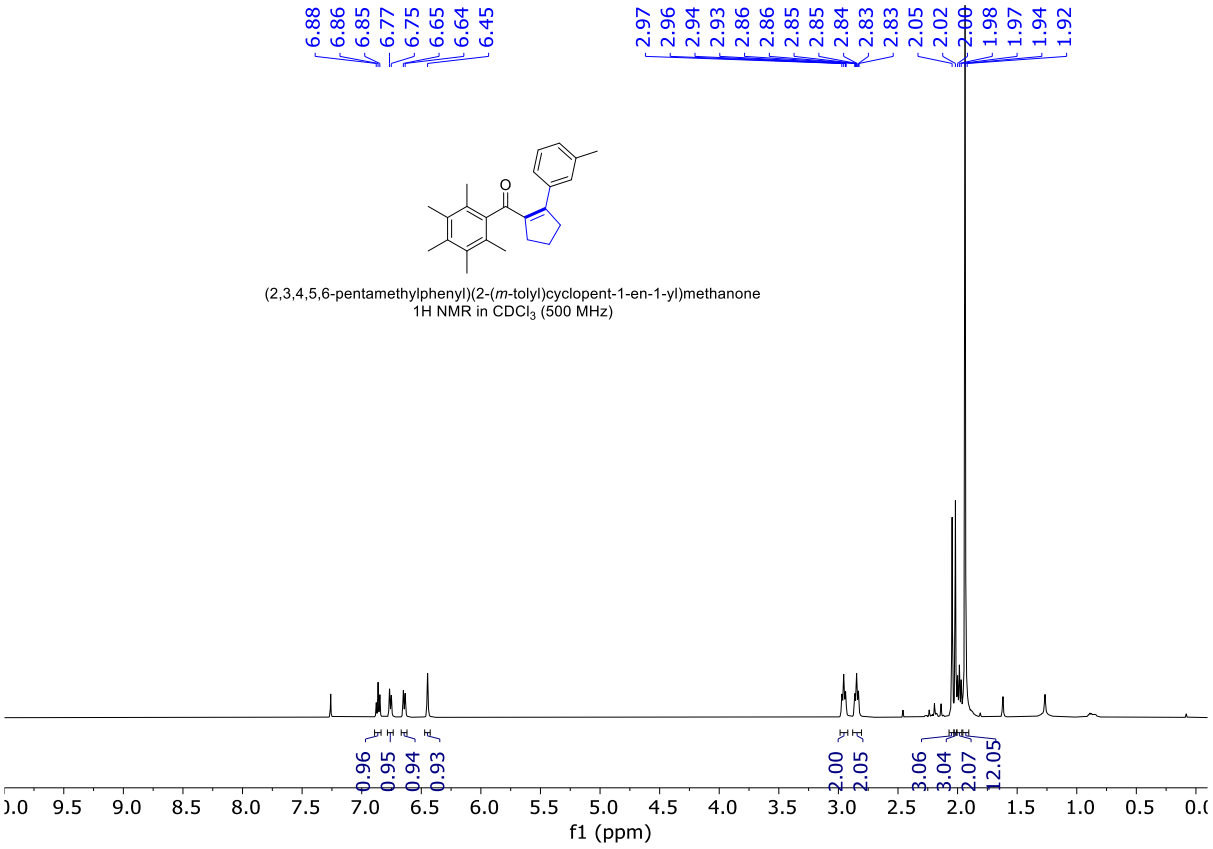

O
(2,3,4,5,6-pentamethylphenyl)(2-phenylcyclopent-1-en-1-yl)methanone
1H NMR in CDCl3 (400 MHz)
f1 (ppm)


200.38
157.06
139.77
139.69
137.24
134.77
132.26
128.40
126.66
126.50
126.19
43.22
34.15
21.52
17.61
16.45
15.71
O
(2,3,4,5,6-pentamethylphenyl)(2-phenylcyclopent-1-en-1-yl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

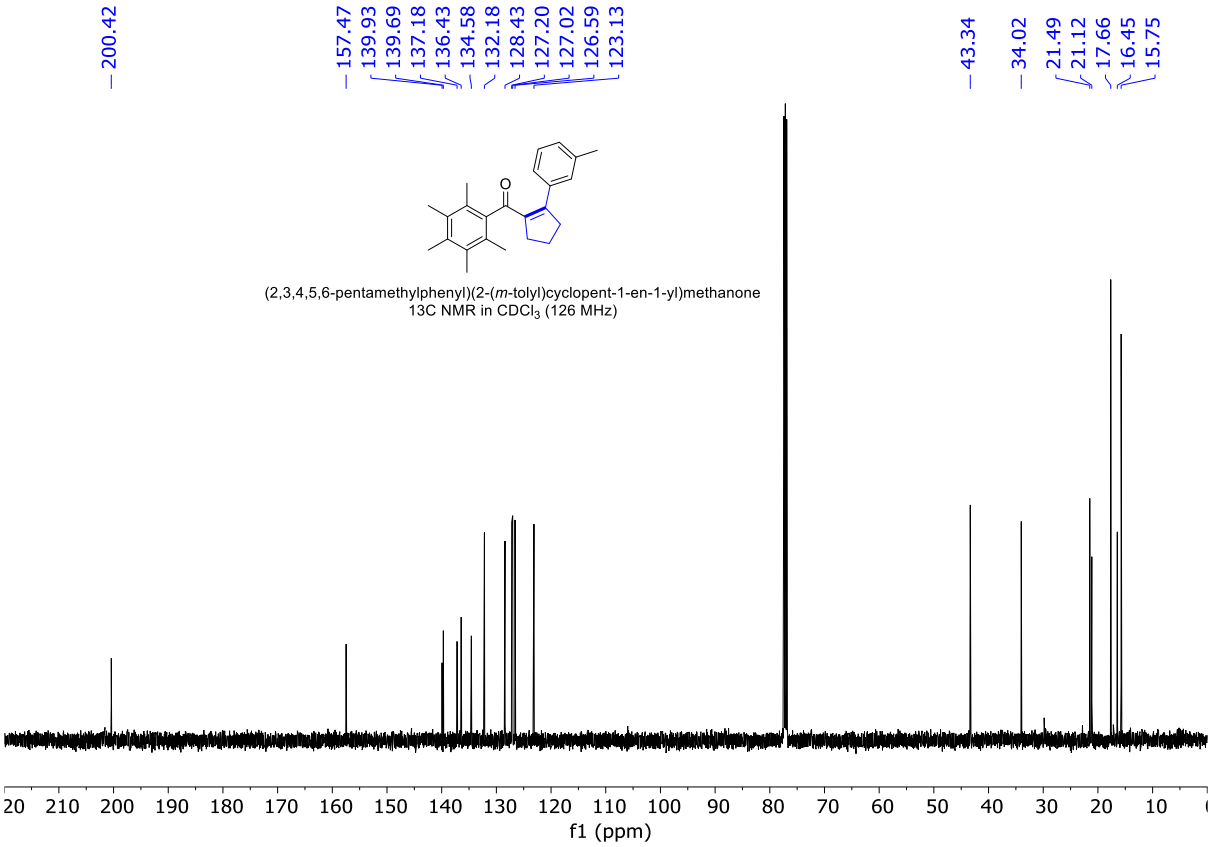

6.88
6.87
6.86
6.84
6.83
6.73
6.71
6.70
6.56
6.54
2.95
2.94
2.93
2.92
2.92
2.75
2.06
2.01
2.00
1.93
O
(2,3,4,5,6-pentamethylphenyl)(2-(o-tolyl)cyclopent-1-en-1-yl)methanone
1H NMR in CDCl3 (500 MHz)
2.04
1.02
1.01
2.00
2.06
3.03
5.06
12.02
f1 (ppm)

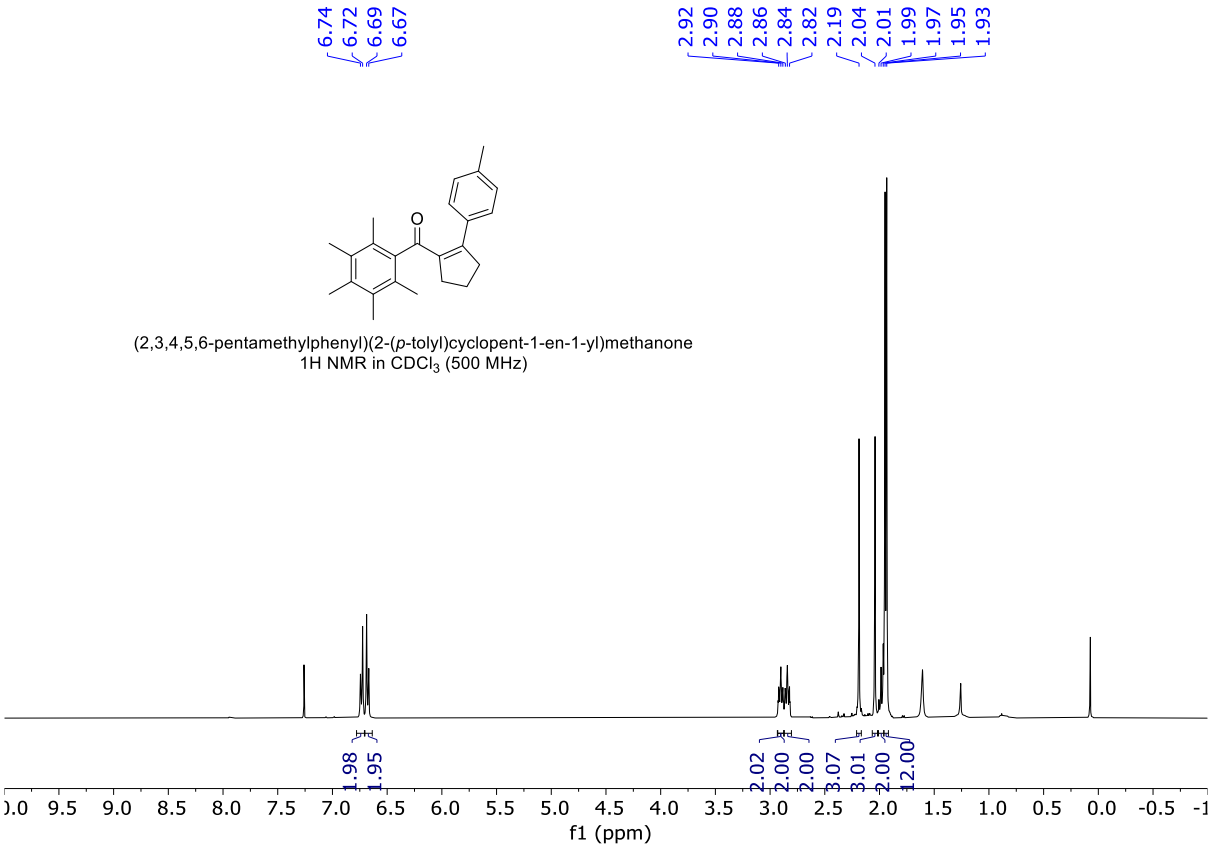


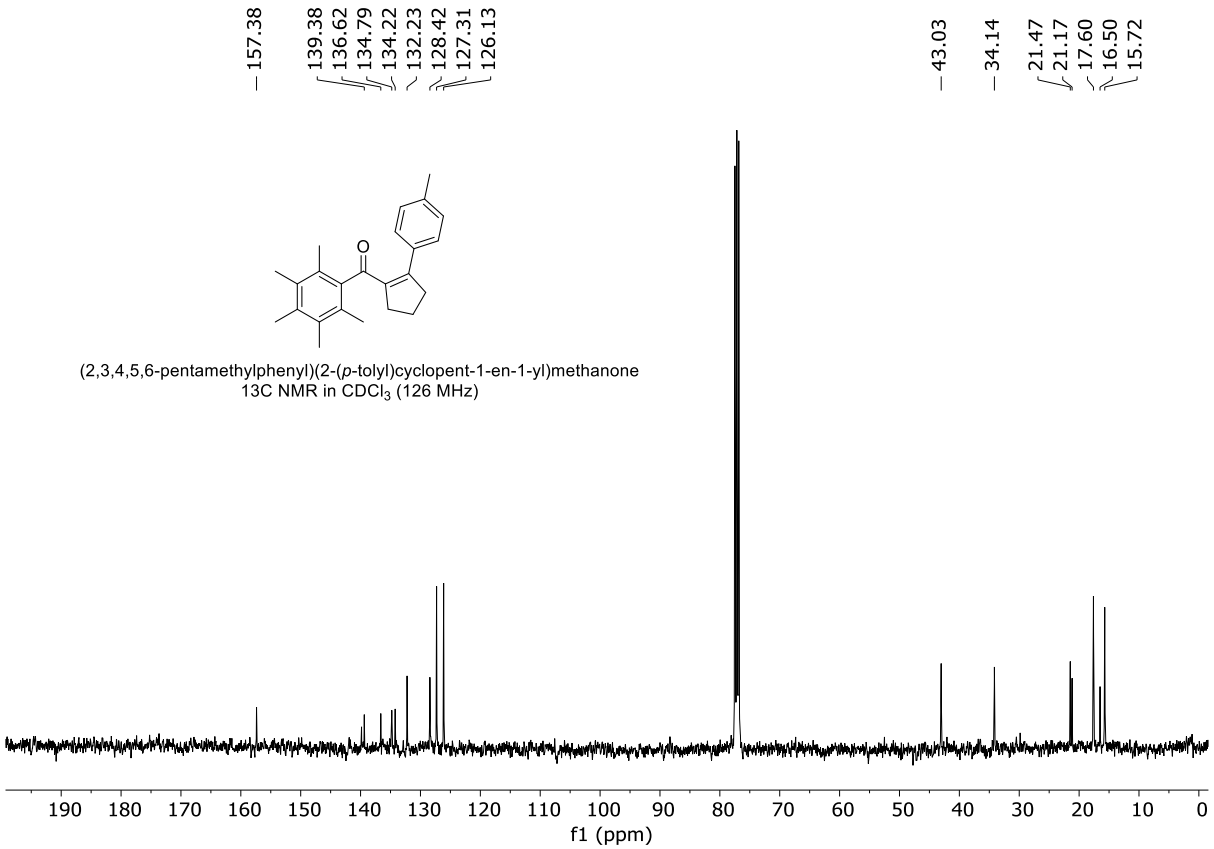
(2,3,4,5,6-pentamethylphenyl)(2-(*o*-tolyl)cyclopent-1-en-1-yl)methanone
13C NMR in $CDCl_3$ (126 MHz)

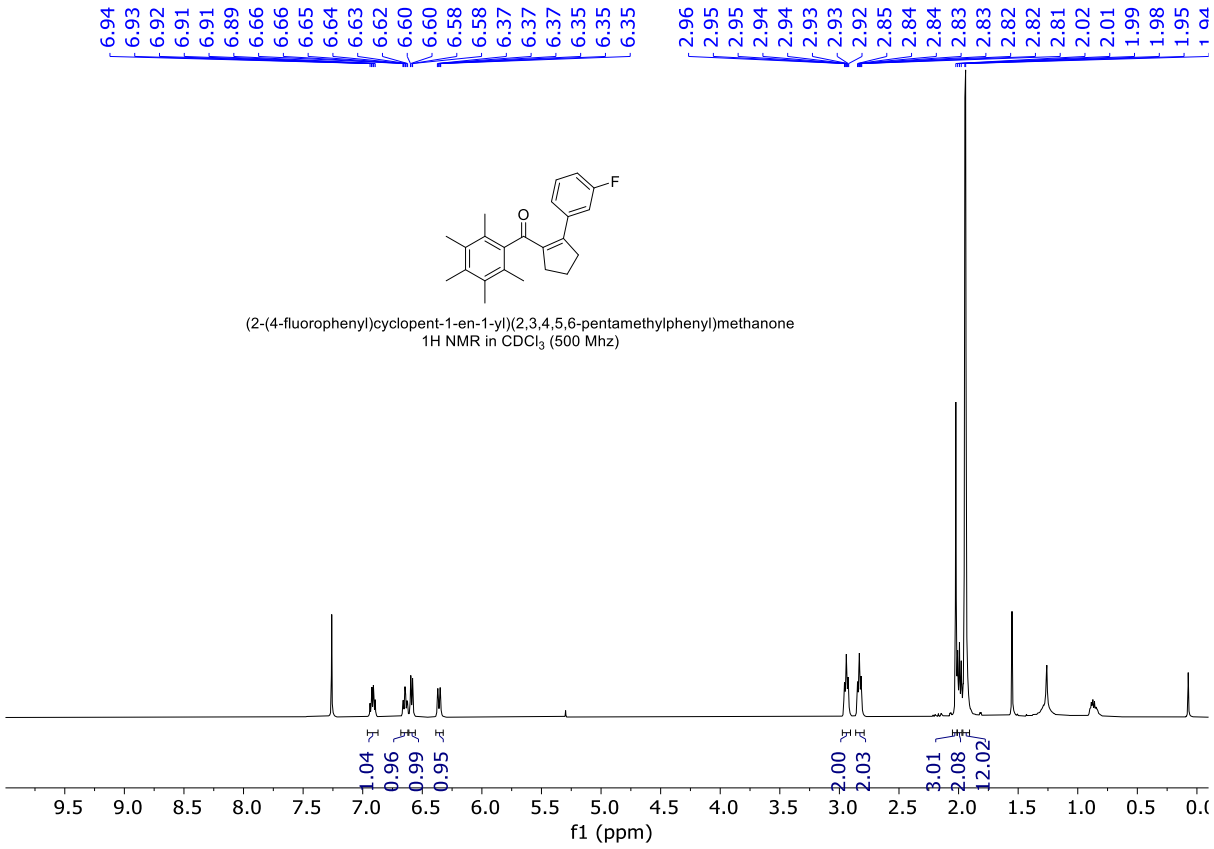


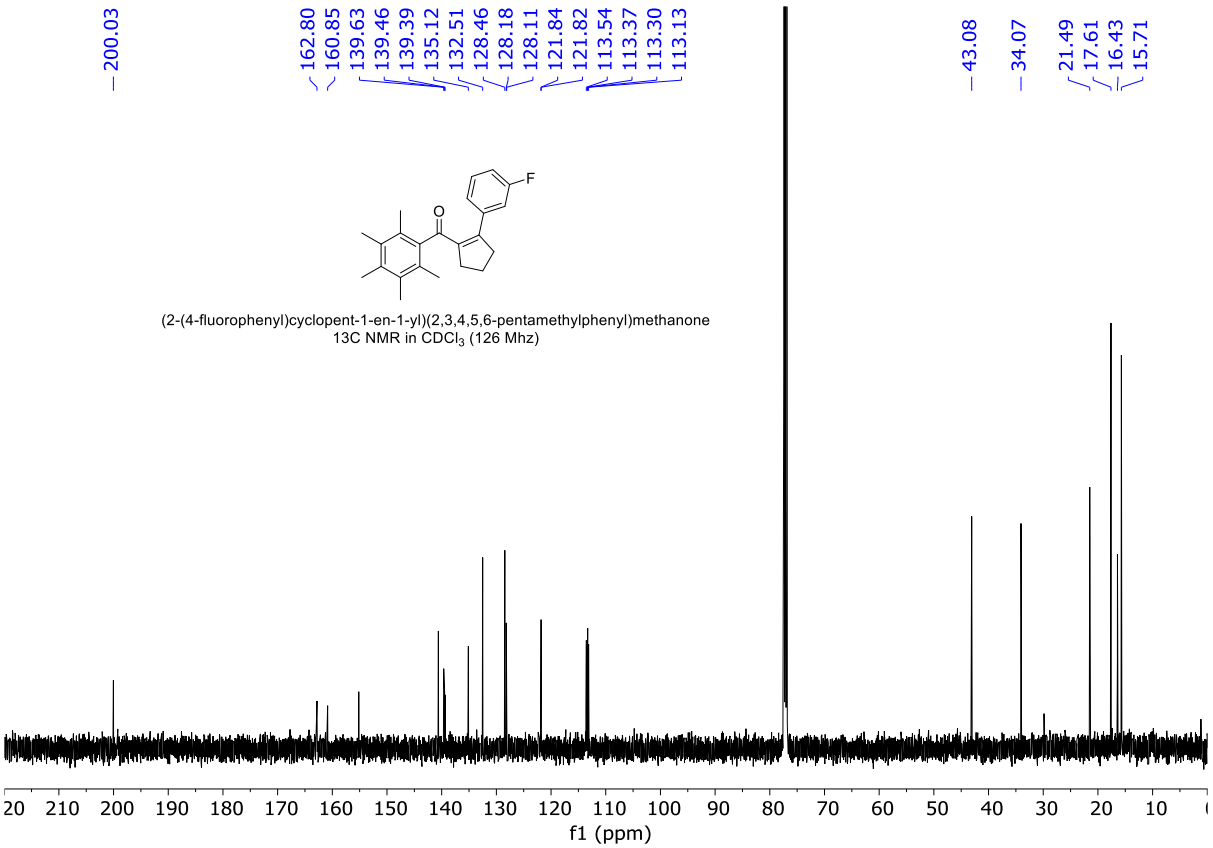
(2,3,4,5,6-pentamethylphenyl)(2-(*m*-tolyl)cyclopent-1-en-1-yl)methanone
1H NMR in $CDCl_3$ (500 MHz)


200.42
157.47
139.93
139.69
137.18
136.43
134.58
132.18
128.43
127.20
127.02
126.59
123.13
43.34
34.02
21.49
21.12
17.66
16.45
15.75
O
(2,3,4,5,6-pentamethylphenyl)(2-(m-tolyl)cyclopent-1-en-1-yl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

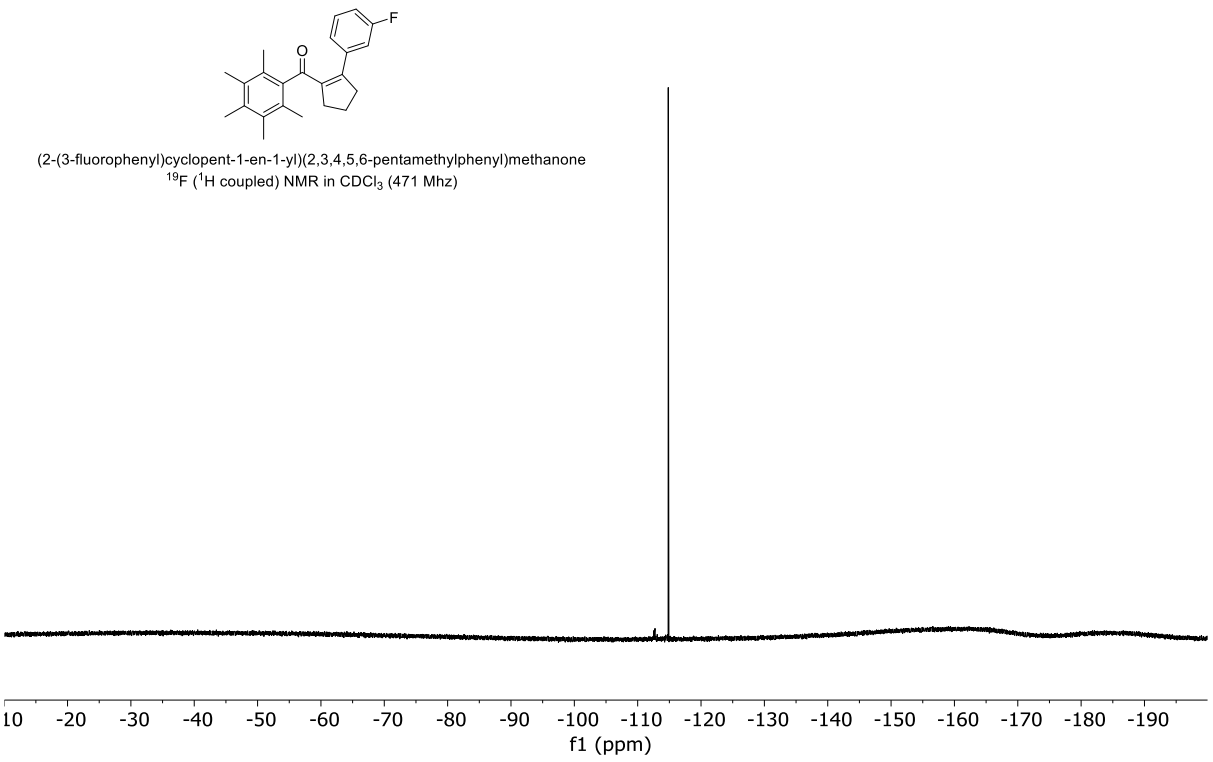

6.74
6.72
6.69
6.67
2.92
2.90
2.88
2.86
2.84
2.82
2.19
2.04
2.01
1.99
1.97
1.95
1.93
O
(2,3,4,5,6-pentamethylphenyl)(2-(p-tolyl)cyclopent-1-en-1-yl)methanone
1H NMR in CDCl3 (500 MHz)
1.98
1.95
2.02
2.00
2.00
3.07
3.01
2.00
12.00
f1 (ppm)


157.38
139.38
136.62
134.79
134.22
132.23
128.42
127.31
126.13
43.03
34.14
21.47
21.17
17.60
16.50
15.72
O
(2,3,4,5,6-pentamethylphenyl)(2-(p-tolyl)cyclopent-1-en-1-yl)methanone
13C NMR in CDCl3 (126 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

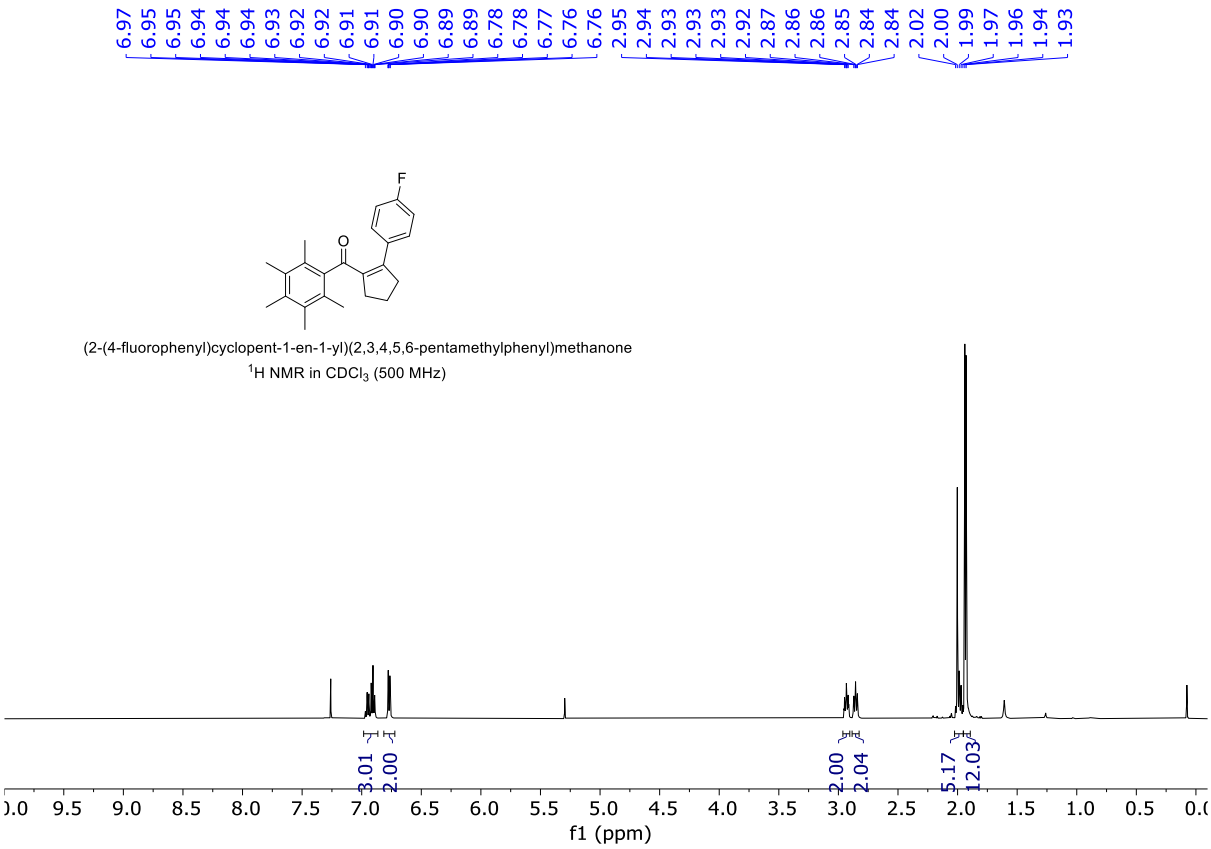

6.94
6.93
6.92
6.91
6.91
6.89
6.66
6.66
6.65
6.64
6.63
6.62
6.60
6.60
6.58
6.58
6.37
6.37
6.37
6.35
6.35
2.96
2.95
2.95
2.94
2.94
2.93
2.93
2.92
2.85
2.84
2.84
2.83
2.83
2.82
2.82
2.81
2.02
2.01
1.99
1.98
1.95
F
O
(2-(4-fluorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 Mhz)
1.04
0.96
0.99
0.95
2.00
2.03
3.01
2.08
12.02
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
f1 (ppm)

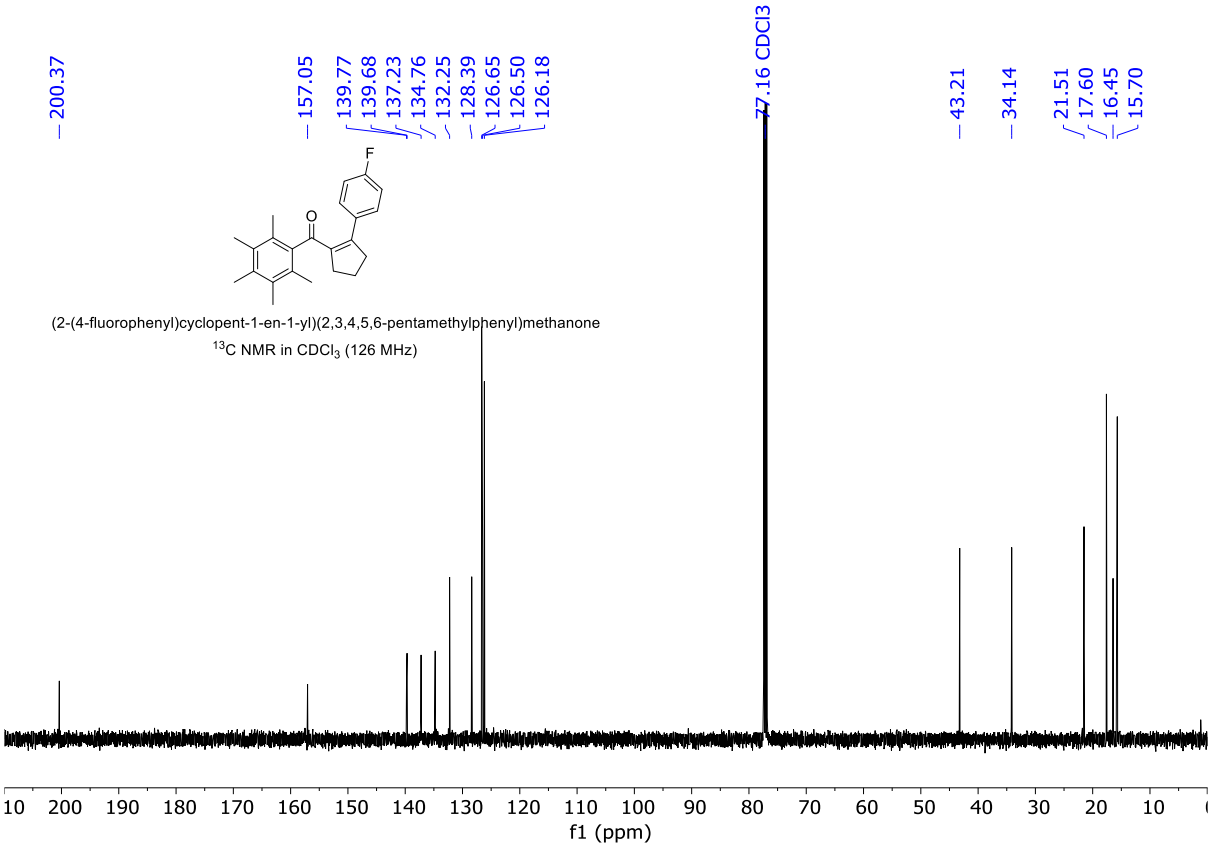


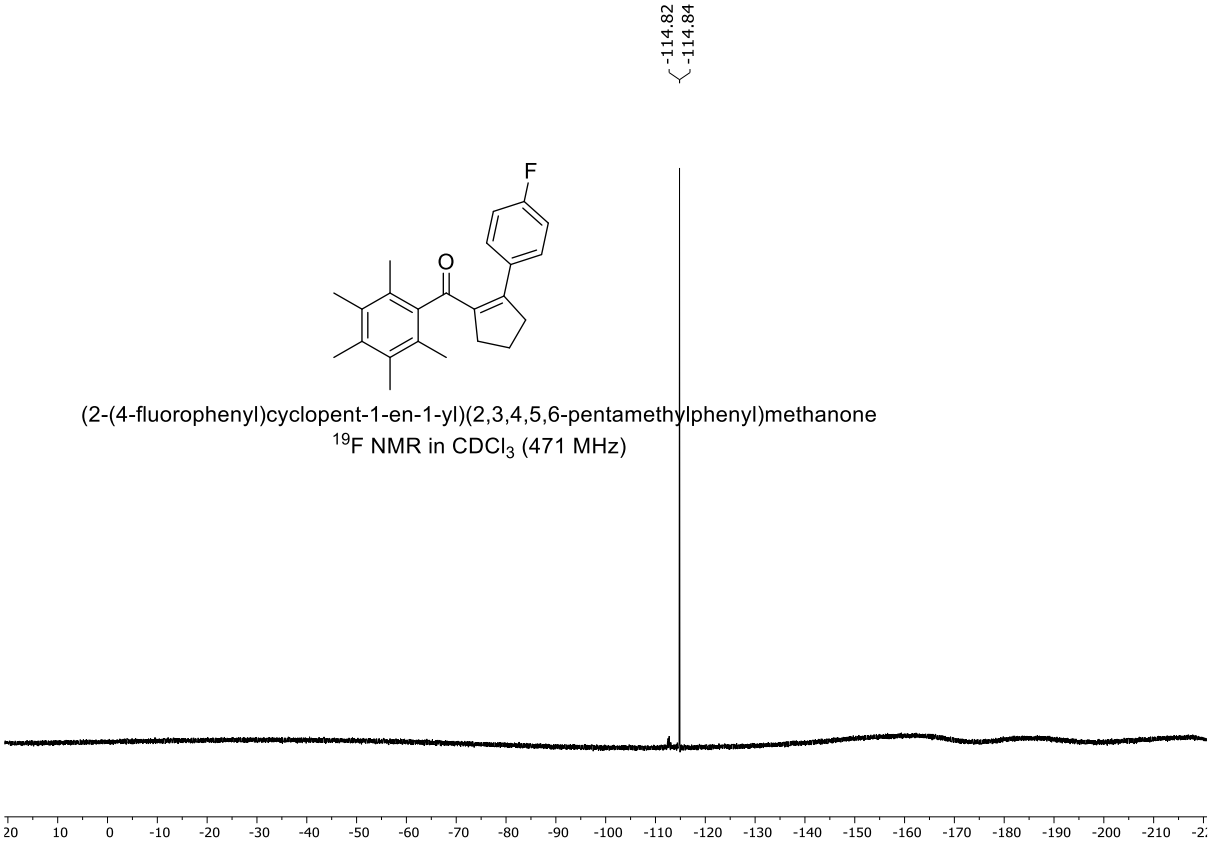
(2-(4-fluorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in $CDCl_3$ (126 Mhz)



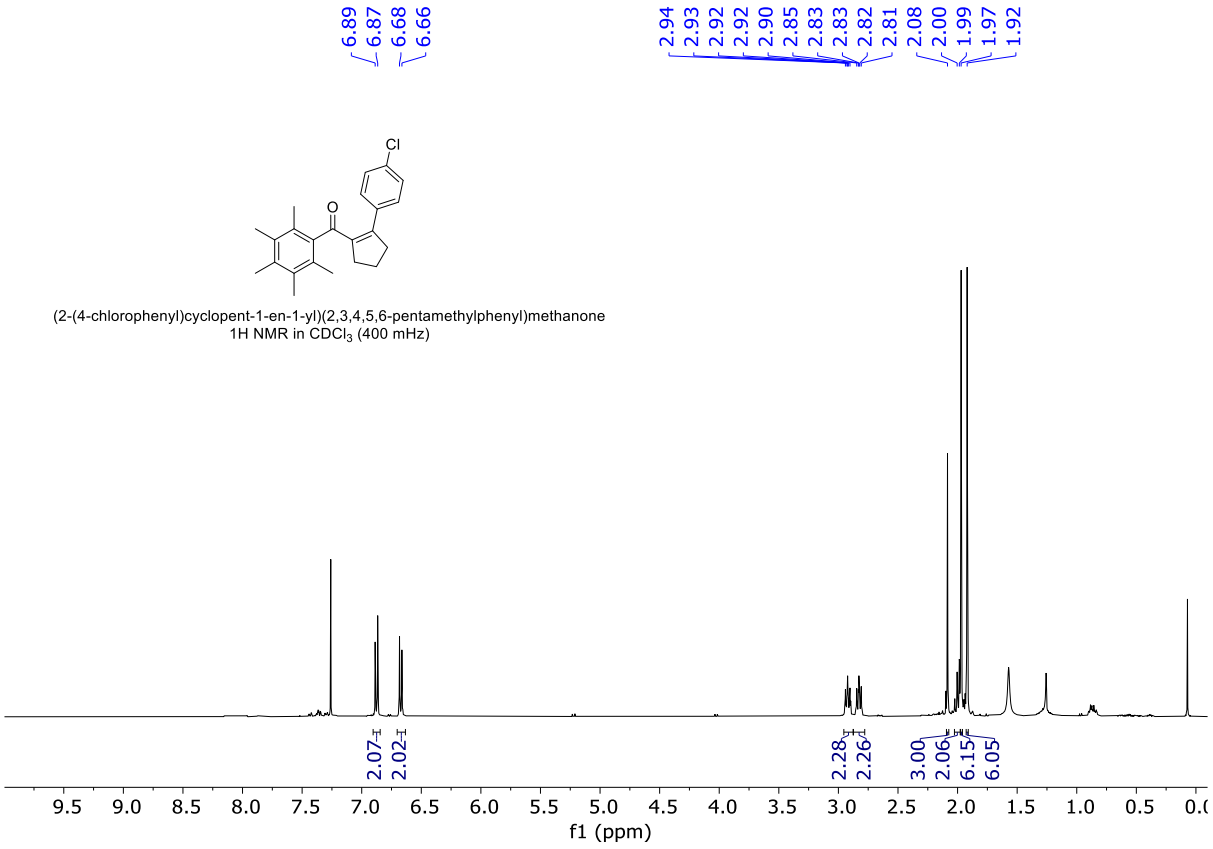
(2-(3-fluorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{19}F (^{1}H coupled) NMR in $CDCl_3$ (471 Mhz)


6.97 6.95 6.95 6.94 6.94 6.94 6.93 6.92 6.92 6.91 6.91 6.90 6.90 6.89 6.89 6.78 6.78 6.77 6.76 6.76
2.95 2.94 2.93 2.93 2.93 2.92 2.87 2.86 2.86 2.85 2.84 2.84
2.02 2.00 1.99 1.97 1.96 1.94 1.93
F
O
(2-(4-fluorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
3.01
2.00
2.00
2.04
5.17
12.03
f1 (ppm)

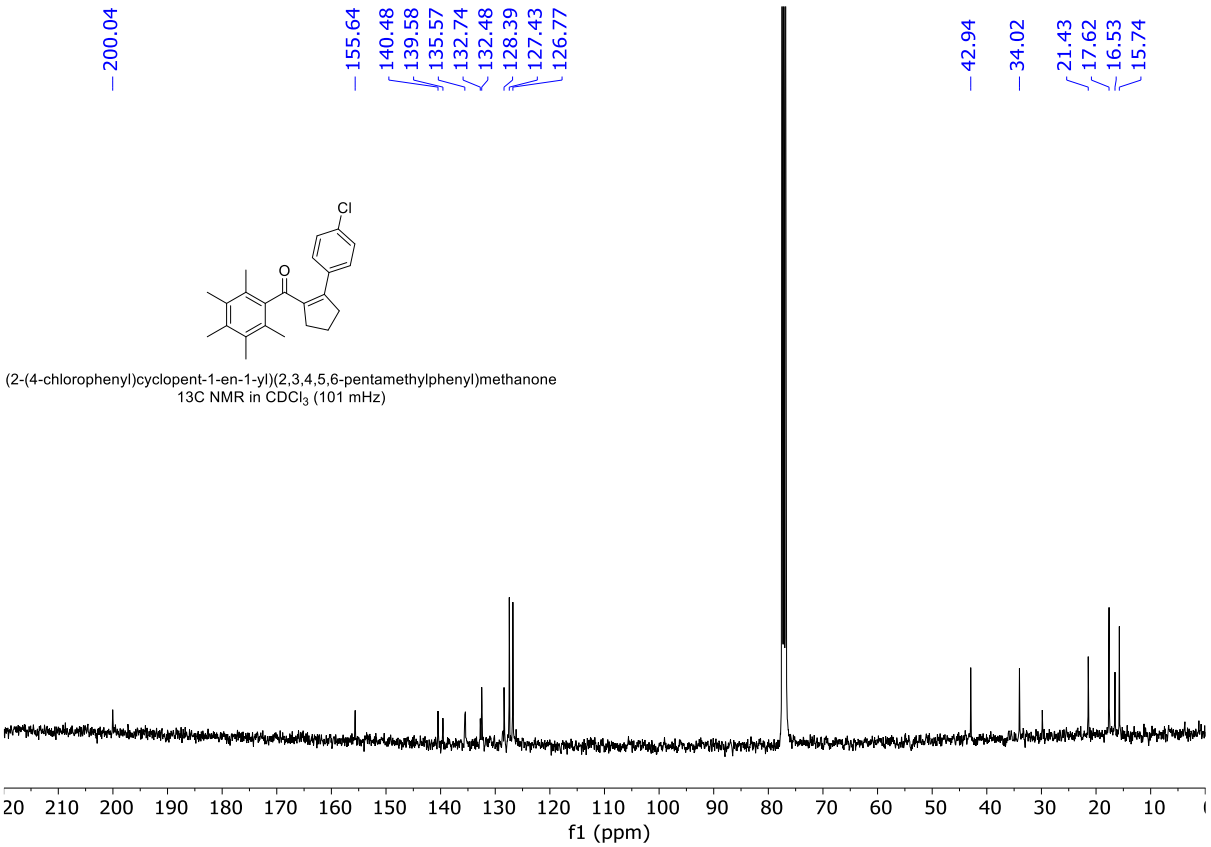

200.37
157.05
139.77
139.68
137.23
134.76
132.25
128.39
126.65
126.50
126.18
77.16 CDCl3
43.21
34.14
21.51
17.60
16.45
15.70
F
O
(2-(4-fluorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)



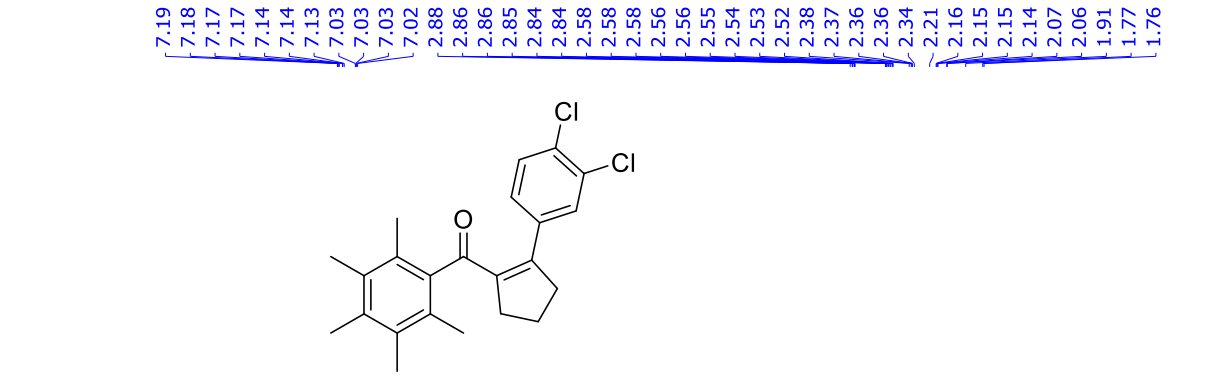
(2-(4-fluorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{19}F NMR in $CDCl_3$ (471 MHz)



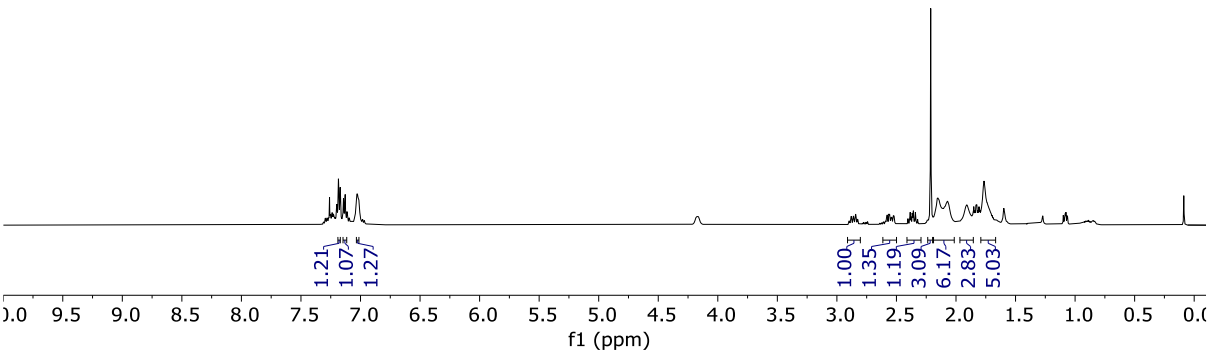
(2-(4-chlorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in $CDCl_3$ (400 mHz)

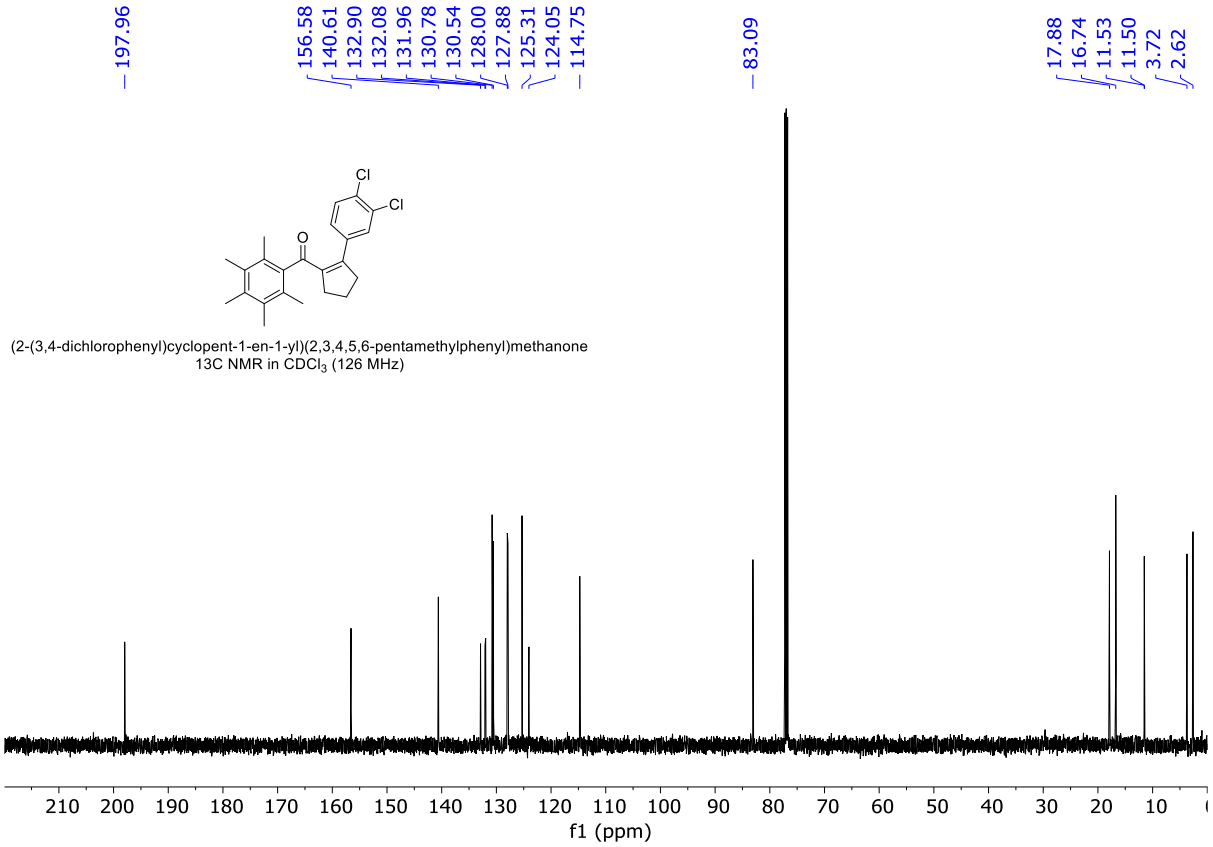


(2-(4-chlorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in $CDCl_3$ (101 mHz)

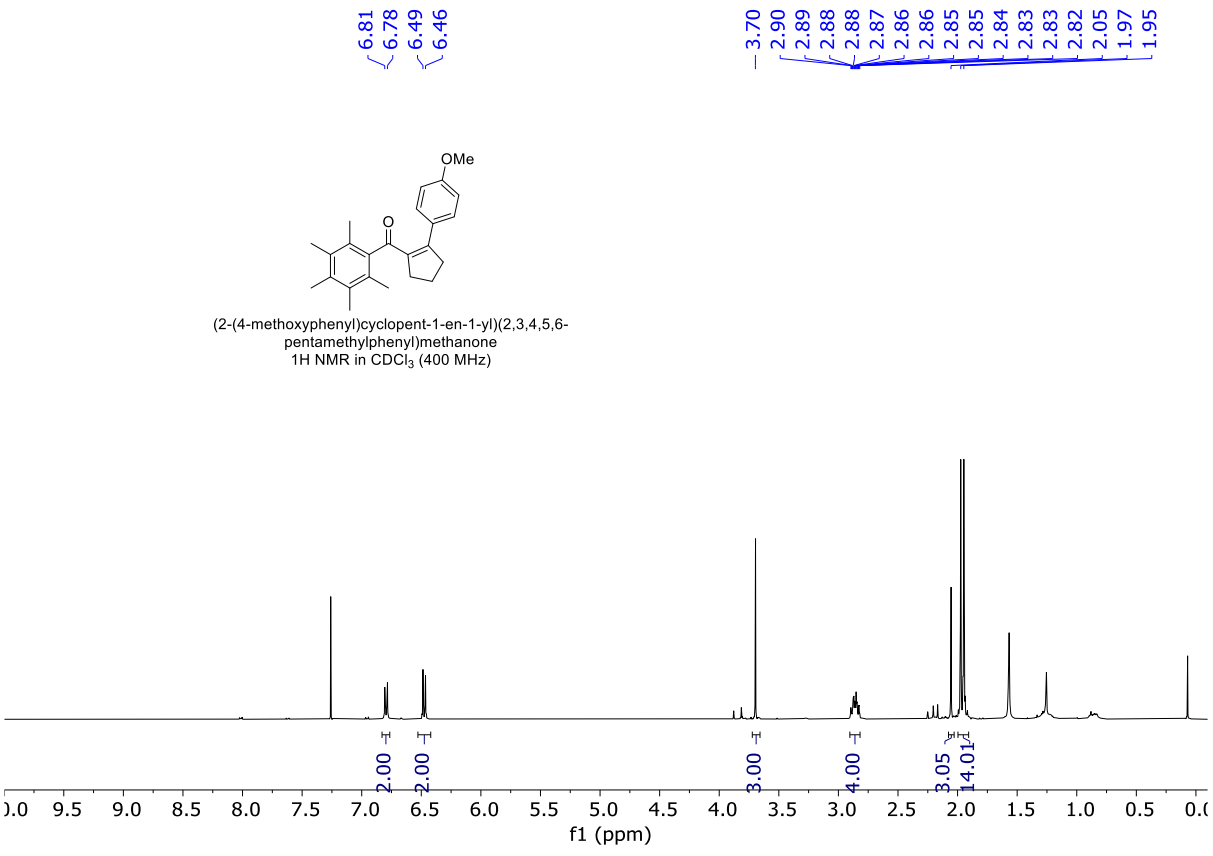


(2-(3,4-dichlorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)



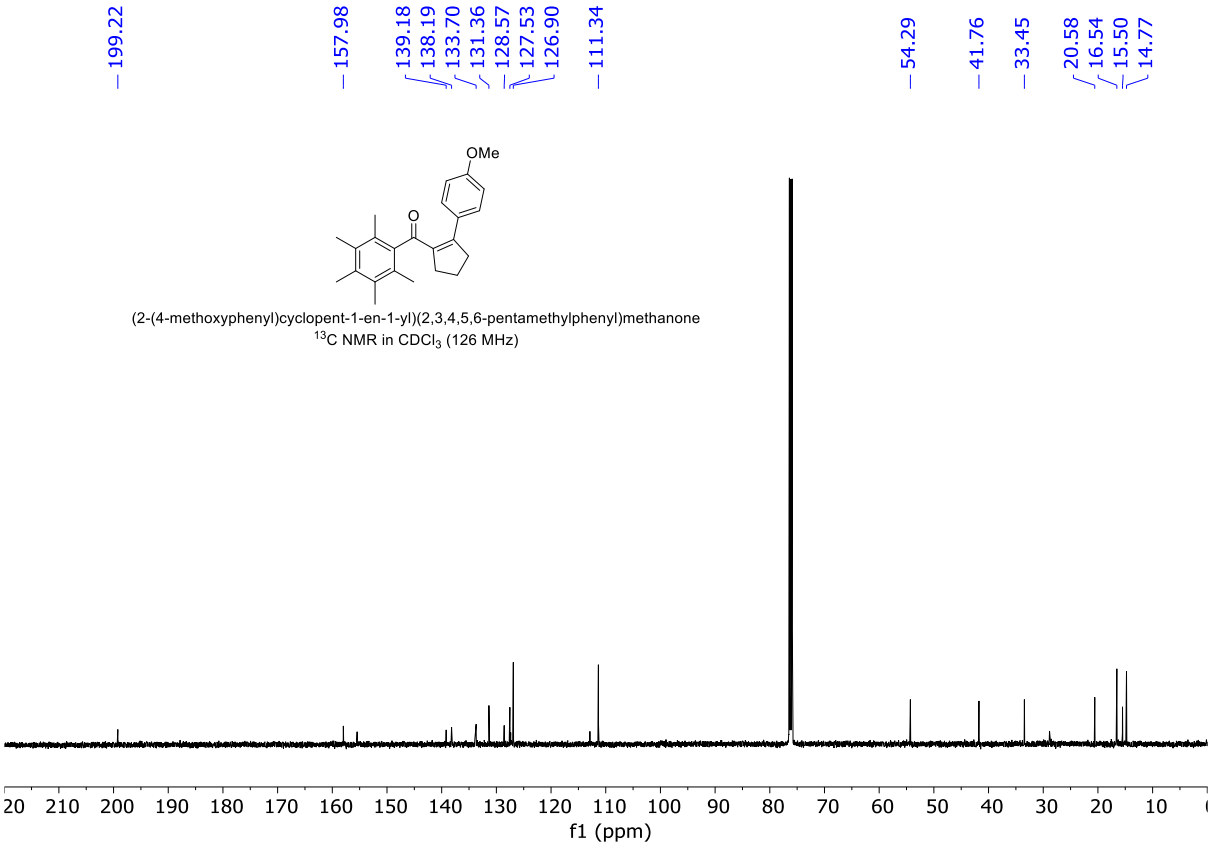


(2-(3,4-dichlorophenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in $CDCl_3$ (126 MHz)

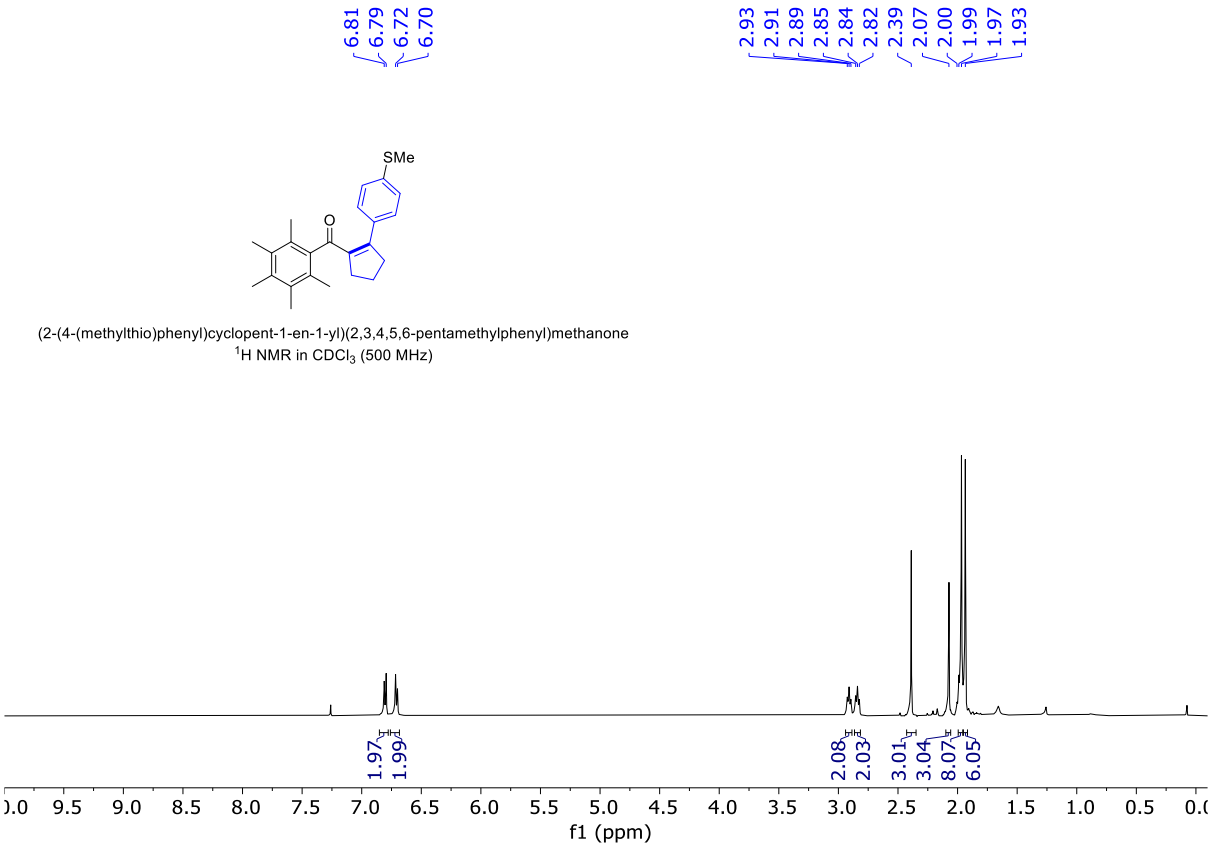


(2-(4-methoxyphenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in $CDCl_3$ (400 MHz)

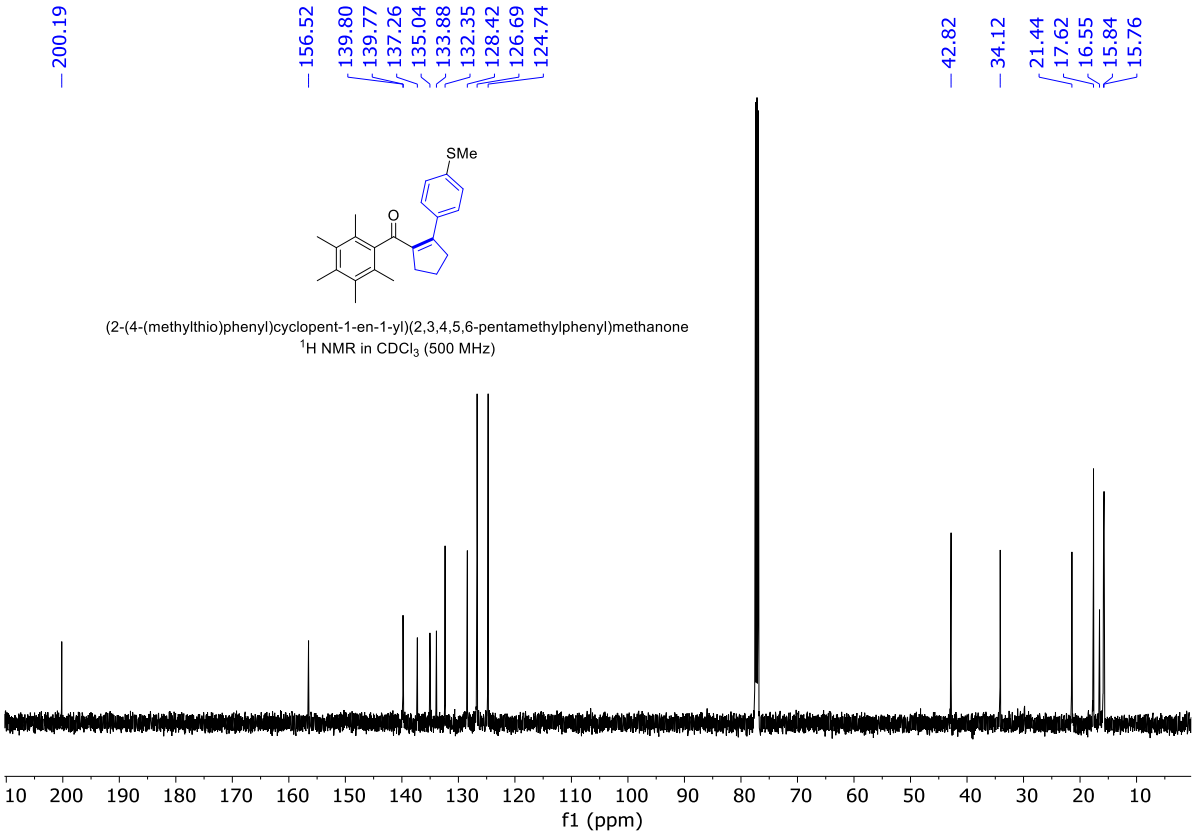
;

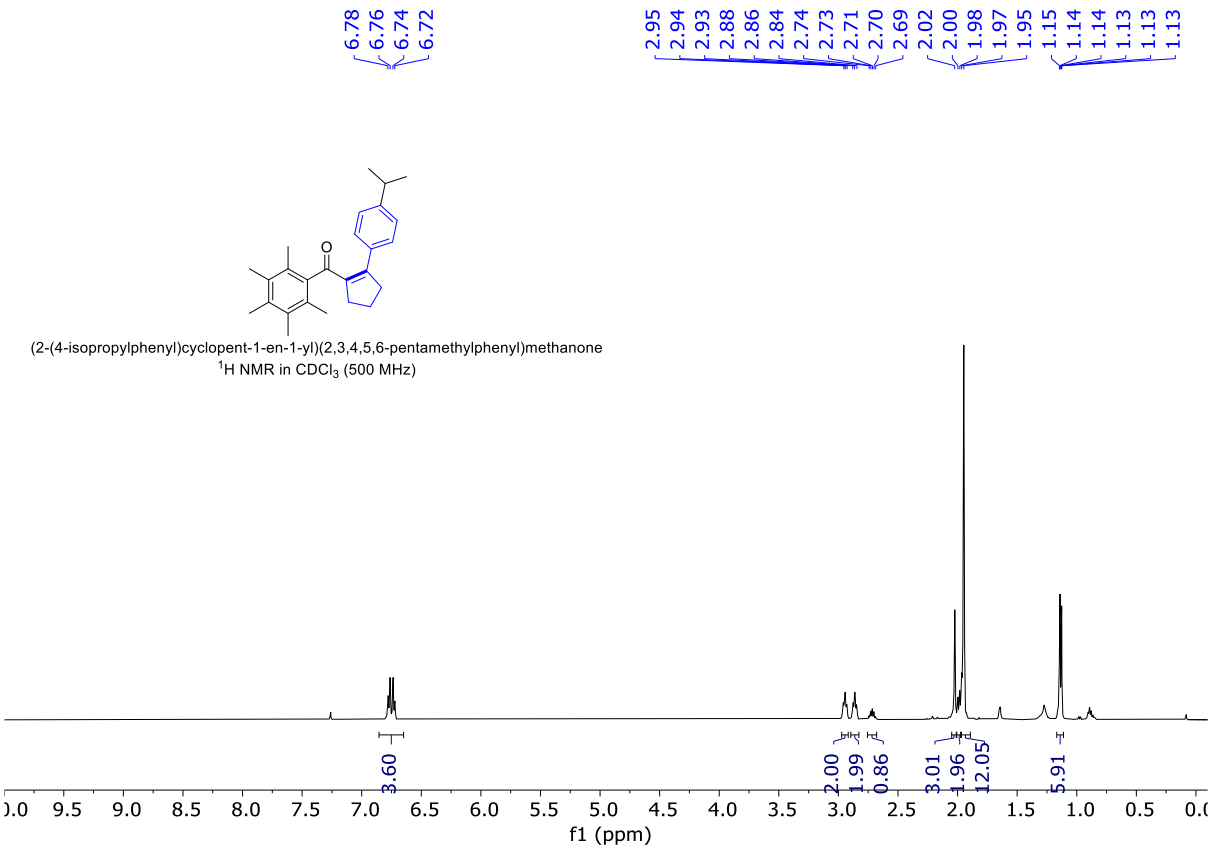


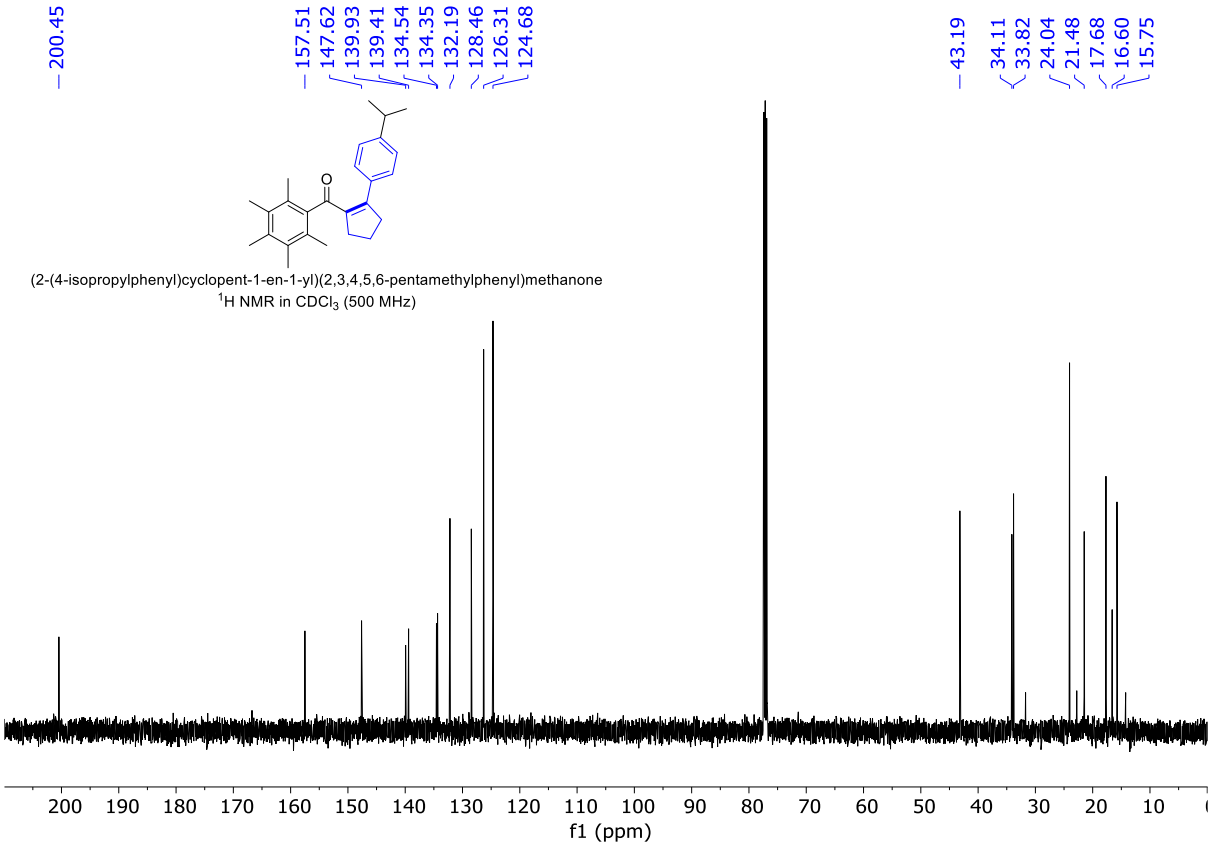
(2-(4-methoxyphenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{13}C NMR in $CDCl_3$ (126 MHz)



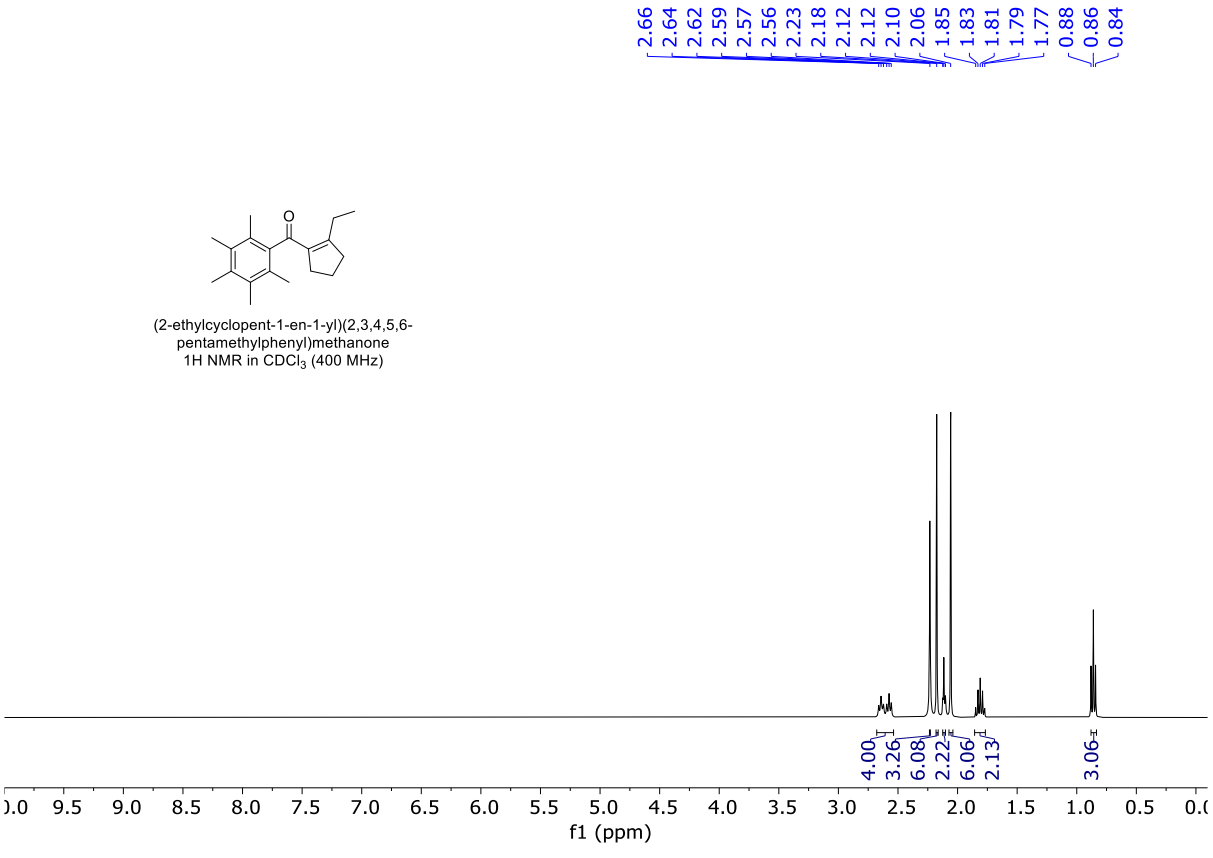
(2-(4-(methylthio)phenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)


200.19
156.52
139.80
139.77
137.26
135.04
133.88
132.35
128.42
126.69
124.74
42.82
34.12
21.44
17.62
16.55
15.84
15.76
SMe
O
(2-(4-(methylthio)phenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
f1 (ppm)

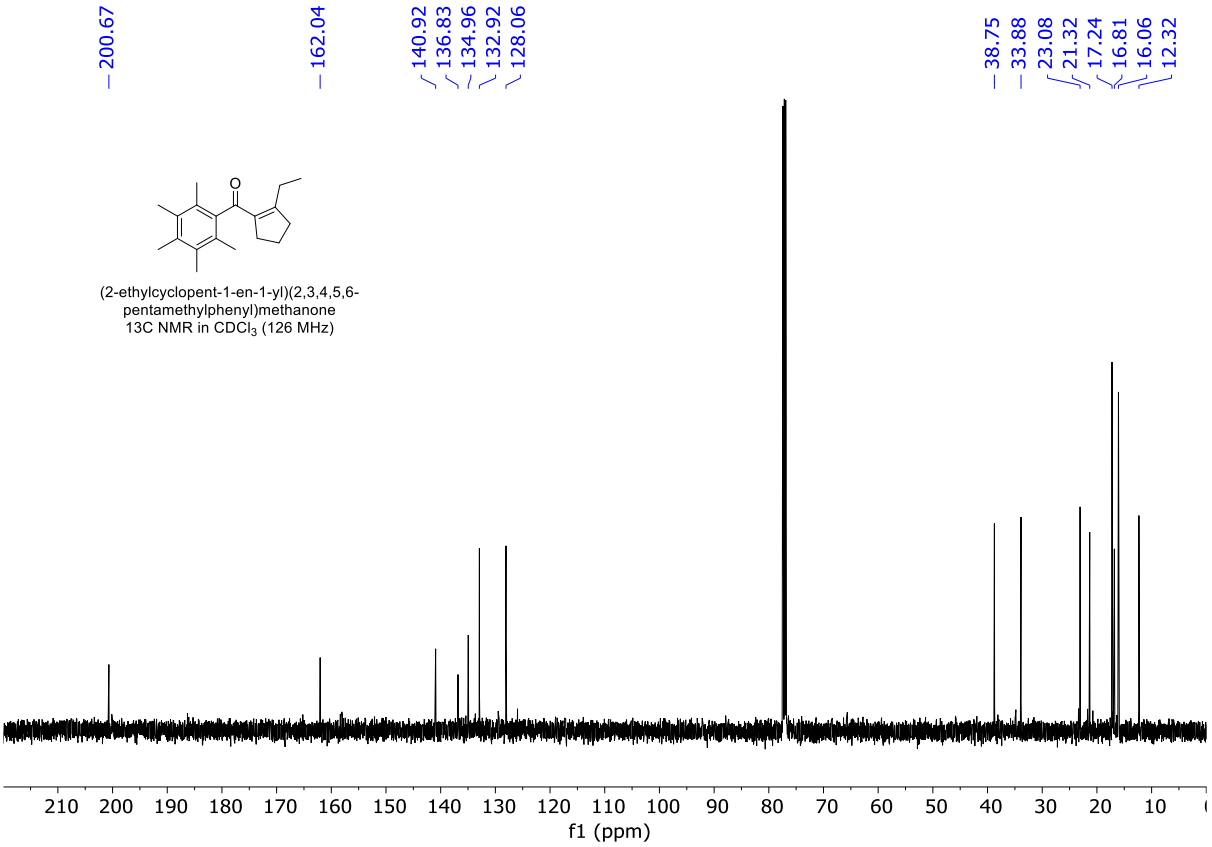

6.78
6.76
6.74
6.72
2.95
2.94
2.93
2.88
2.86
2.84
2.74
2.73
2.71
2.70
2.69
2.02
2.00
1.98
1.97
1.95
1.15
1.14
1.14
1.13
1.13
1.13
O
(2-(4-isopropylphenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
3.60
2.00
1.99
0.86
3.01
1.96
12.05
5.91
f1 (ppm)

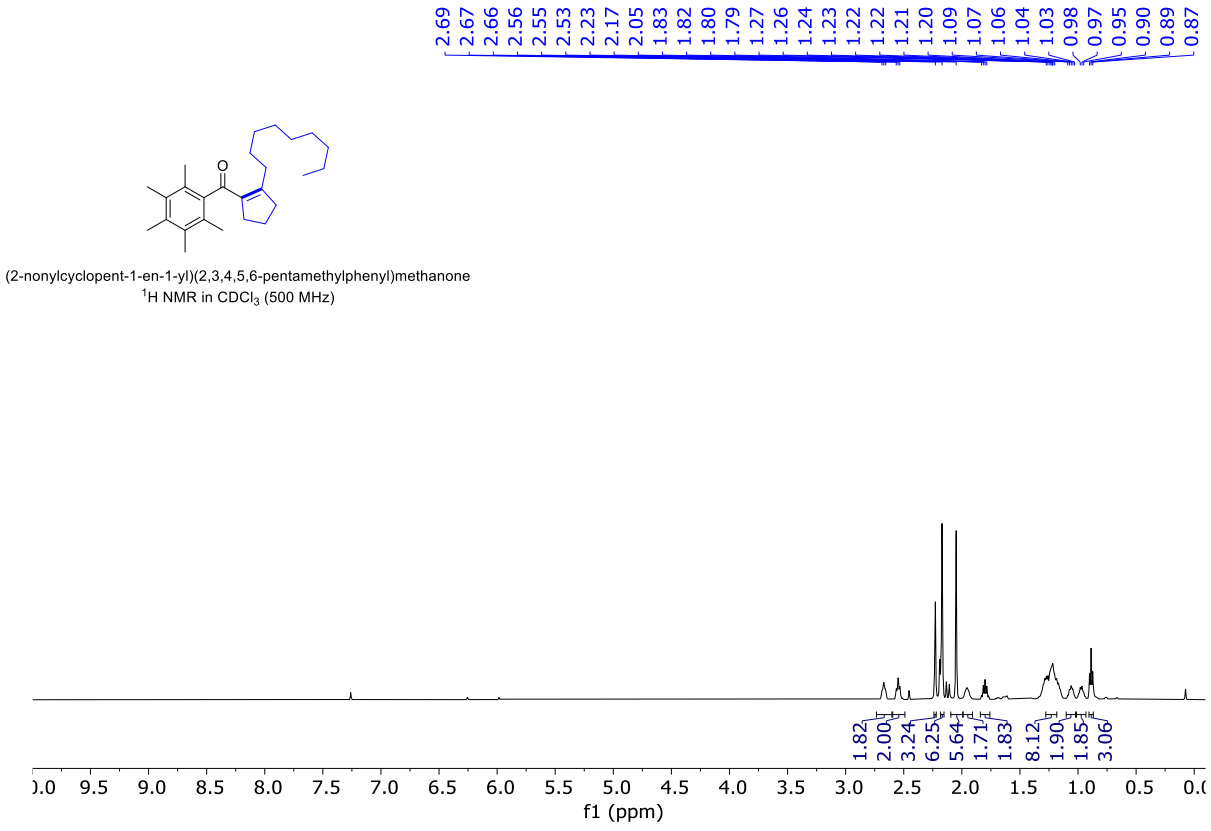


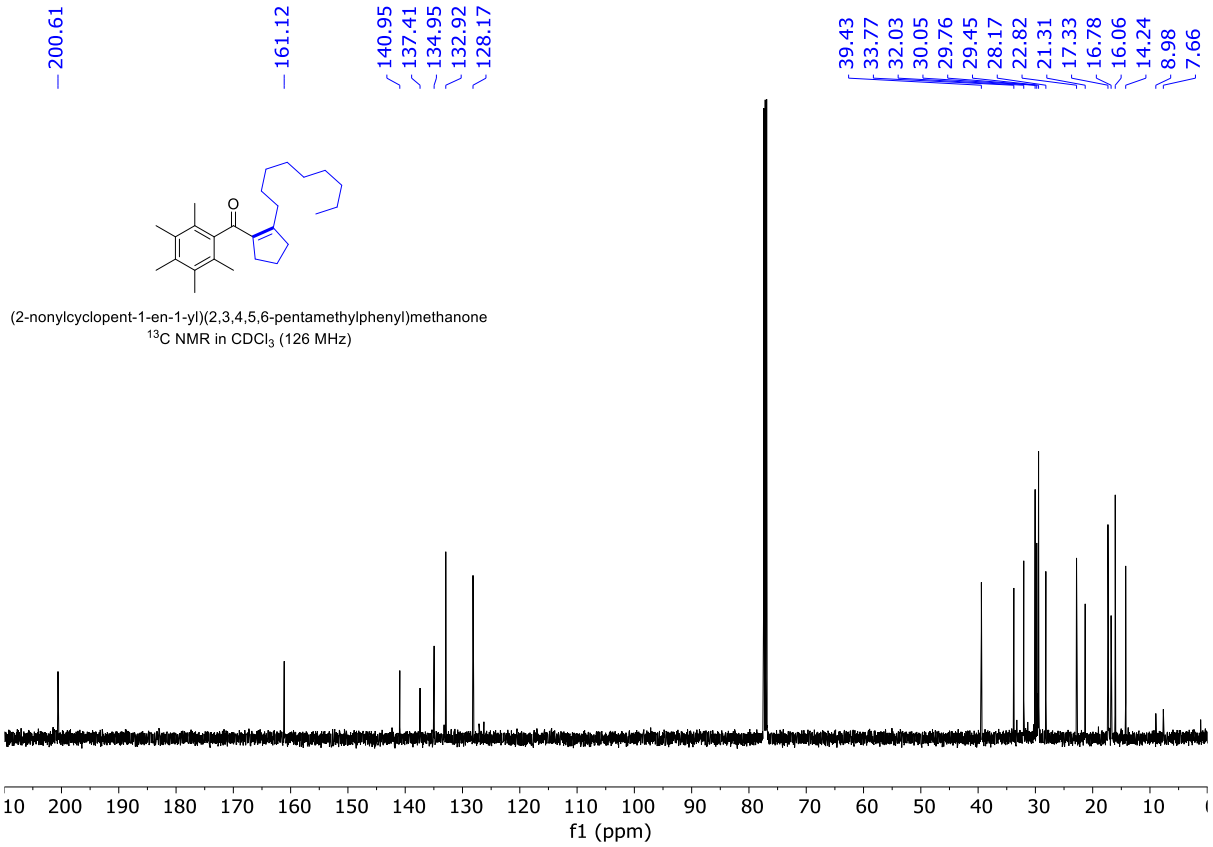
(2-(4-isopropylphenyl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)



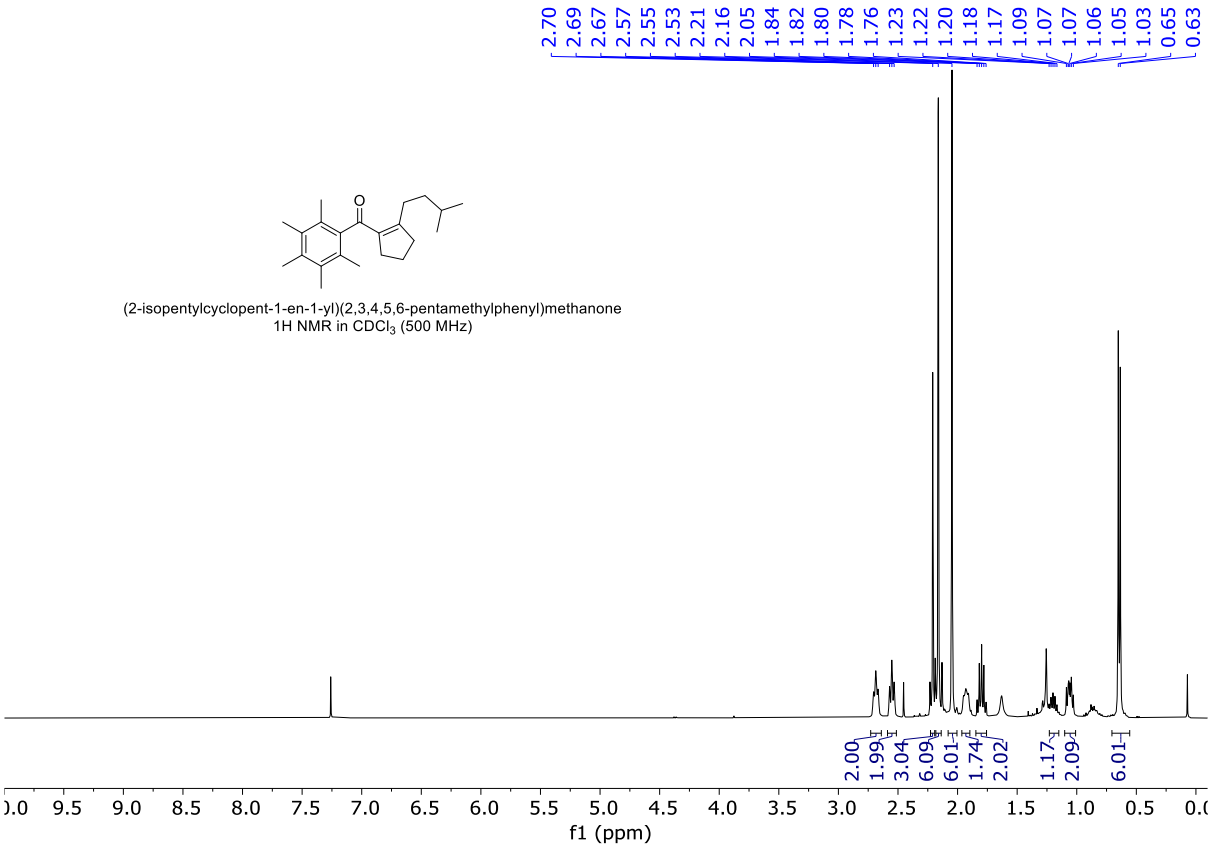
(2-ethylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in $CDCl_3$ (400 MHz)


200.67
162.04
140.92
136.83
134.96
132.92
128.06
38.75
33.88
23.08
21.32
17.24
16.81
16.06
12.32
O
(2-ethylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in CDCl3 (126 MHz)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

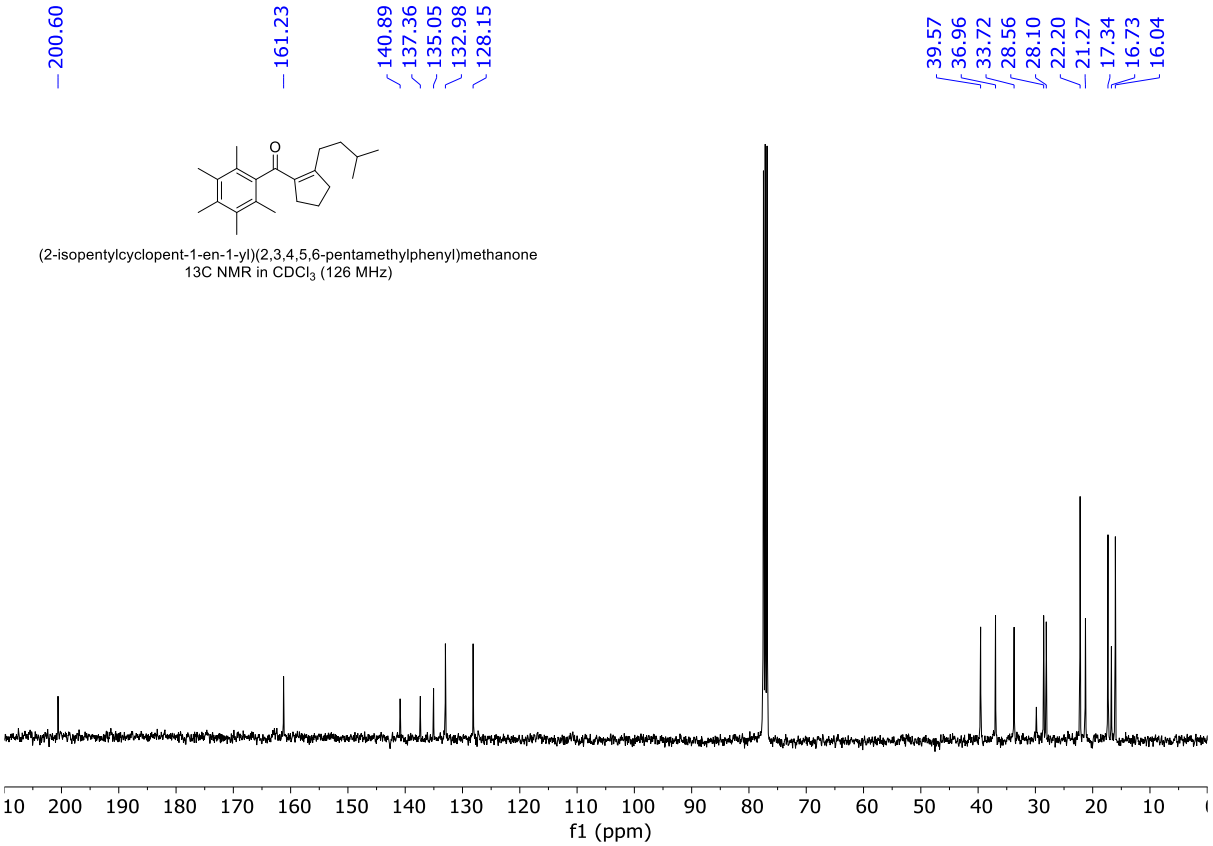

2.69
2.67
2.66
2.56
2.55
2.53
2.23
2.17
2.05
1.83
1.82
1.80
1.79
1.27
1.26
1.24
1.23
1.22
1.22
1.21
1.20
1.09
1.07
1.06
1.04
1.03
0.98
0.97
0.95
0.90
0.89
0.87
O
(2-nonylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
1.82
2.00
3.24
6.25
5.64
1.71
1.83
8.12
1.90
1.85
3.06
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
f1 (ppm)

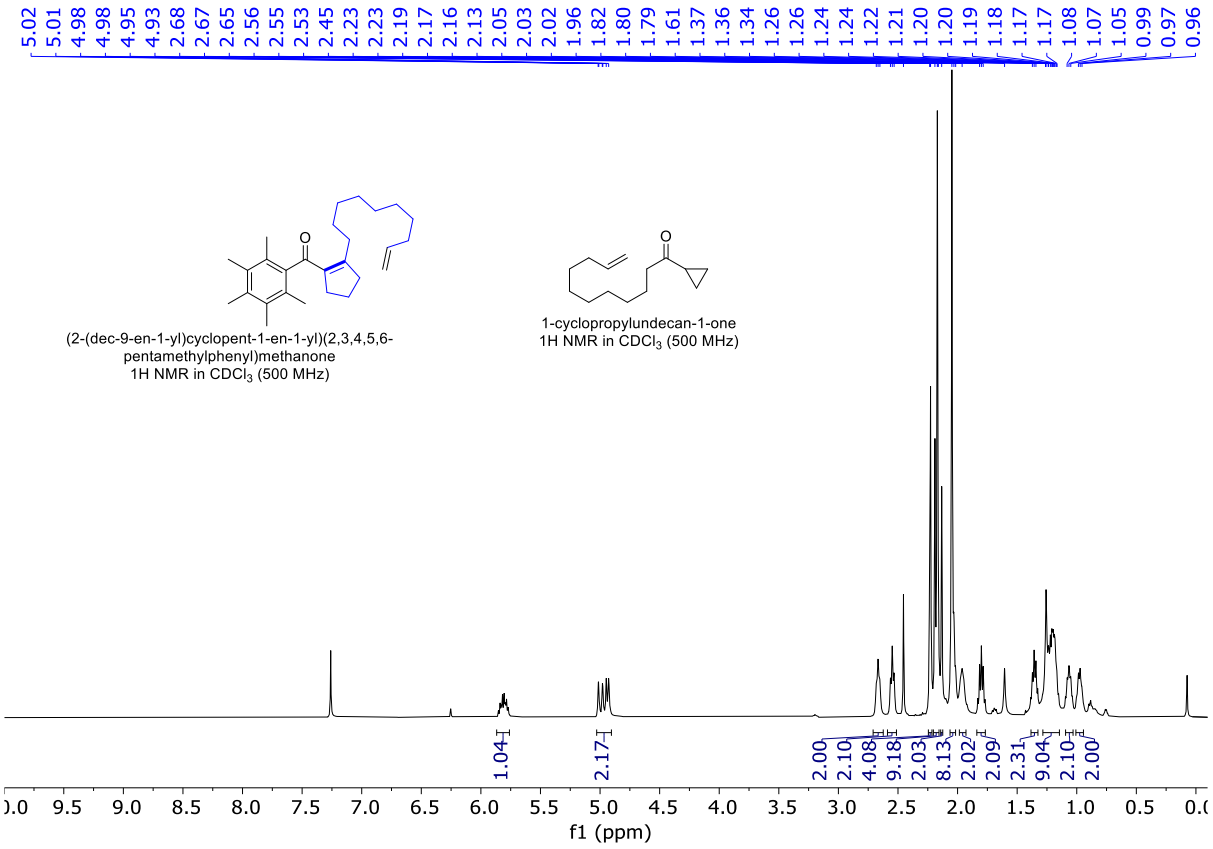


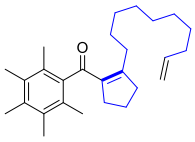
(2-nonylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{13}C NMR in $CDCl_3$ (126 MHz)



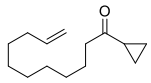
(2-isopentylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in $CDCl_3$ (500 MHz)


200.60
161.23
140.89
137.36
135.05
132.98
128.15
39.57
36.96
33.72
28.56
28.10
22.20
21.27
17.34
16.73
16.04
(2-isopentylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

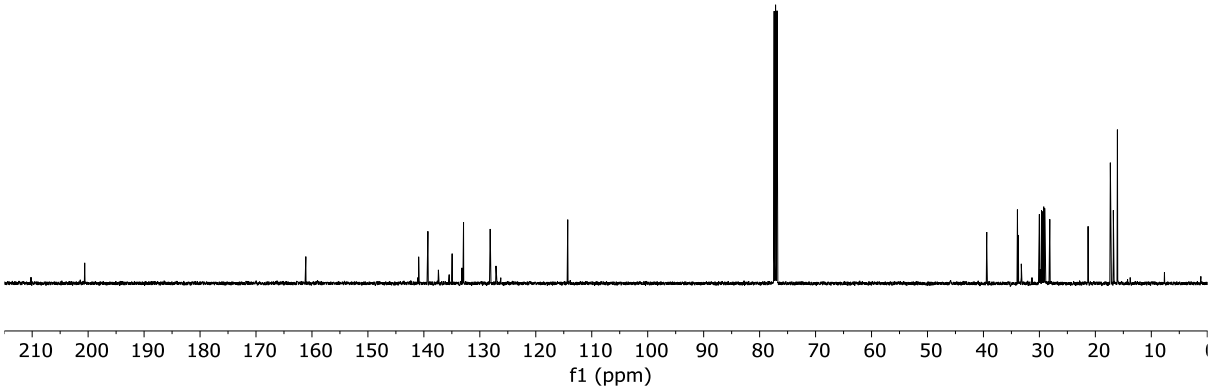

(2-(dec-9-en-1-yl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
1-cyclopropylundecan-1-one
1H NMR in CDCl3 (500 MHz)
f1 (ppm)

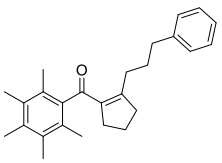


(2-(dec-9-en-1-yl)cyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in $CDCl_3$ (126 MHz)

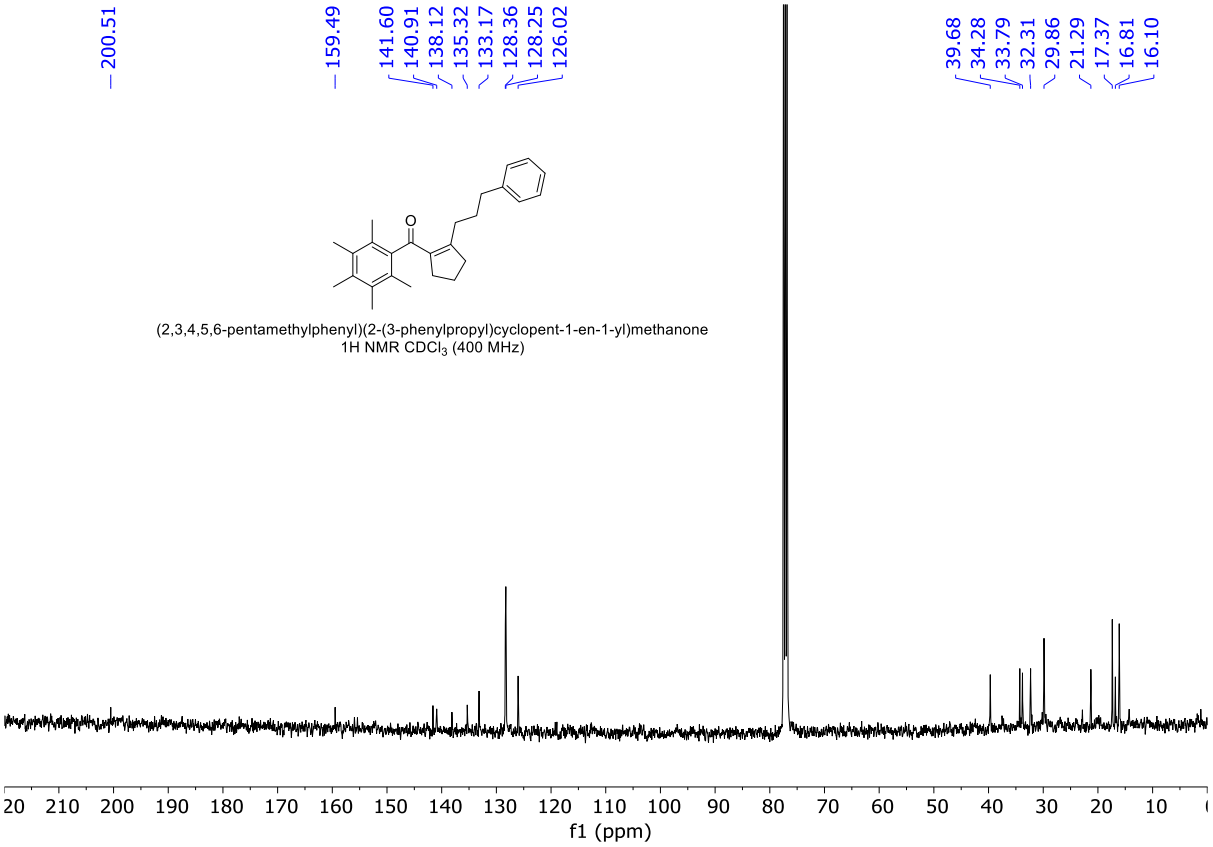


1-cyclopropylundecan-1-one
13C NMR in $CDCl_3$ (126 MHz)

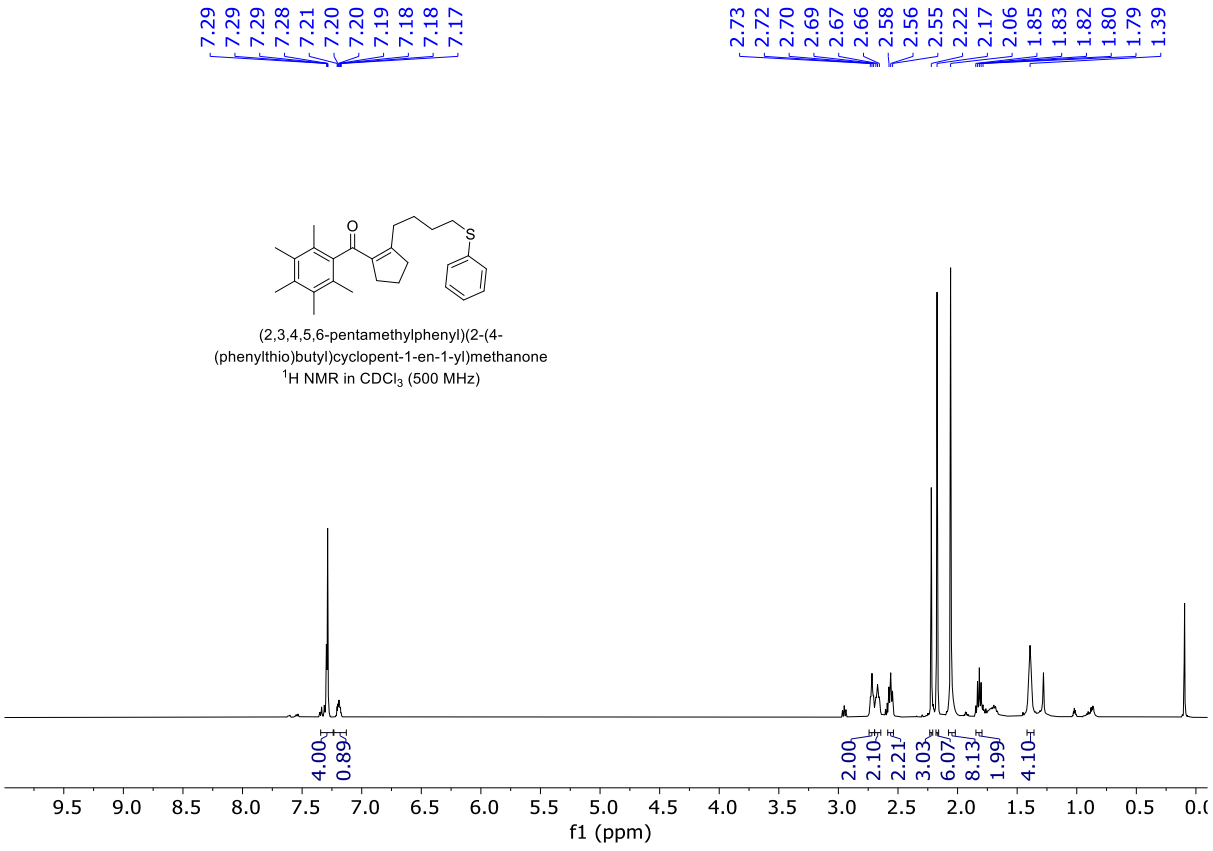




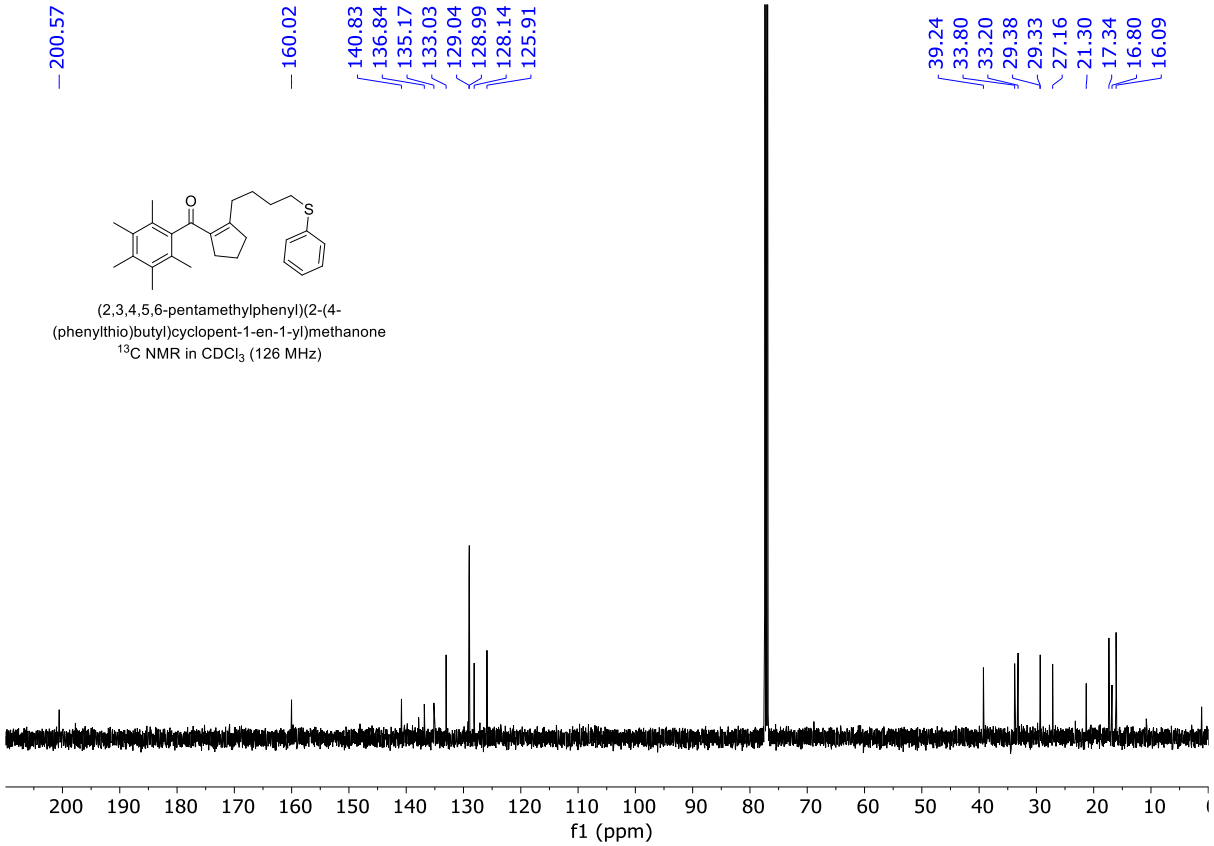
(2,3,4,5,6-pentamethylphenyl)(2-(3-phenylpropyl)cyclopent-1-en-1-yl)methanone
13C NMR $CDCl_3$ (101 MHz)



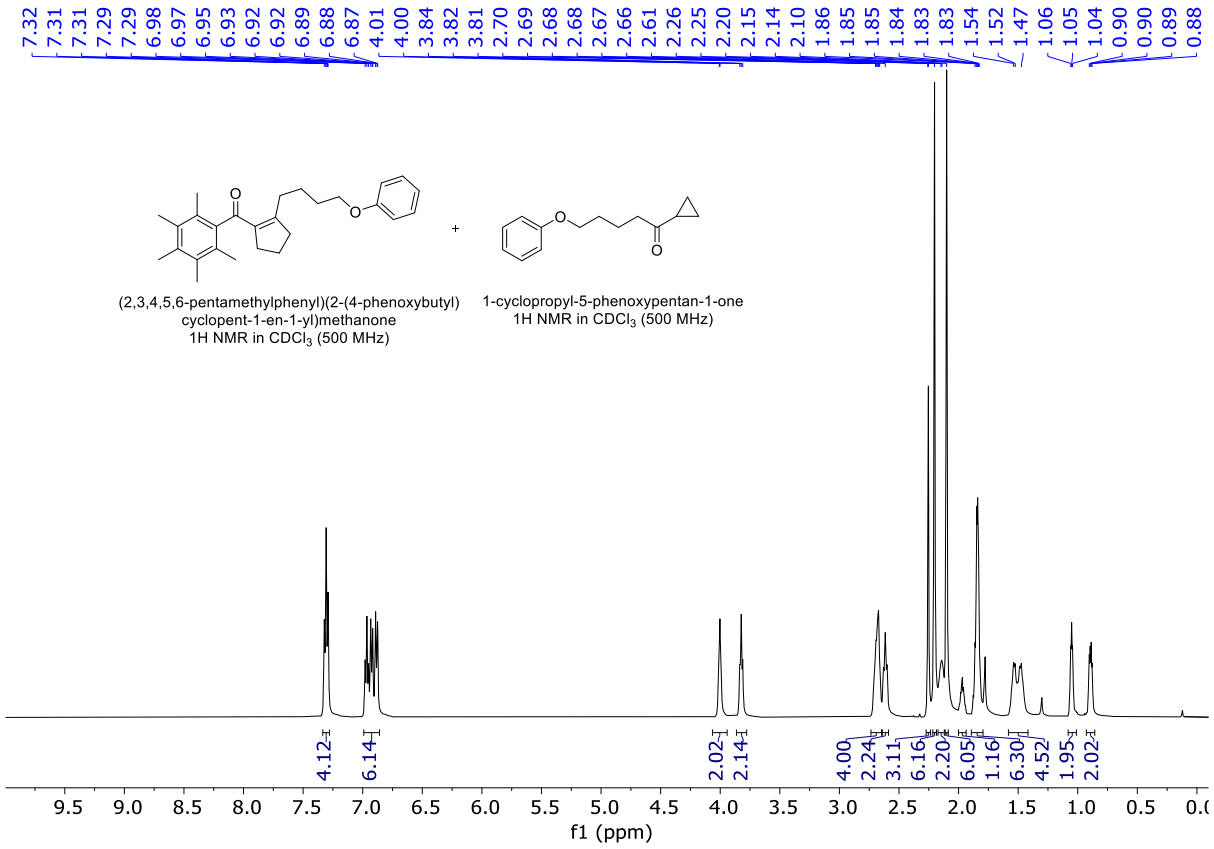
(2,3,4,5,6-pentamethylphenyl)(2-(3-phenylpropyl)cyclopent-1-en-1-yl)methanone
1H NMR $CDCl_3$ (400 MHz)



(2,3,4,5,6-pentamethylphenyl)(2-(4-(phenylthio)butyl)cyclopent-1-en-1-yl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)

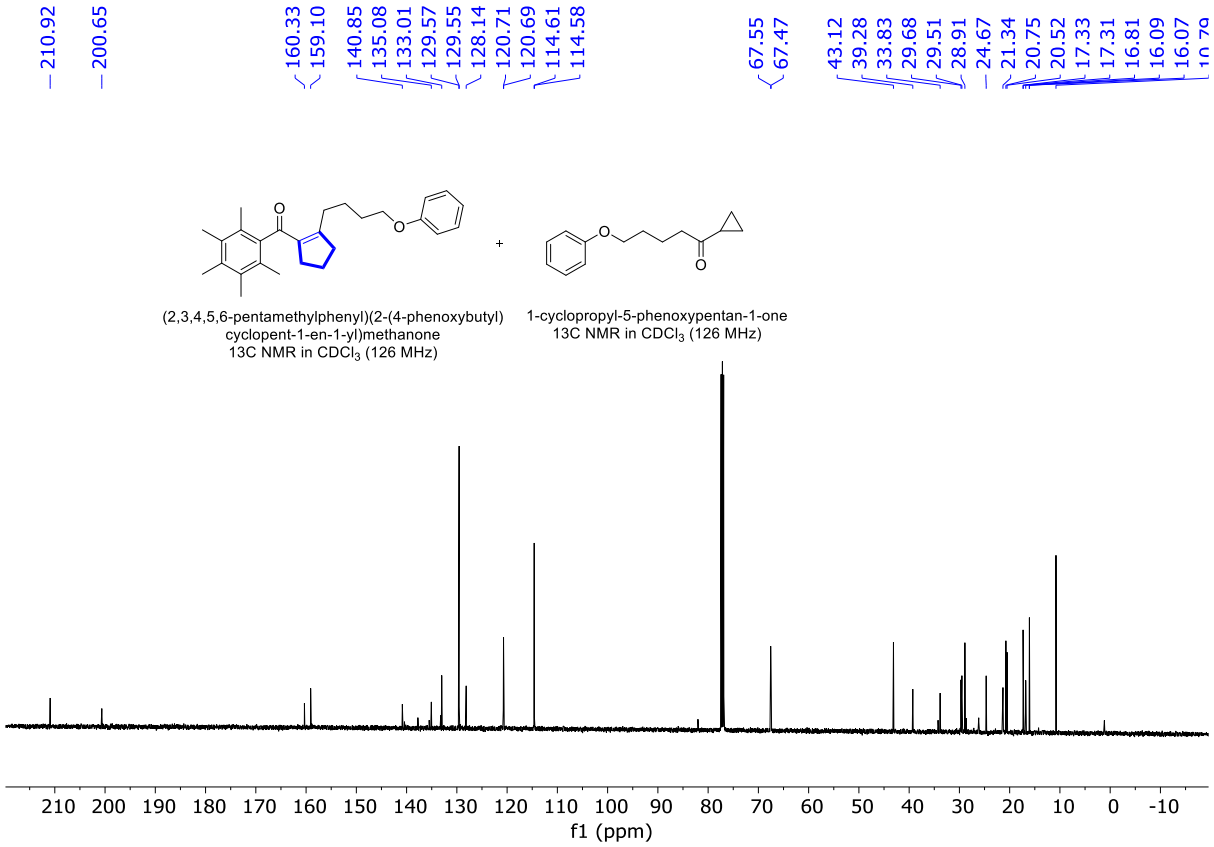


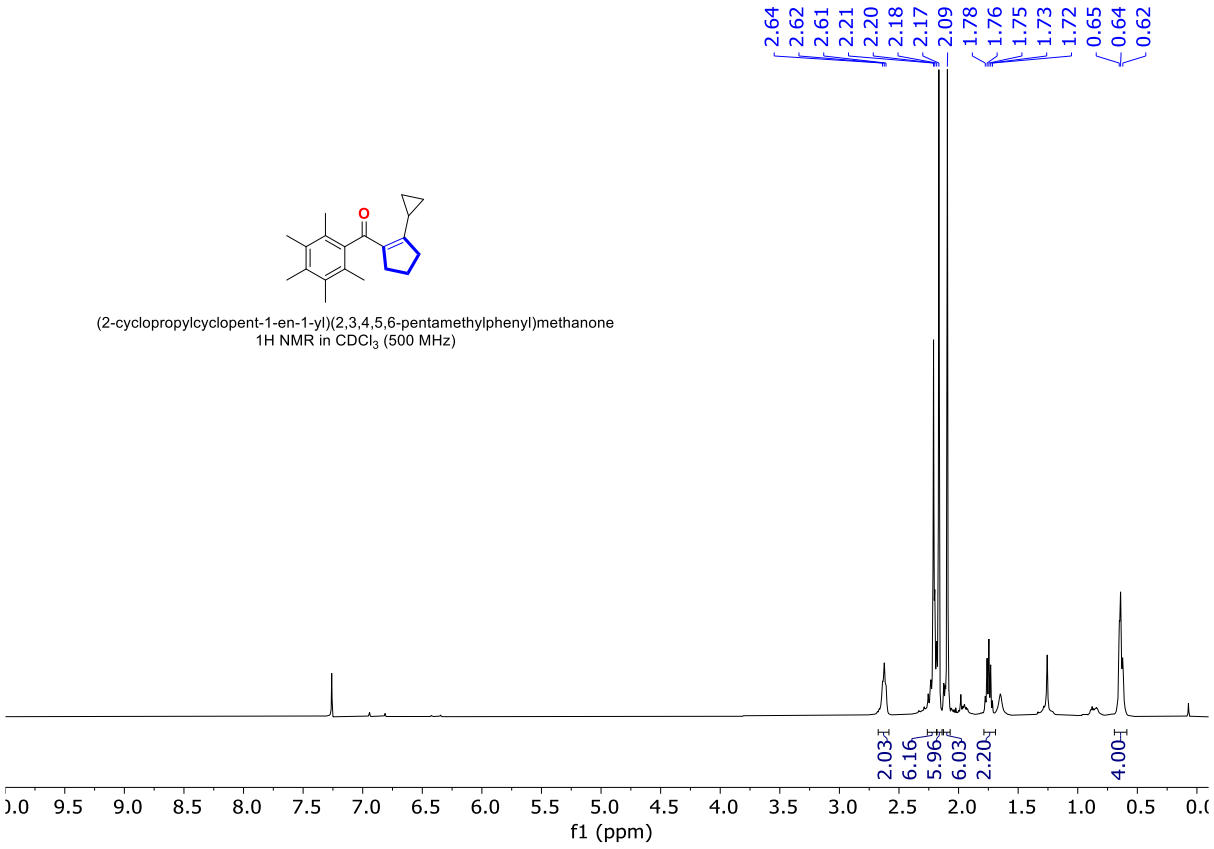
(2,3,4,5,6-pentamethylphenyl)(2-(4-(phenylthio)butyl)cyclopent-1-en-1-yl)methanone
^{13}C NMR in $CDCl_3$ (126 MHz)

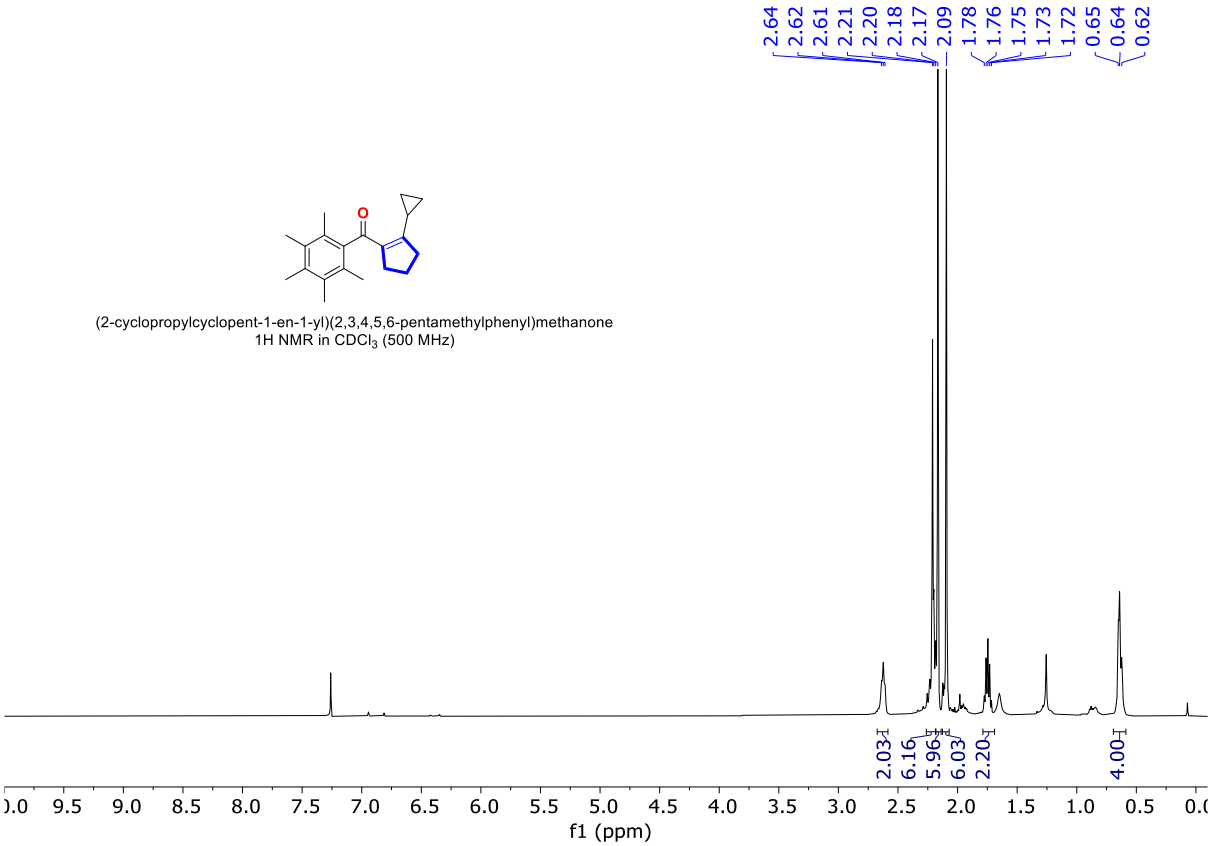


(2,3,4,5,6-pentamethylphenyl)(2-(4-phenoxybutyl)cyclopent-1-en-1-yl)methanone
1H NMR in $CDCl_3$ (500 MHz)

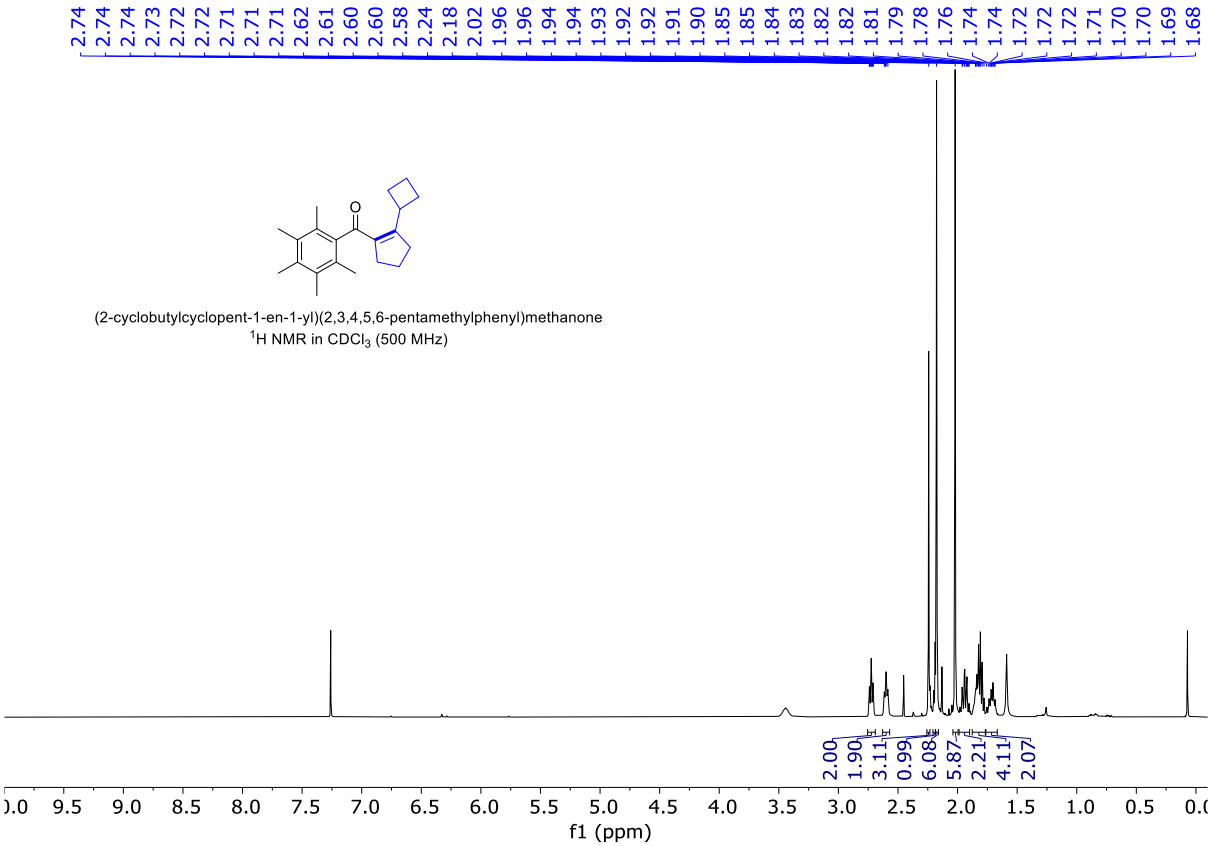
1-cyclopropyl-5-phenoxypentan-1-one
1H NMR in $CDCl_3$ (500 MHz)


210.92
200.65
160.33
159.10
140.85
135.08
133.01
129.57
129.55
128.14
120.71
120.69
114.61
114.58
67.55
67.47
43.12
39.28
33.83
29.68
29.51
28.91
24.67
21.34
20.75
20.52
17.33
17.31
16.81
16.09
16.07
(2,3,4,5,6-pentamethylphenyl)(2-(4-phenoxybutyl) cyclopent-1-en-1-yl)methanone
13C NMR in CDCl3 (126 MHz)
1-cyclopropyl-5-phenoxypentan-1-one
13C NMR in CDCl3 (126 MHz)
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)

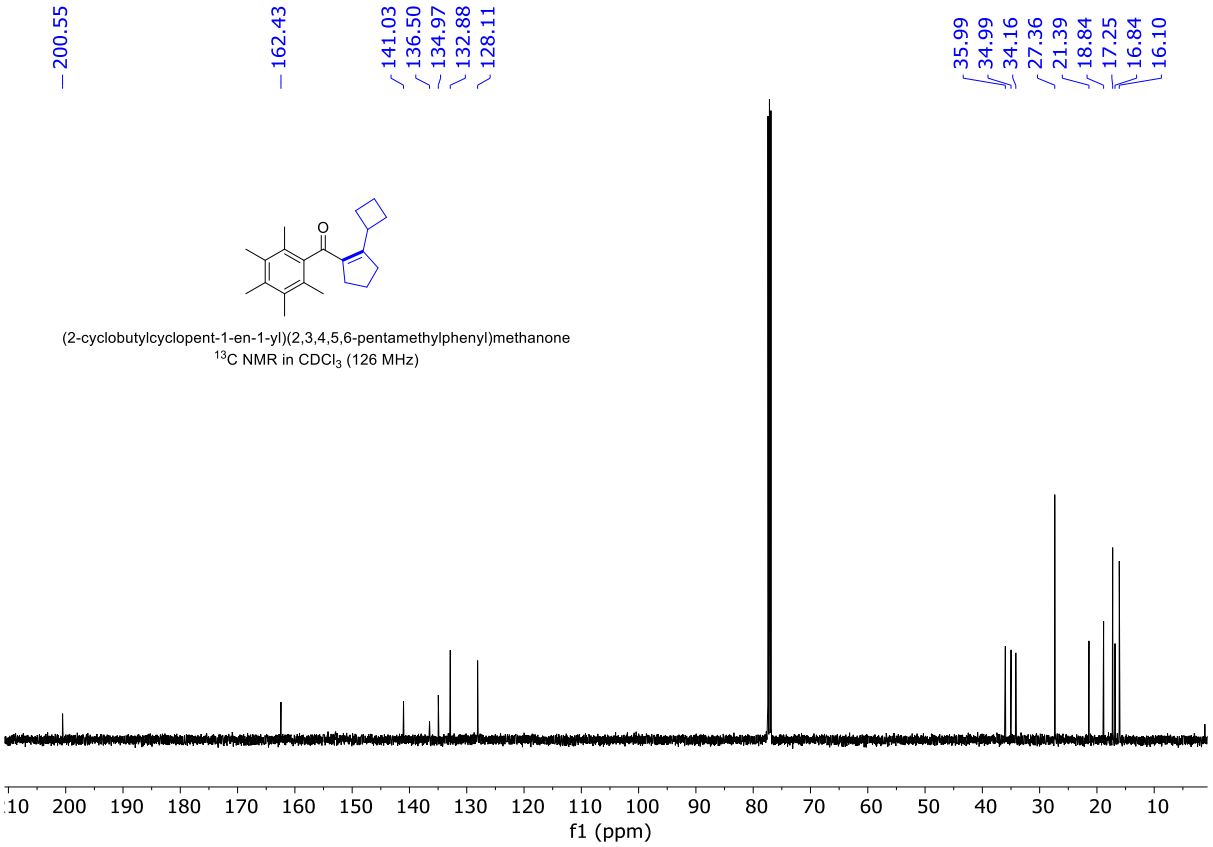

2.64
2.62
2.61
2.21
2.20
2.18
2.17
2.09
1.78
1.76
1.75
1.73
1.72
0.65
0.64
0.62
(2-cyclopropylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
2.03
6.16
5.96
6.03
2.20
4.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

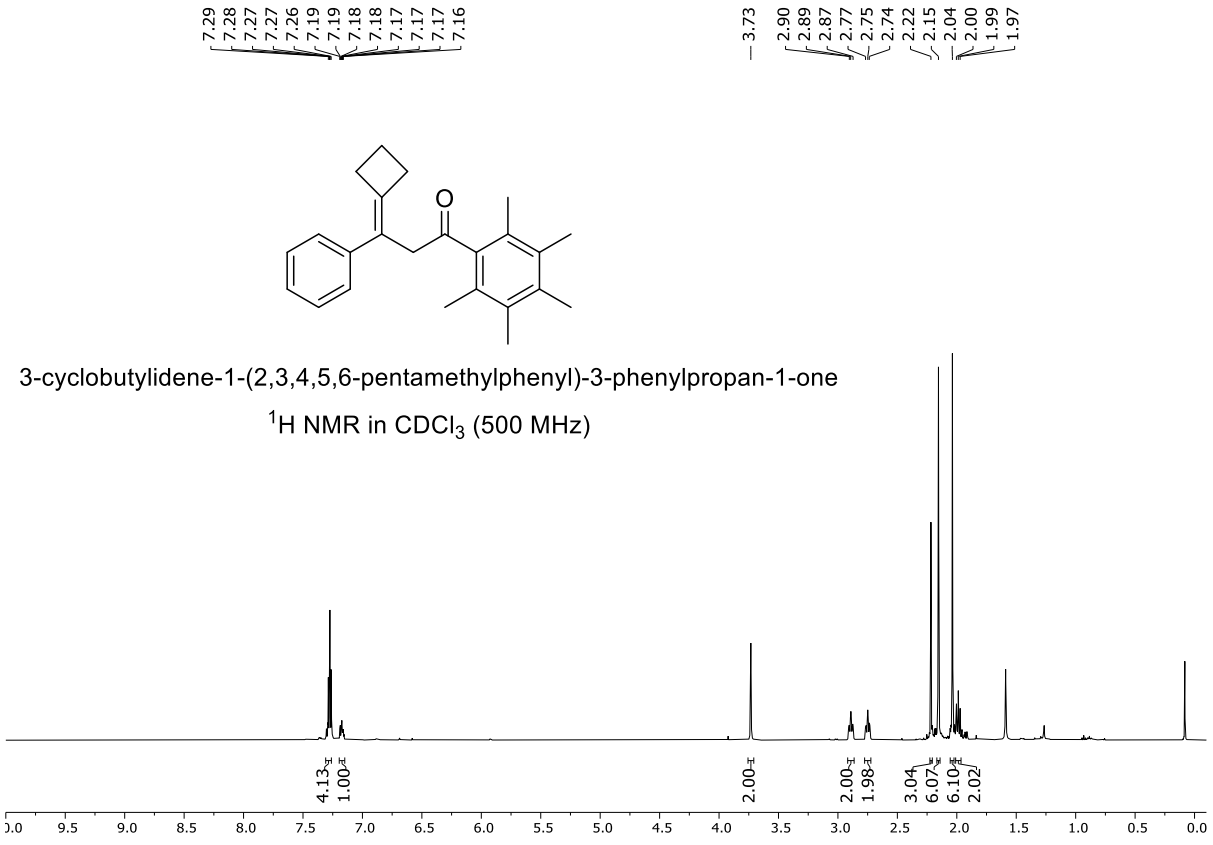


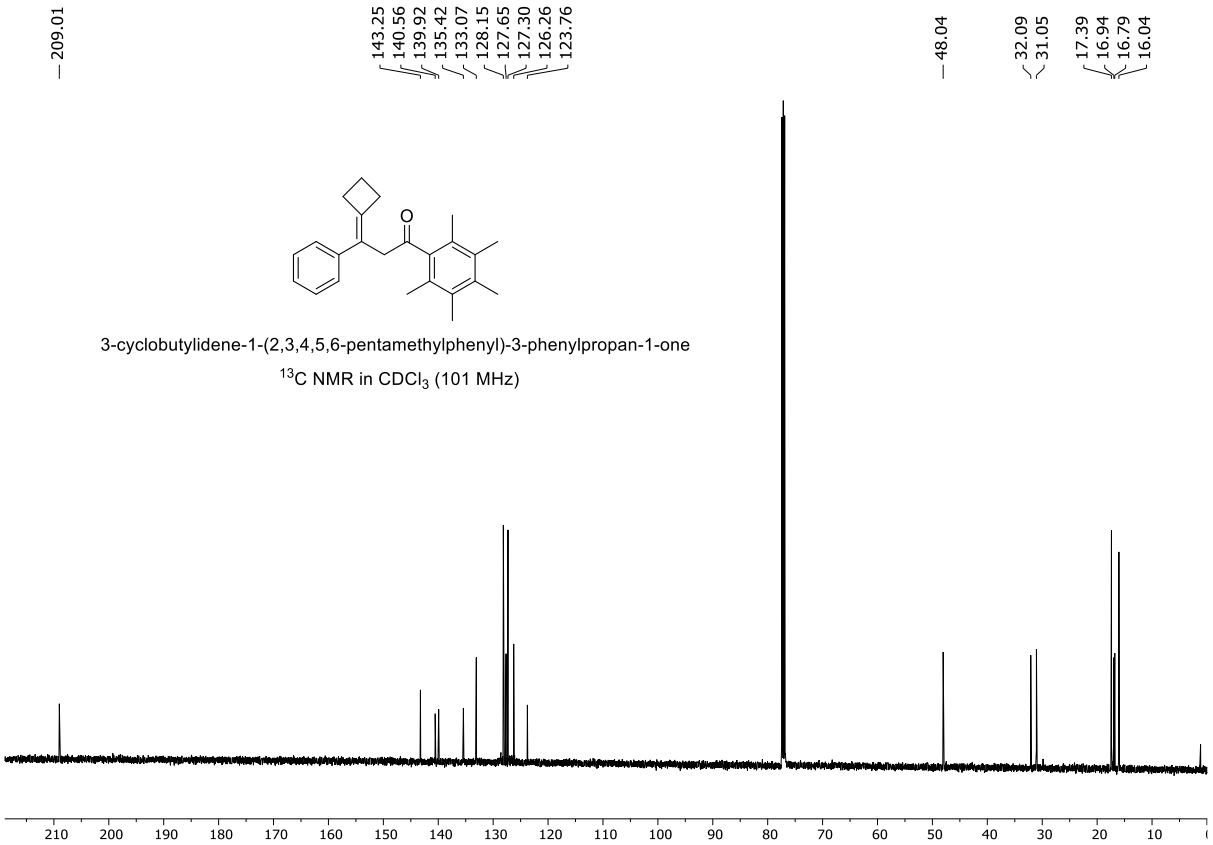
(2-cyclopropylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in $CDCl_3$ (500 MHz)



(2-cyclobutylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)

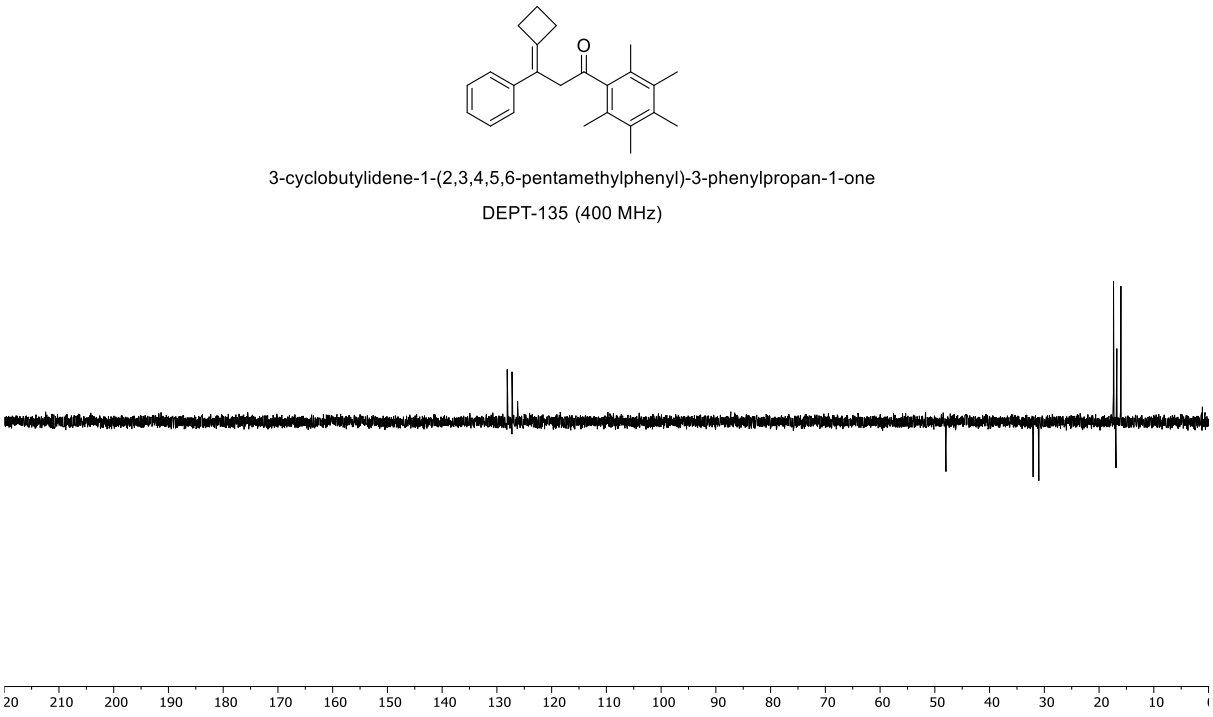

200.55
162.43
141.03
136.50
134.97
132.88
128.11
35.99
34.99
34.16
27.36
21.39
18.84
17.25
16.84
16.10
O
(2-cyclobutylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


7.29
7.28
7.27
7.27
7.26
7.19
7.19
7.18
7.18
7.17
7.17
7.17
7.16
3.73
2.90
2.89
2.87
2.77
2.75
2.74
2.22
2.15
2.04
2.00
1.99
1.97
O
3-cyclobutylidene-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one
1H NMR in CDCl3 (500 MHz)
4.13
1.00
2.00
2.00
1.98
3.04
6.07
6.10
2.02



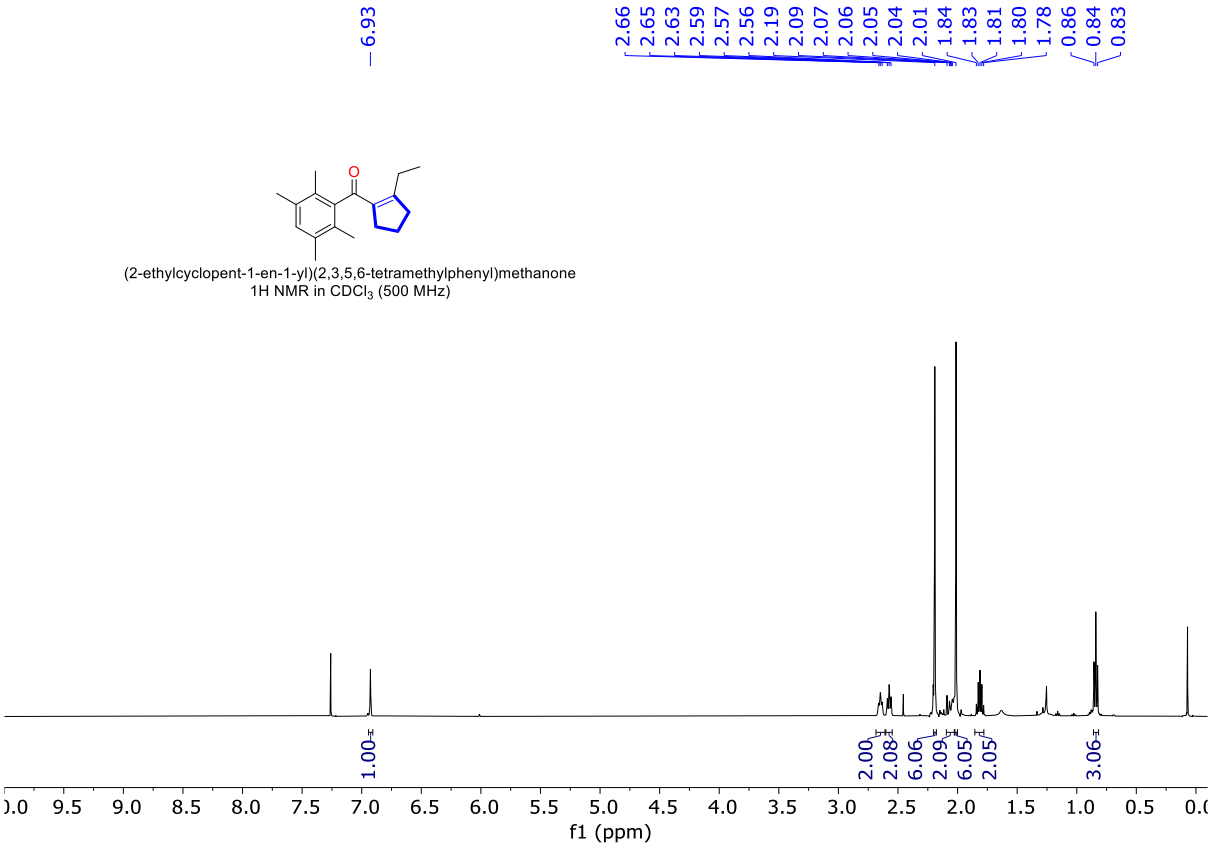
3-cyclobutylidene-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one

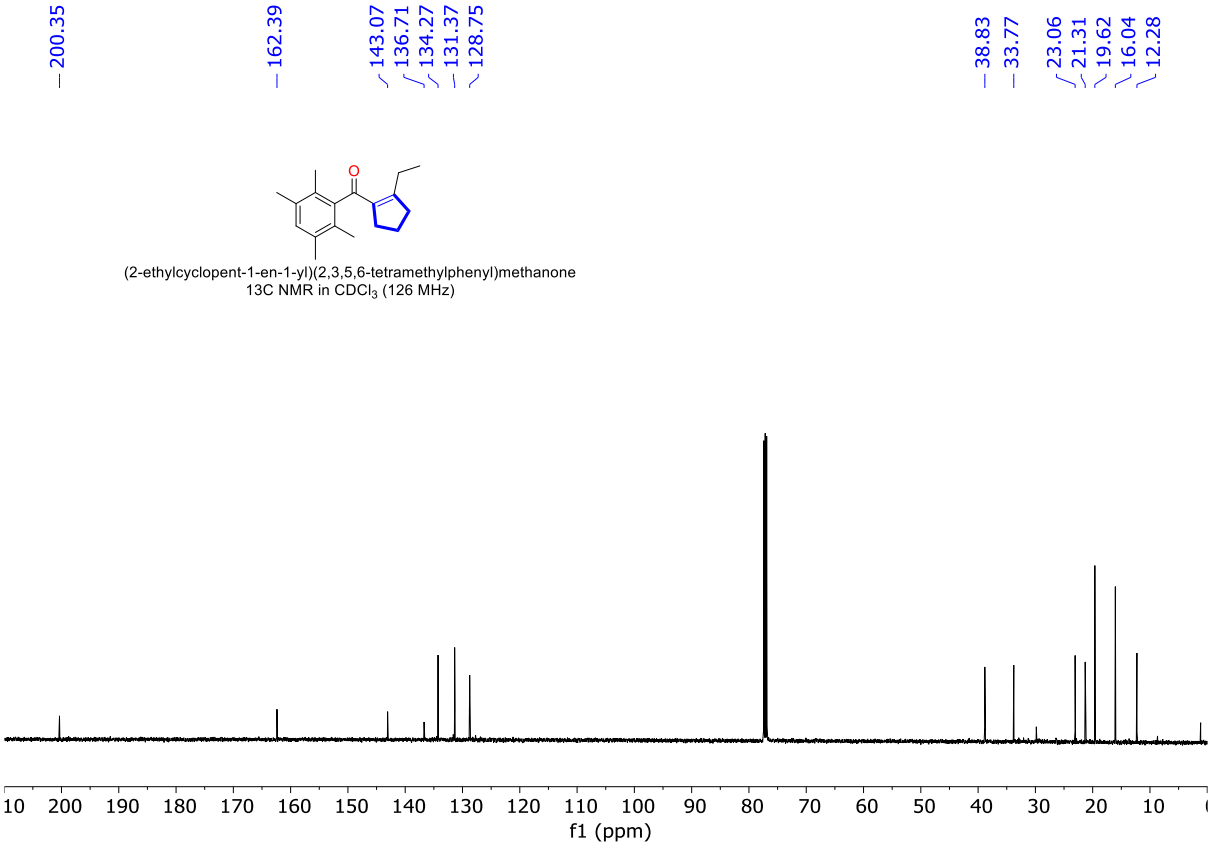
^{13}C NMR in $CDCl_3$ (101 MHz)

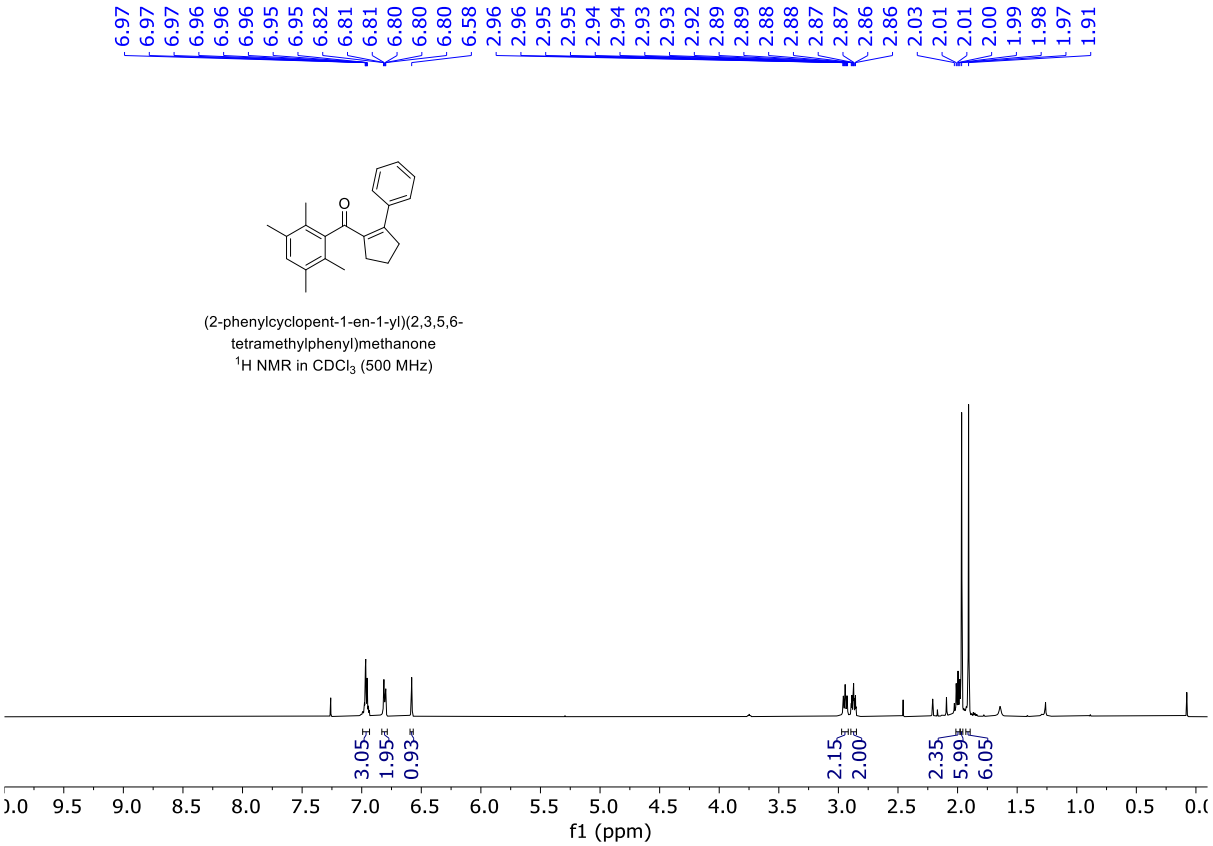


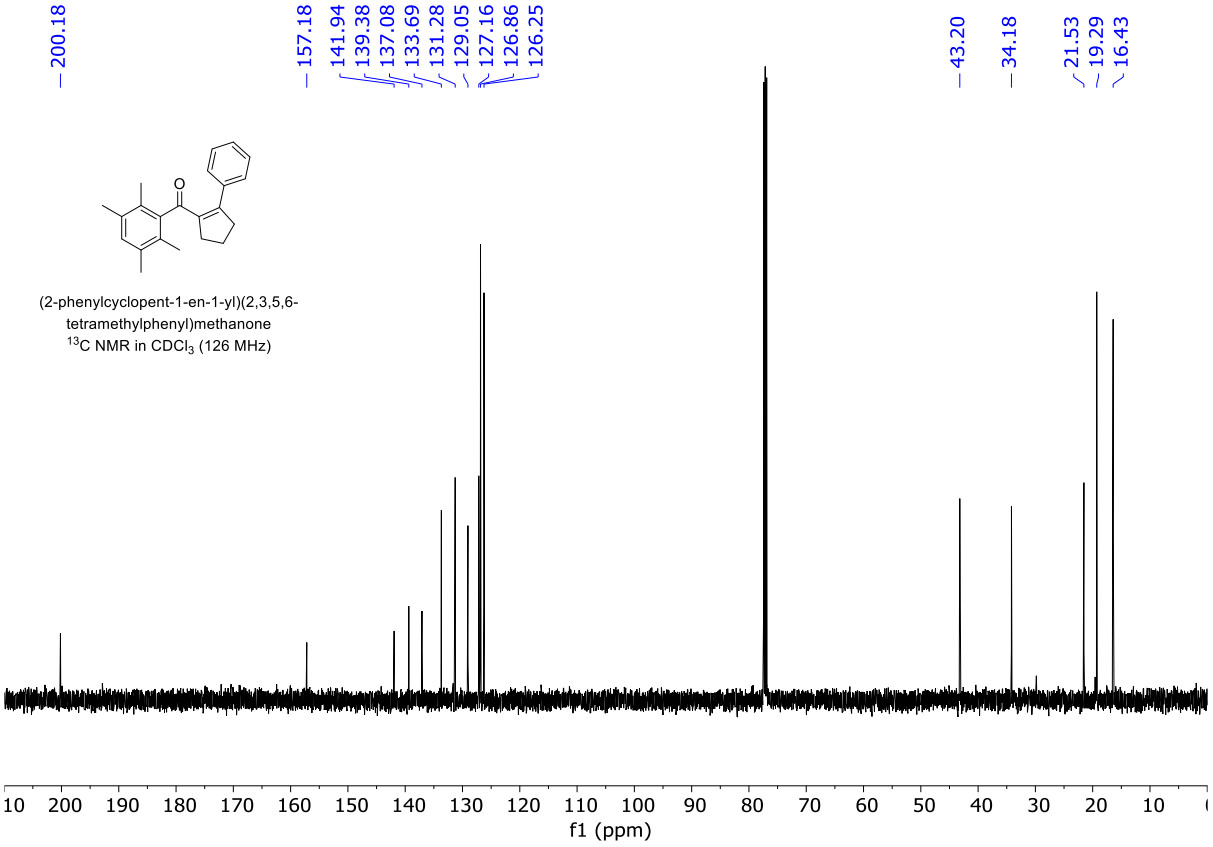
3-cyclobutylidene-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one

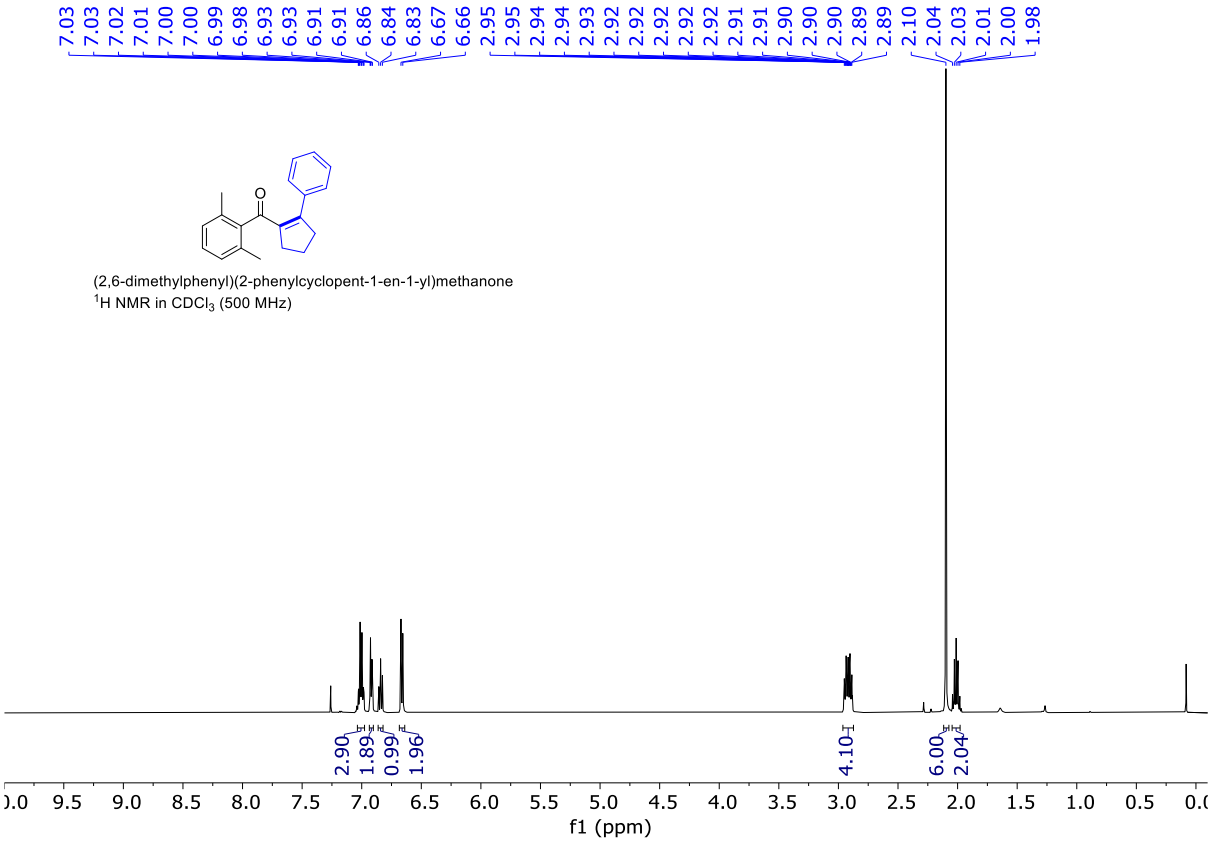
DEPT-135 (400 MHz)

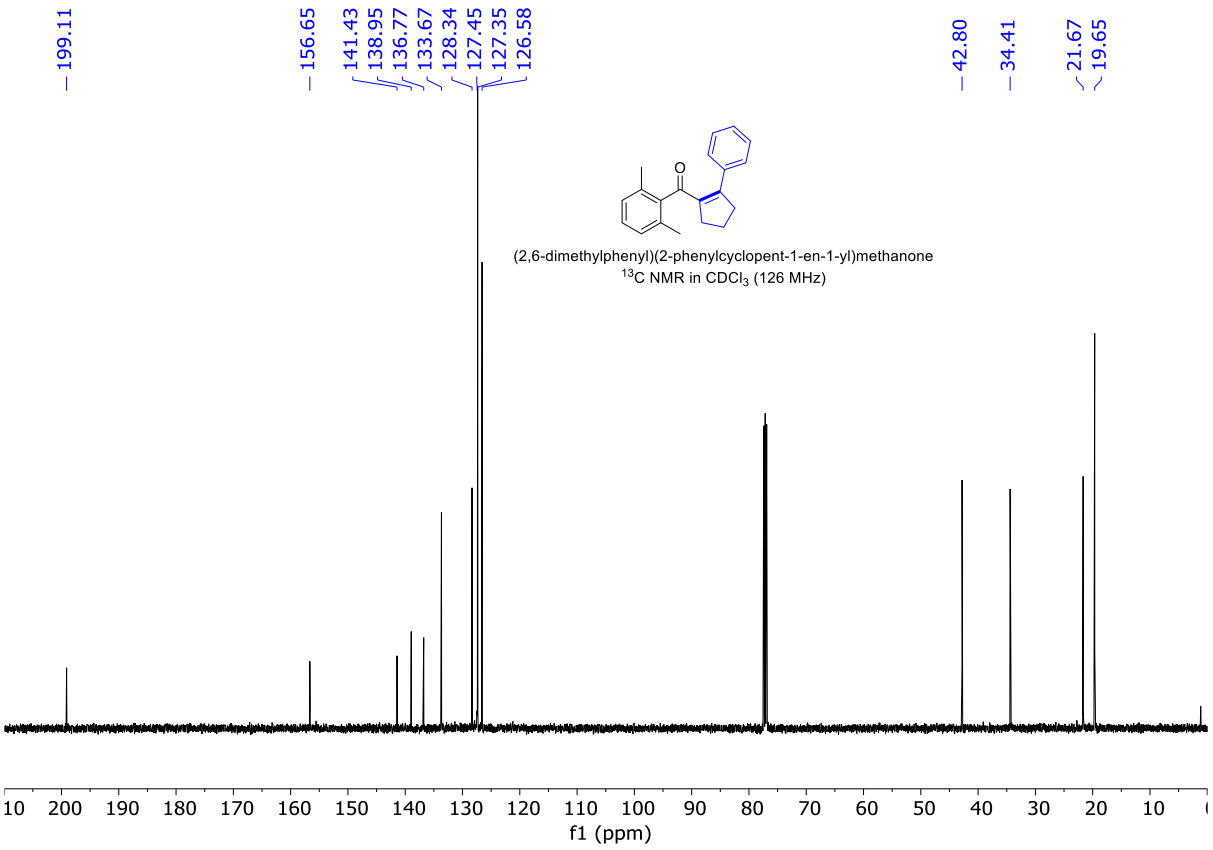

6.93
2.66
2.65
2.63
2.59
2.57
2.56
2.19
2.09
2.07
2.06
2.05
2.04
2.01
1.84
1.83
1.81
1.80
1.78
0.86
0.84
0.83
O
(2-ethylcyclopent-1-en-1-yl)(2,3,5,6-tetramethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
1.00
2.00
2.08
6.06
2.09
6.05
2.05
3.06
f1 (ppm)

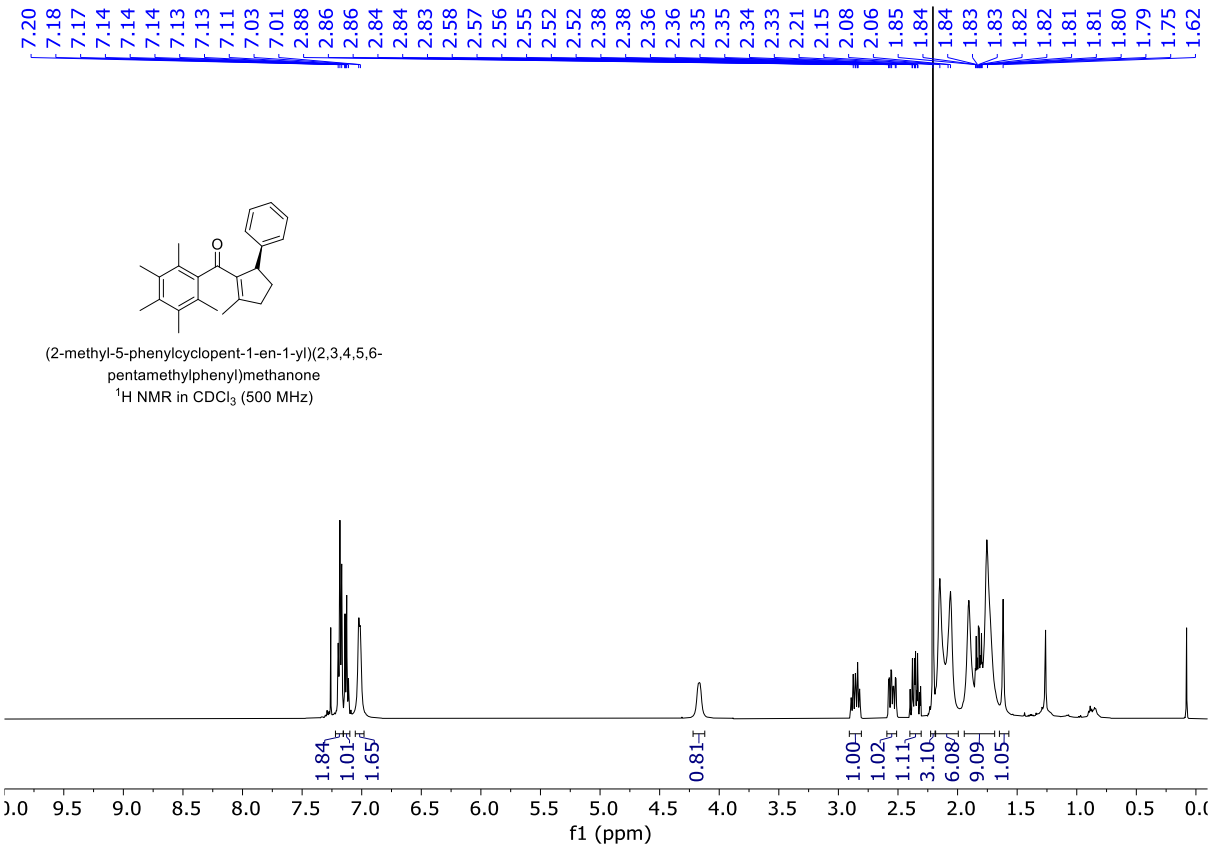

200.35
162.39
143.07
136.71
134.27
131.37
128.75
38.83
33.77
23.06
21.31
19.62
16.04
12.28
O
(2-ethylcyclopent-1-en-1-yl)(2,3,5,6-tetramethylphenyl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

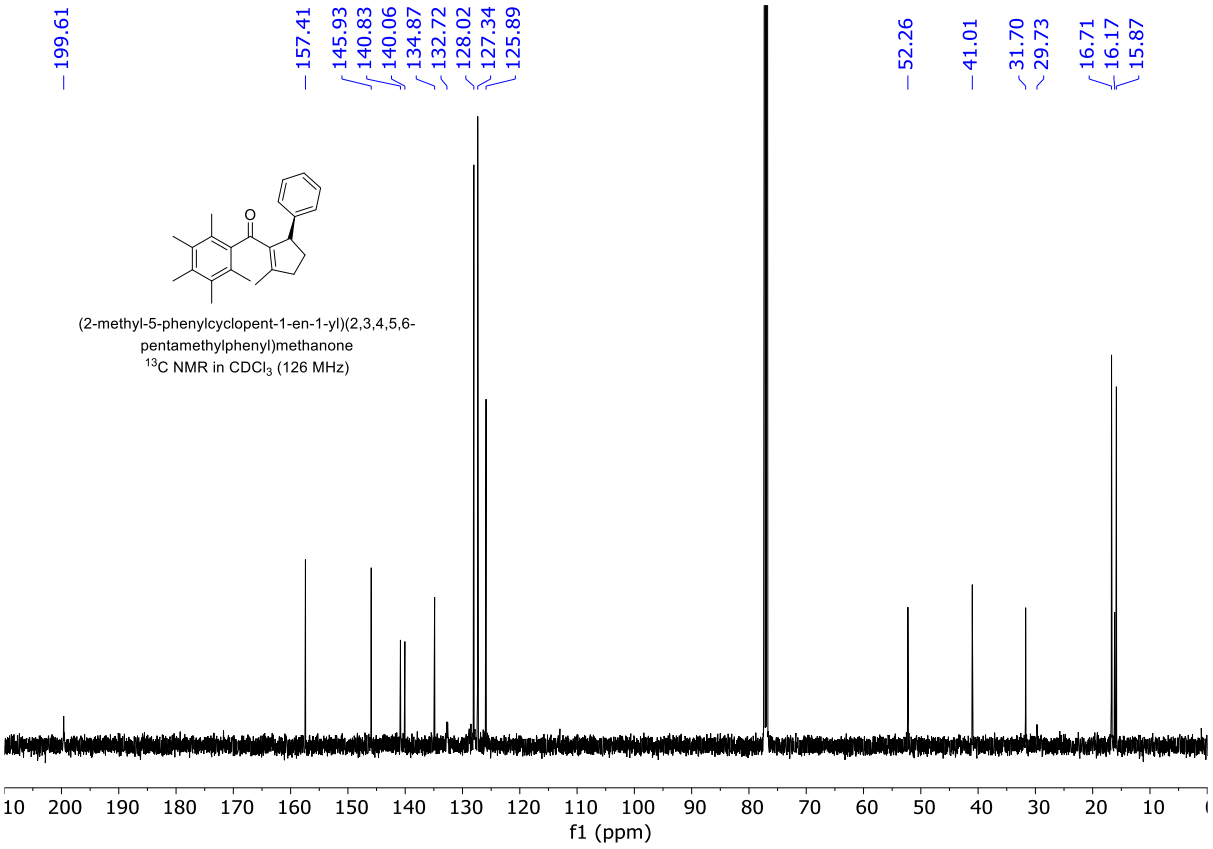

6.97 6.97 6.97 6.96 6.96 6.96 6.95 6.95 6.82 6.81 6.81 6.80 6.80 6.80 6.58
2.96 2.96 2.95 2.95 2.94 2.94 2.93 2.93 2.92 2.89 2.89 2.88 2.88 2.87 2.87 2.86 2.86
2.03 2.01 2.01 2.00 1.99 1.98 1.97 1.91
O
(2-phenylcyclopent-1-en-1-yl)(2,3,5,6-tetramethylphenyl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)
3.05 1.95 0.93 2.15 2.00 2.35 5.99 6.05
f1 (ppm)

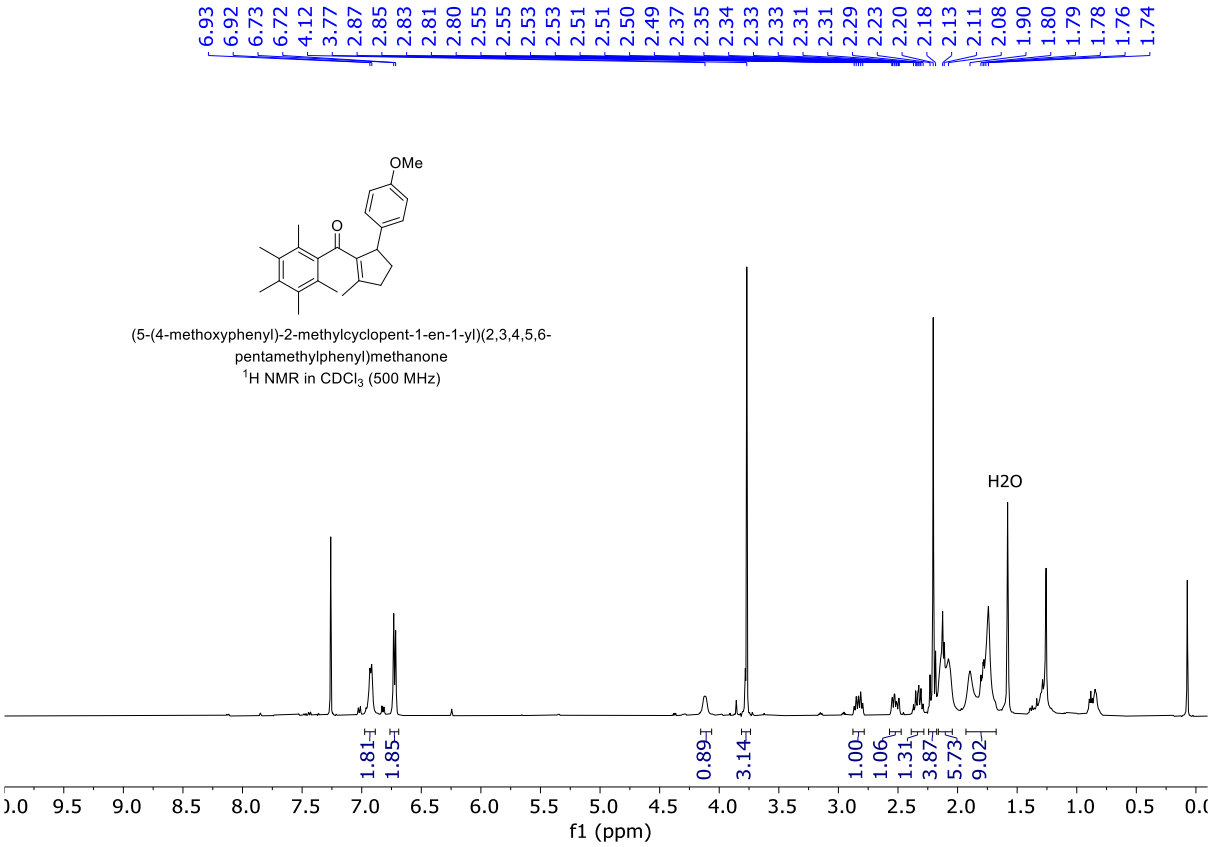

200.18
157.18 141.94 139.38 137.08 133.69 131.28 129.05 127.16 126.86 126.25
43.20 34.18 21.53 19.29 16.43
O
(2-phenylcyclopent-1-en-1-yl)(2,3,5,6-tetramethylphenyl)methanone
^{13}C NMR in $CDCl_3$ (126 MHz)
f1 (ppm)

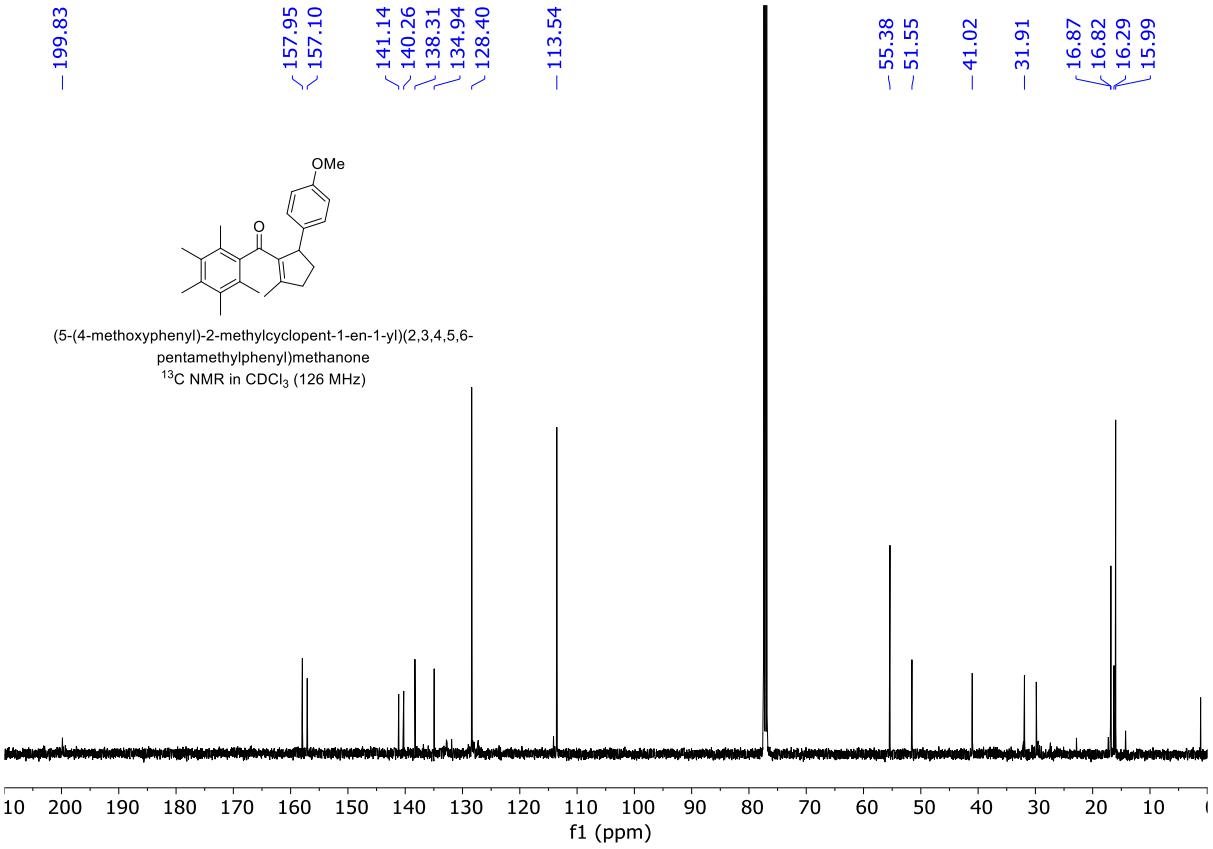

7.03 7.03 7.02 7.01 7.00 7.00 6.99 6.98 6.93 6.93 6.91 6.91 6.86 6.84 6.83 6.67 6.66
2.95 2.95 2.94 2.94 2.93 2.92 2.92 2.92 2.92 2.92 2.91 2.91 2.90 2.90 2.90 2.89 2.89
2.10 2.04 2.03 2.01 2.00 1.98
O
(2,6-dimethylphenyl)(2-phenylcyclopent-1-en-1-yl)methanone
1H NMR in CDCl3 (500 MHz)
2.90 1.89 0.99 1.96 4.10 6.00 2.04
f1 (ppm)

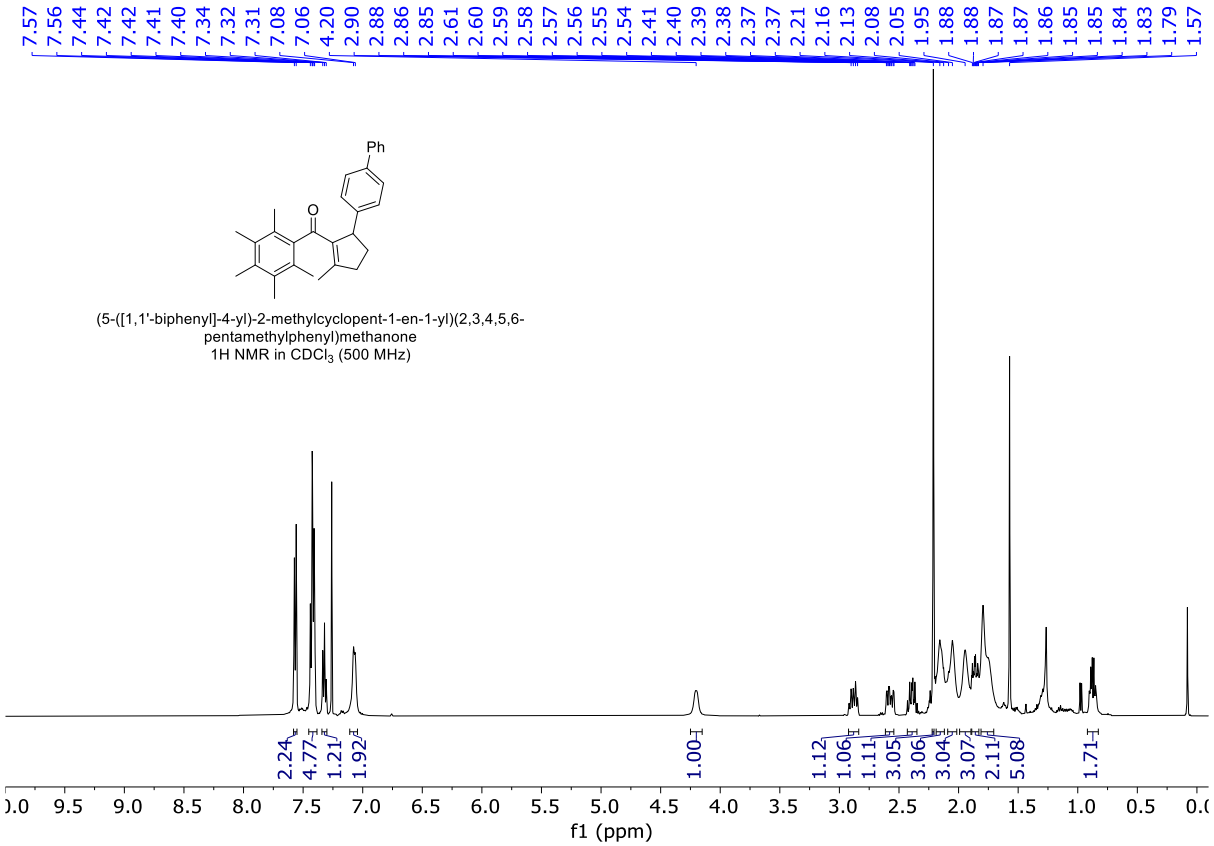

199.11
156.65
141.43 138.95 136.77 133.67 128.34 127.45 127.35 126.58
42.80 34.41 21.67 19.65
O
(2,6-dimethylphenyl)(2-phenylcyclopent-1-en-1-yl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

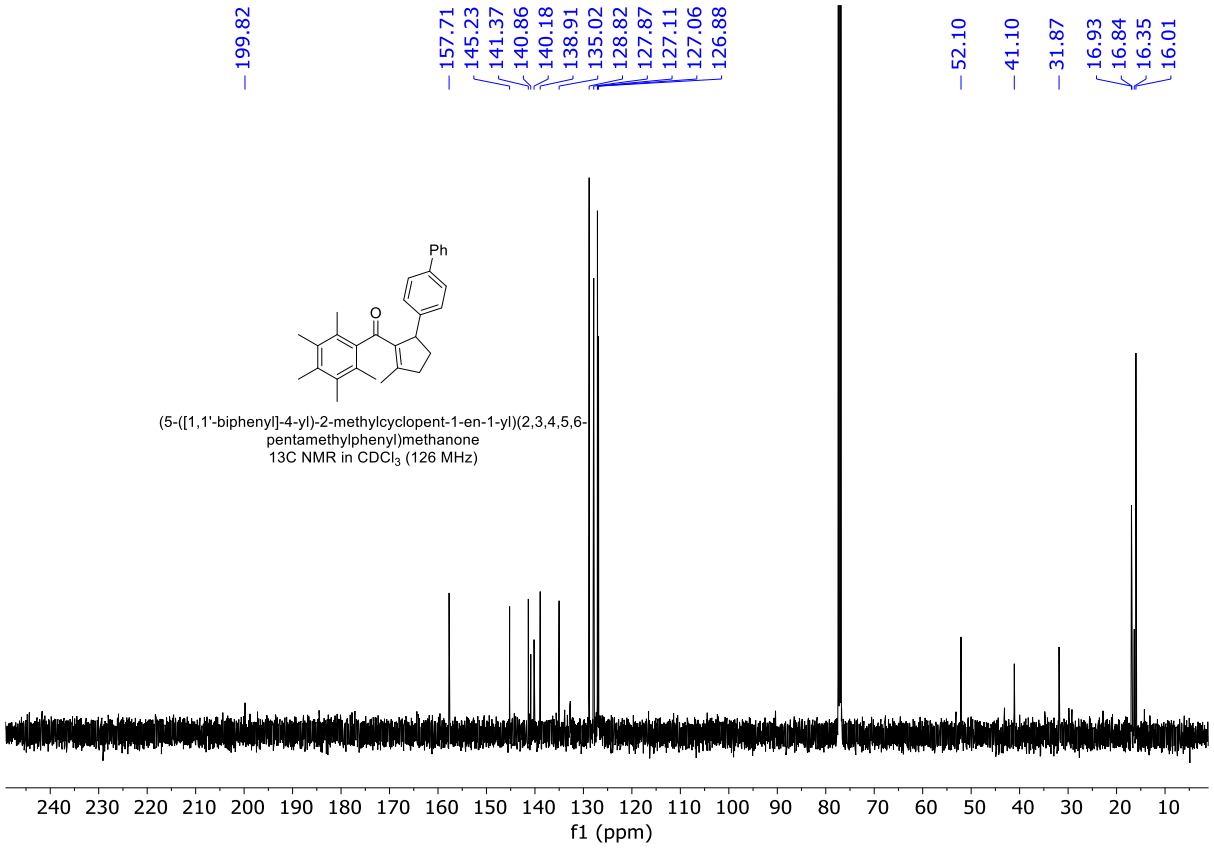

7.20 7.18 7.17 7.14 7.14 7.14 7.13 7.13 7.11 7.03 7.01 2.88 2.86 2.86 2.84 2.84 2.83 2.58 2.57 2.56 2.55 2.52 2.52 2.38 2.38 2.36 2.36 2.35 2.35 2.34 2.33 2.21 2.15 2.08 2.06 1.85 1.84 1.84 1.83 1.83 1.82 1.82 1.81 1.81 1.80 1.79 1.75 1.62
O
(2-methyl-5-phenylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)
1.84 1.01 1.65 0.81 1.00 1.02 1.11 3.10 6.08 9.09 1.05
f1 (ppm)

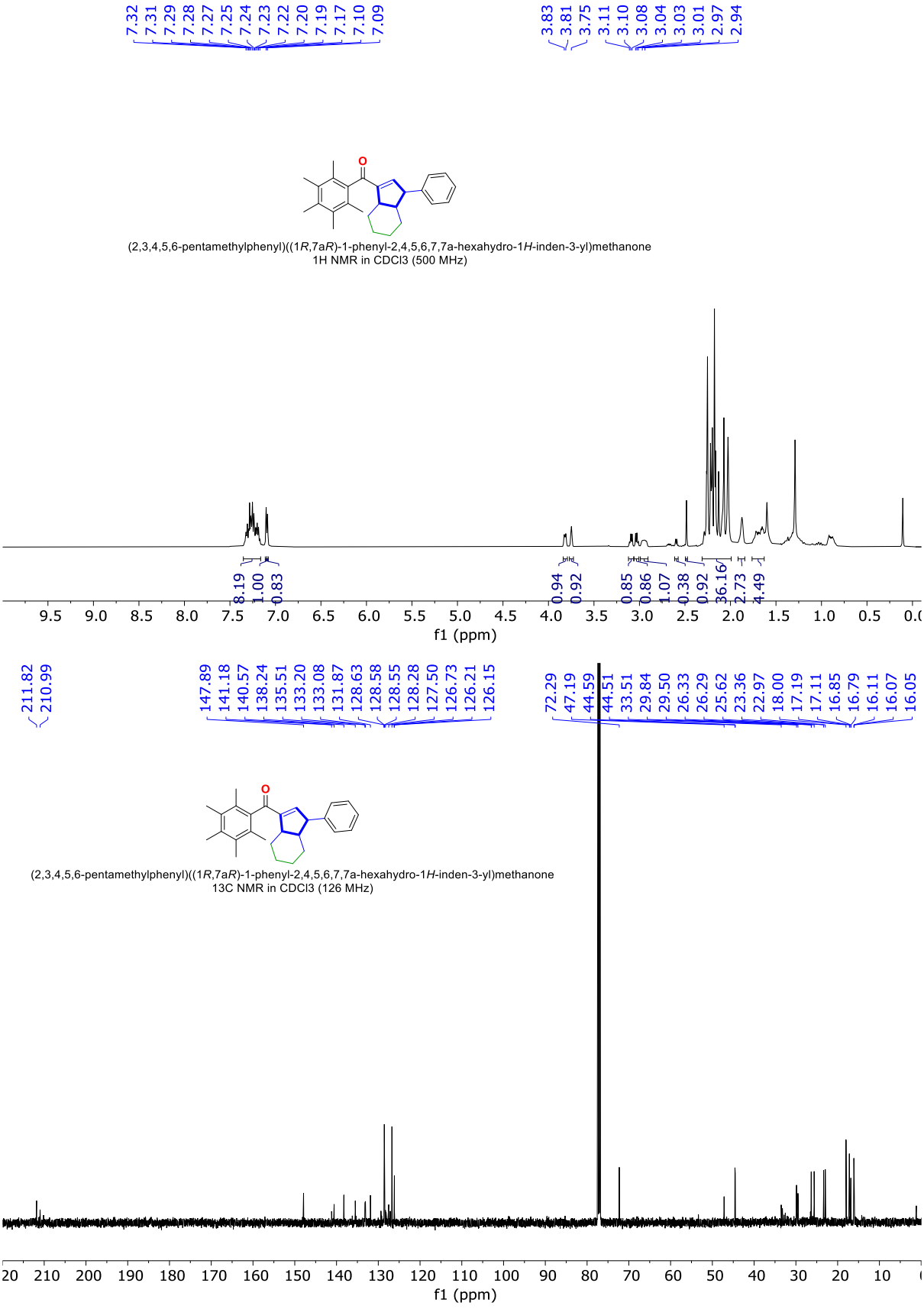

199.61 157.41 145.93 140.83 140.06 134.87 132.72 128.02 127.34 125.89 52.26 41.01 31.70 29.73 16.71 16.17 15.87
O
(2-methyl-5-phenylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
^{13}C NMR in $CDCl_3$ (126 MHz)
f1 (ppm)

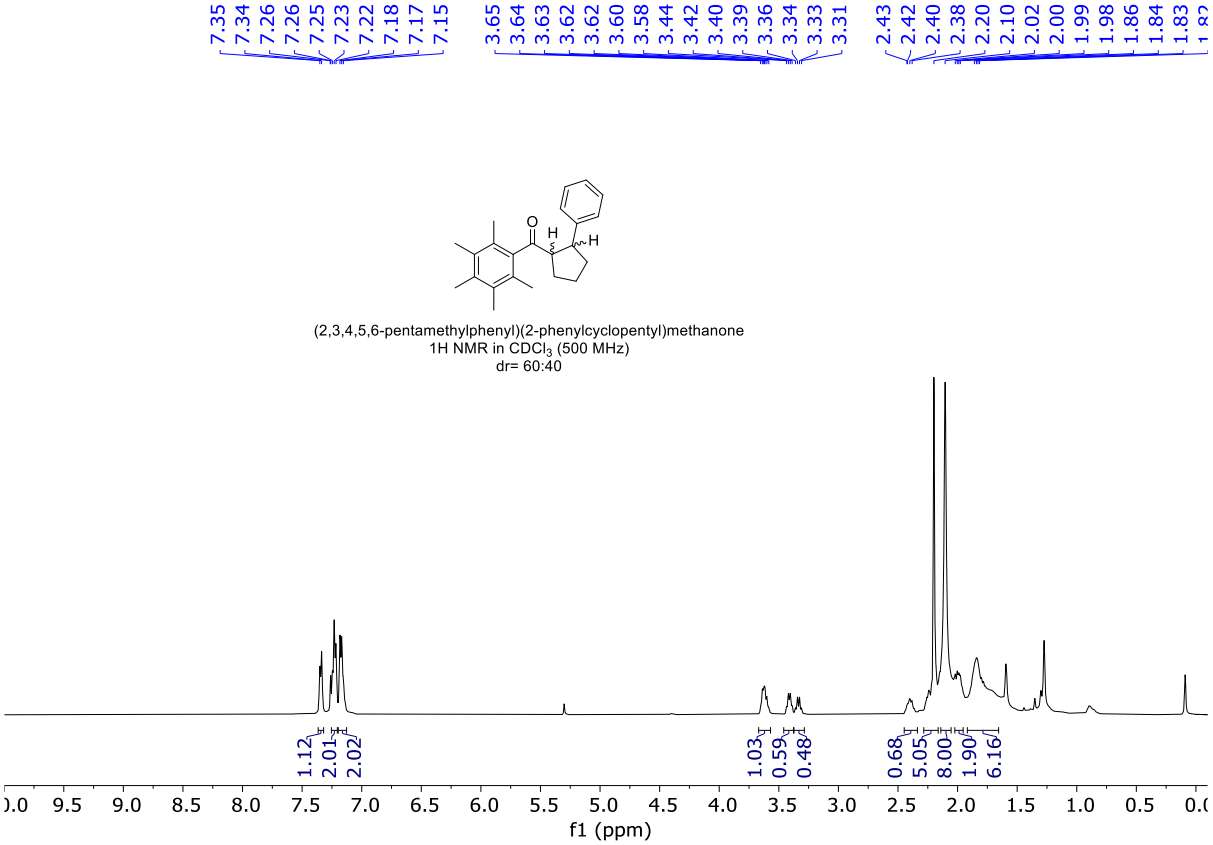

6.93 6.92 6.73 6.72 4.12 3.77 2.87 2.85 2.83 2.81 2.80 2.55 2.55 2.53 2.53 2.51 2.51 2.50 2.49 2.37 2.35 2.34 2.33 2.33 2.31 2.31 2.29 2.23 2.20 2.18 2.13 2.11 2.08 1.90 1.80 1.79 1.78 1.76 1.74
OMe
O
(5-(4-methoxyphenyl)-2-methylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
H2O
1.81 1.85 0.89 3.14 1.00 1.06 1.31 3.87 5.73 9.02
f1 (ppm)

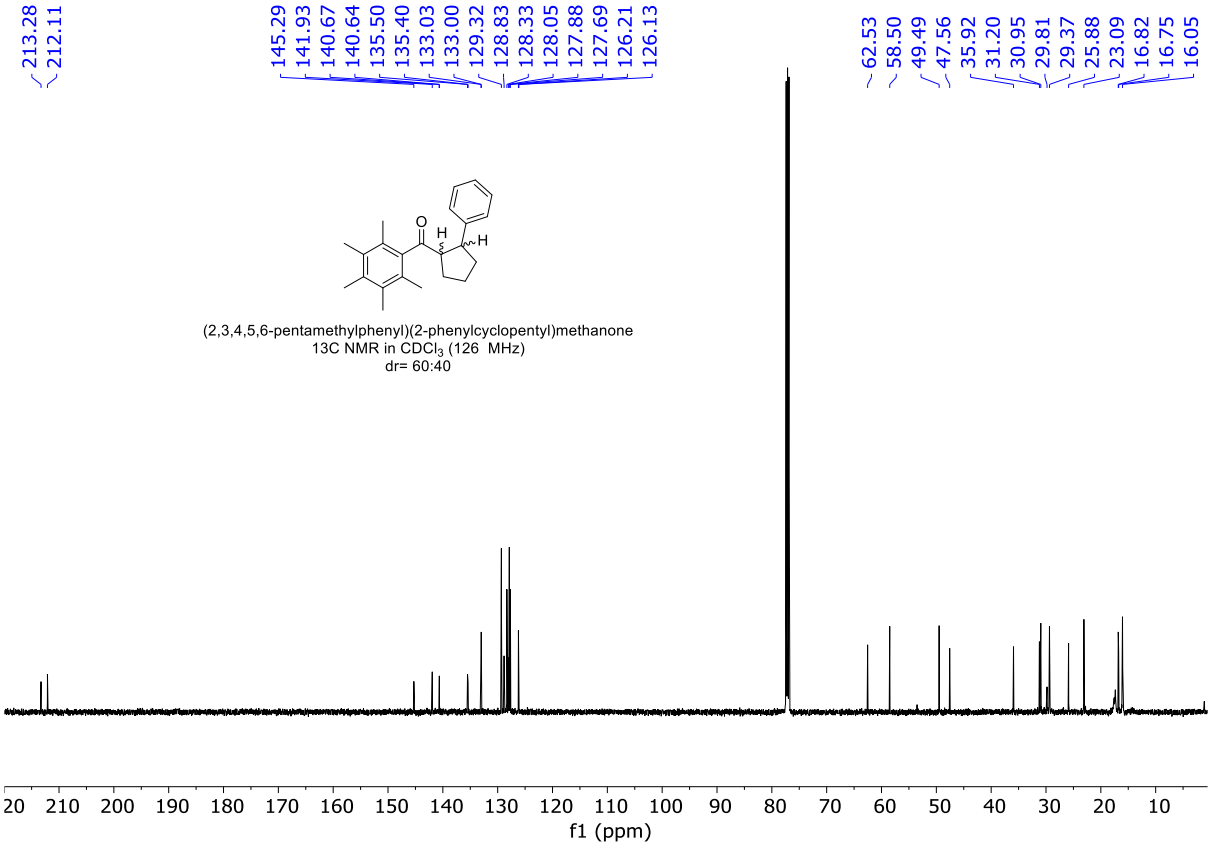

199.83
157.95 157.10 141.14 140.26 138.31 134.94 128.40 113.54
55.38 51.55 41.02 31.91 16.87 16.82 16.29 15.99
OMe
O
(5-(4-methoxyphenyl)-2-methylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

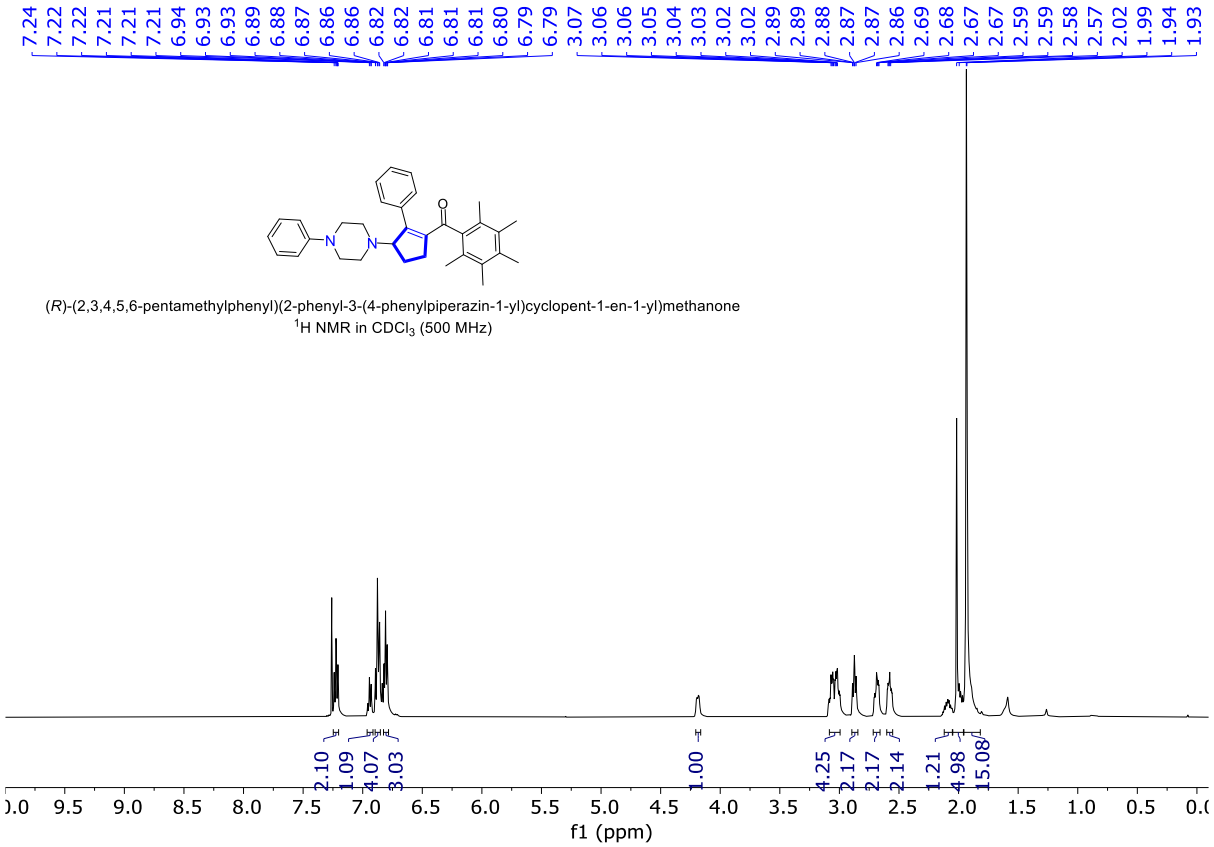

7.57 7.56 7.44 7.42 7.42 7.41 7.40 7.34 7.32 7.31 7.08 7.06 4.20 2.90 2.88 2.86 2.85 2.61 2.60 2.59 2.58 2.57 2.56 2.55 2.54 2.41 2.40 2.39 2.38 2.37 2.37 2.21 2.16 2.13 2.08 2.05 1.95 1.88 1.88 1.87 1.87 1.86 1.85 1.85 1.84 1.83 1.79 1.57
Ph
O
(5-([1,1'-biphenyl]-4-yl)-2-methylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in CDCl3 (500 MHz)
2.24 4.77 1.21 1.92 1.00 1.12 1.06 1.11 3.05 3.06 3.04 3.07 2.11 5.08 1.71
f1 (ppm)


199.82 157.71 145.23 141.37 140.86 140.18 138.91 135.02 128.82 127.87 127.11 127.06 126.88 52.10 41.10 31.87 16.93 16.84 16.35 16.01
Ph
O
(5-([1,1'-biphenyl]-4-yl)-2-methylcyclopent-1-en-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

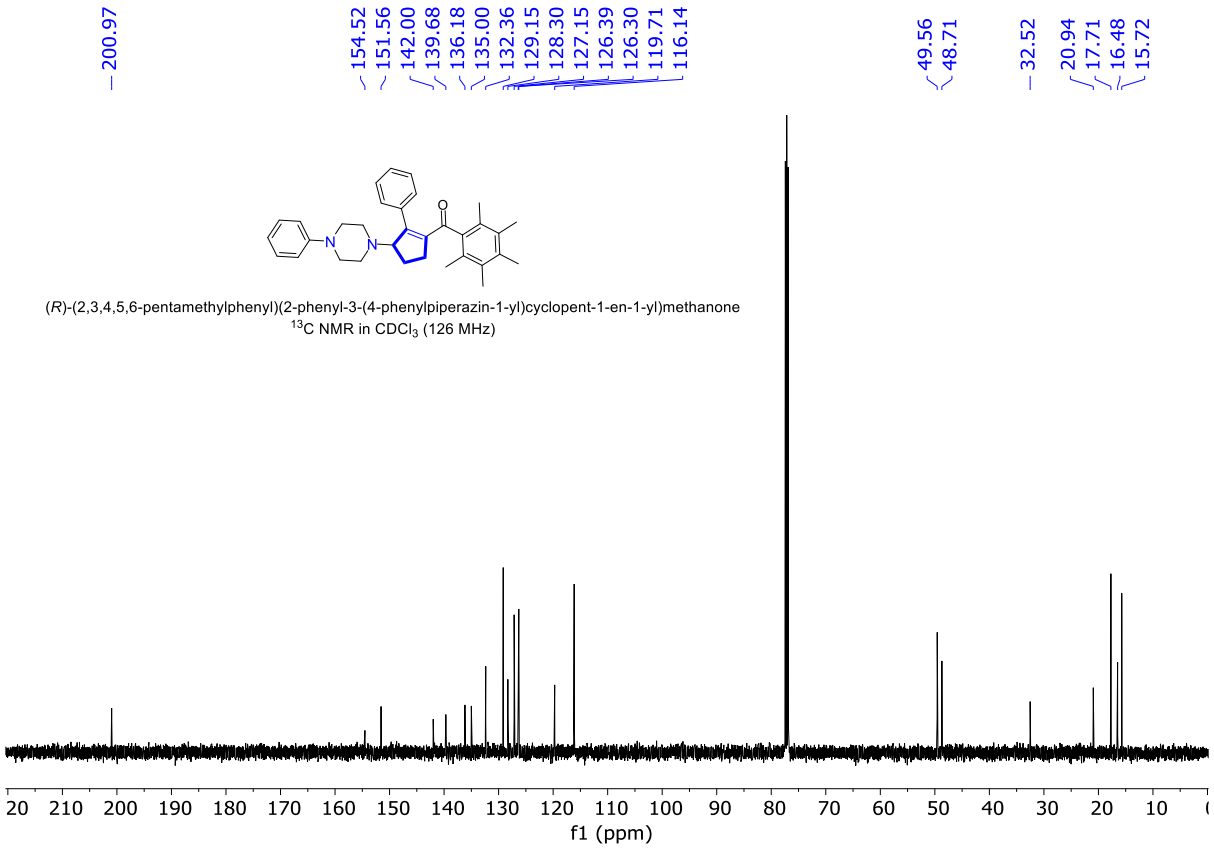

7.32
7.31
7.29
7.28
7.27
7.25
7.24
7.23
7.22
7.20
7.19
7.17
7.10
7.09
3.83
3.81
3.75
3.11
3.10
3.08
3.04
3.03
3.01
2.97
2.94
O
(2,3,4,5,6-pentamethylphenyl)((1R,7aR)-1-phenyl-2,4,5,6,7,7a-hexahydro-1H-inden-3-yl)methanone
1H NMR in CDCl3 (500 MHz)
8.19
1.00
0.83
0.94
0.92
0.85
0.86
1.07
0.38
0.92
36.16
2.73
4.49
f1 (ppm)
211.82
210.99
147.89
141.18
140.57
138.24
135.51
133.20
133.08
131.87
128.63
128.58
128.55
128.28
127.50
126.73
126.21
126.15
72.29
47.19
44.59
44.51
33.51
29.84
29.50
26.33
26.29
25.62
23.36
22.97
18.00
17.19
17.11
16.85
16.79
16.11
16.07
16.05
O
(2,3,4,5,6-pentamethylphenyl)((1R,7aR)-1-phenyl-2,4,5,6,7,7a-hexahydro-1H-inden-3-yl)methanone
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


7.35 7.34 7.26 7.26 7.25 7.23 7.22 7.18 7.17 7.15
3.65 3.64 3.63 3.62 3.62 3.60 3.58 3.44 3.42 3.40 3.39 3.36 3.34 3.33 3.31
2.43 2.42 2.40 2.38 2.20 2.10 2.02 2.00 1.99 1.98 1.86 1.84 1.83
O
H
H
(2,3,4,5,6-pentamethylphenyl)(2-phenylcyclopentyl)methanone
1H NMR in CDCl3 (500 MHz)
dr= 60:40
1.12 2.01 2.02 1.03 0.59 0.48 0.68 5.05 8.00 1.90 6.16
f1 (ppm)

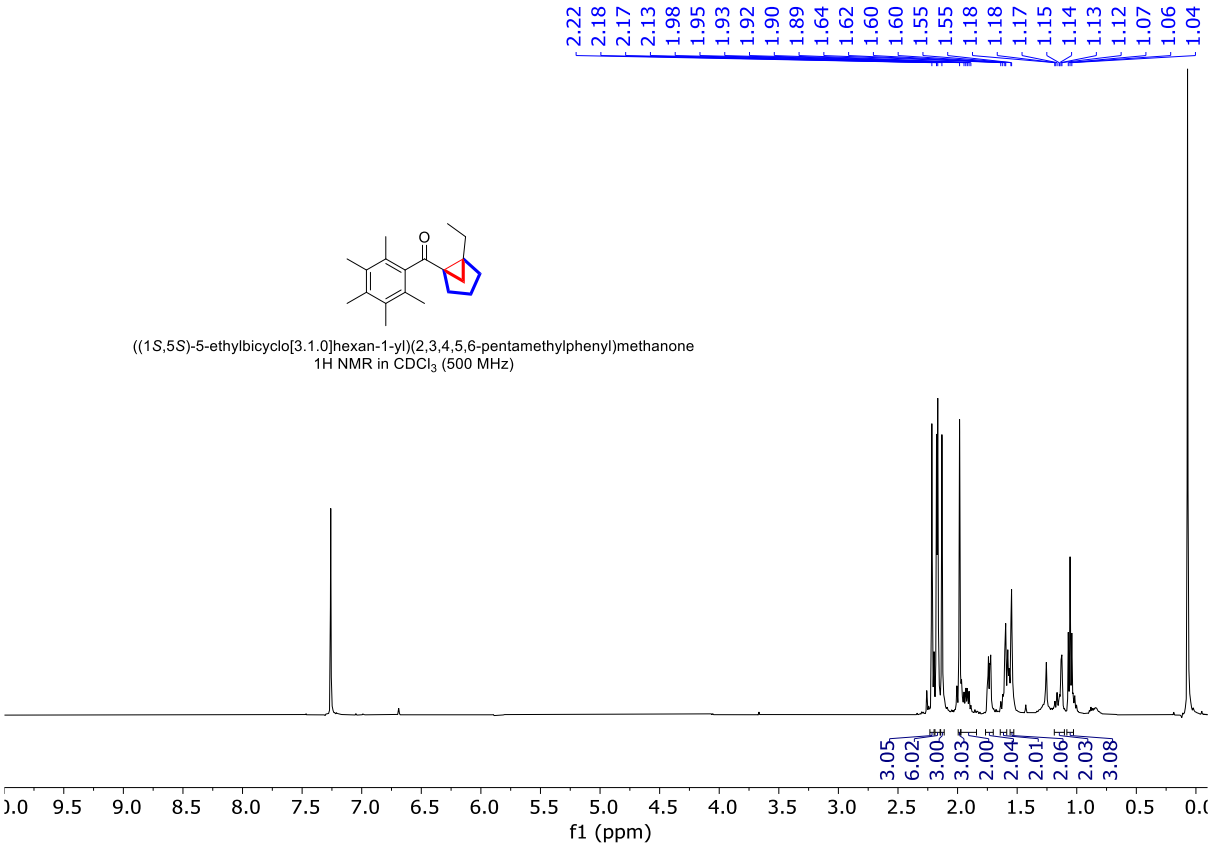

213.28 212.11
145.29 141.93 140.67 140.64 135.50 135.40 133.03 133.00 129.32 128.83 128.33 128.05 127.88 127.69 126.21 126.13
62.53 58.50 49.49 47.56 35.92 31.20 30.95 29.81 29.37 25.88 23.09 16.82 16.75 16.05
O
H
H
(2,3,4,5,6-pentamethylphenyl)(2-phenylcyclopentyl)methanone
13C NMR in CDCl3 (126 MHz)
dr= 60:40
f1 (ppm)



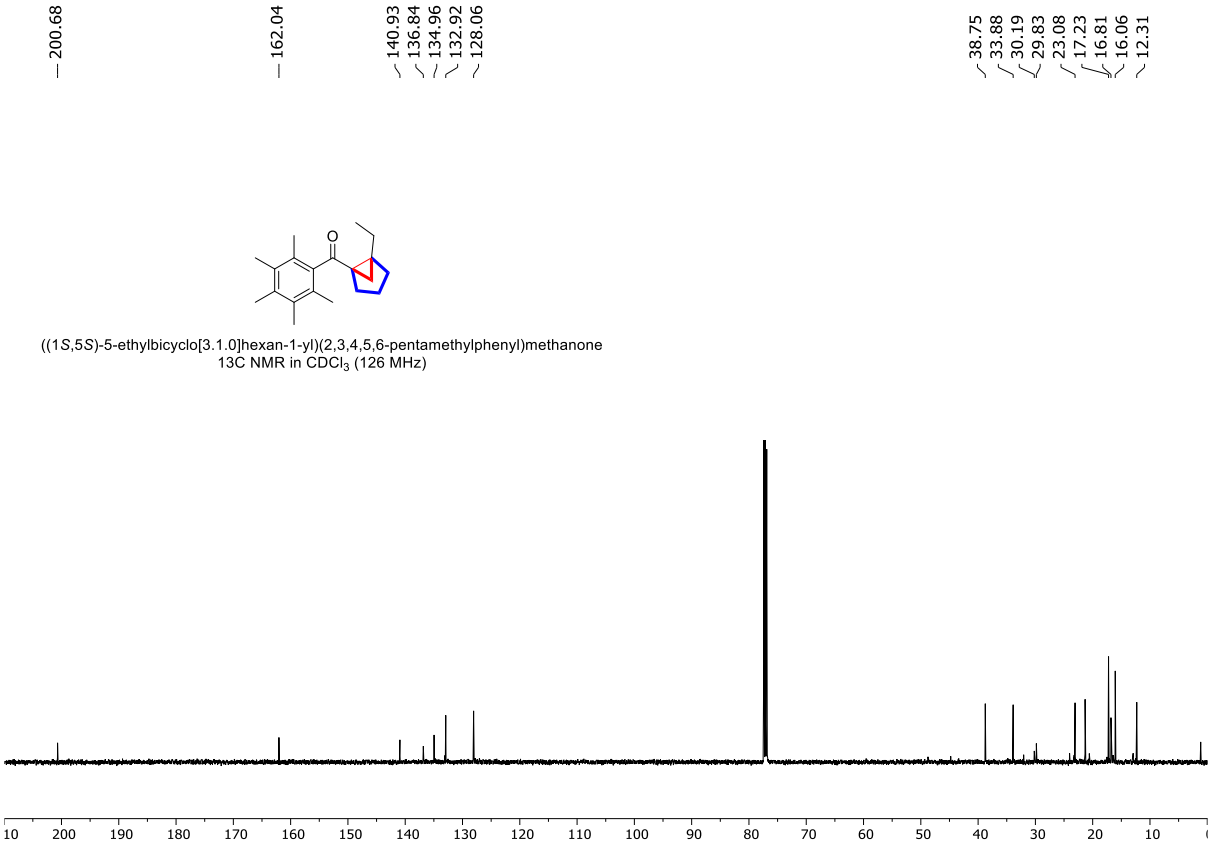
(*R*)-(2,3,4,5,6-pentamethylphenyl)(2-phenyl-3-(4-phenylpiperazin-1-yl)cyclopent-1-en-1-yl)methanone
^{1}H NMR in $CDCl_3$ (500 MHz)



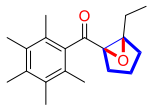
(*R*)-(2,3,4,5,6-pentamethylphenyl)(2-phenyl-3-(4-phenylpiperazin-1-yl)cyclopent-1-en-1-yl)methanone
^{13}C NMR in $CDCl_3$ (126 MHz)



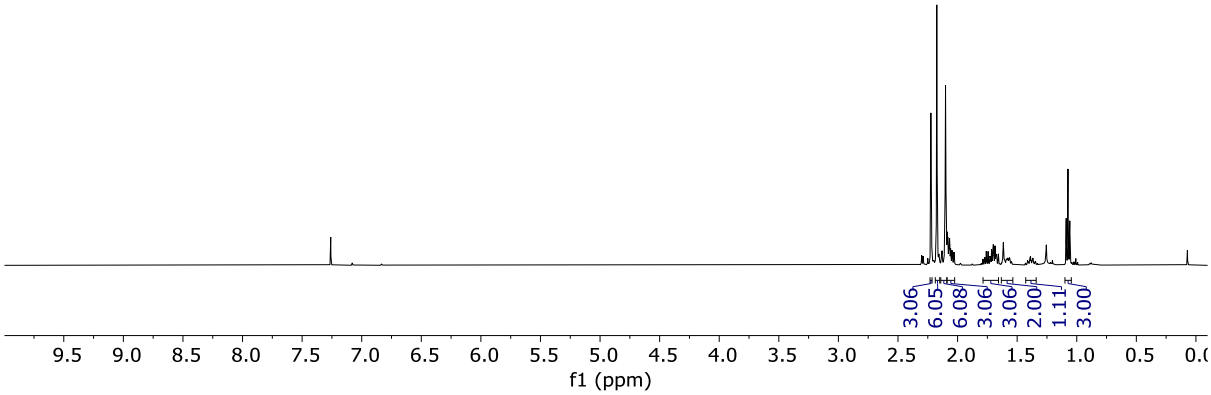
((1*S*,5*S*)-5-ethylbicyclo[3.1.0]hexan-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in $CDCl_3$ (500 MHz)

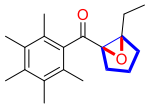


((1*S*,5*S*)-5-ethylbicyclo[3.1.0]hexan-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in $CDCl_3$ (126 MHz)

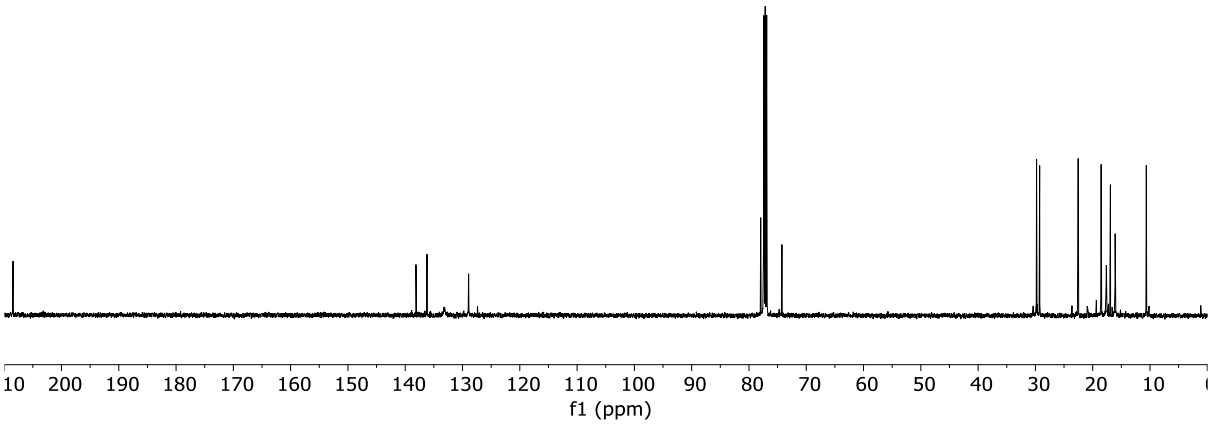


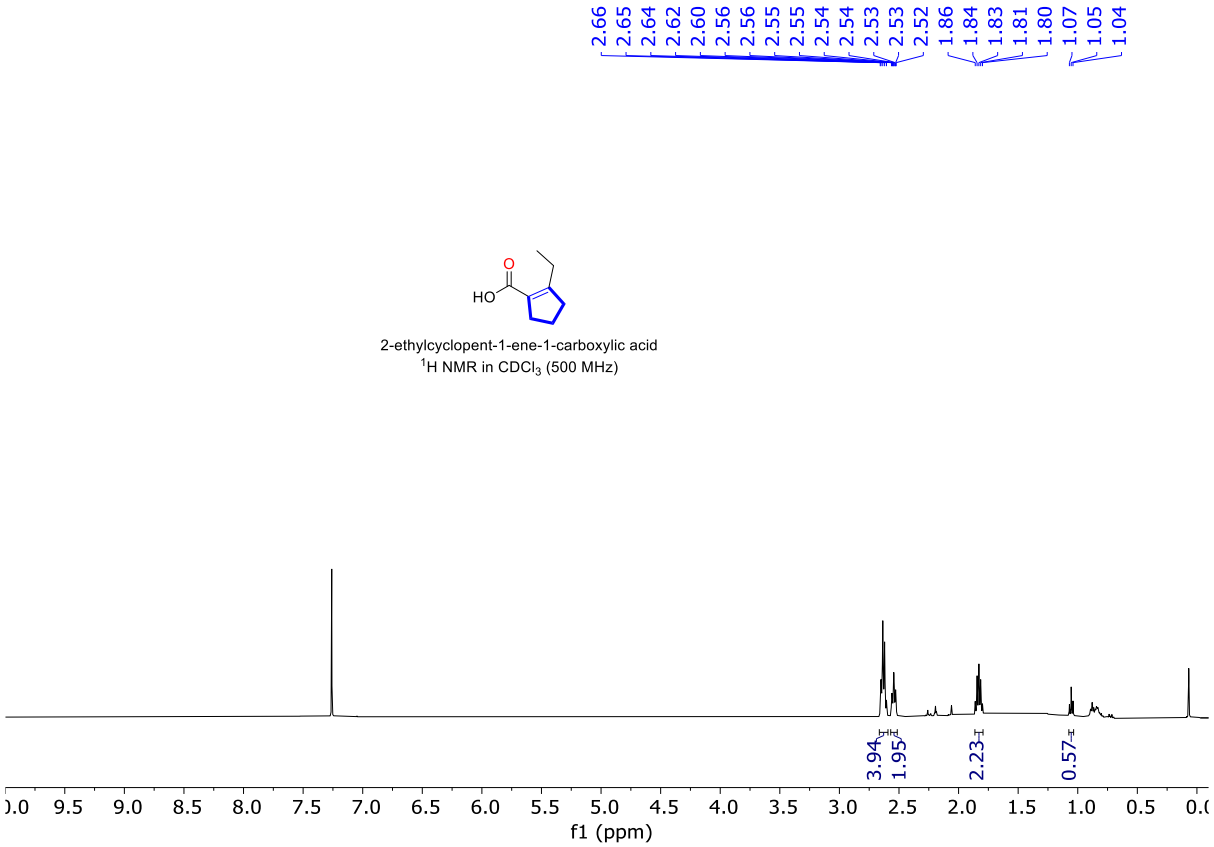
((1*S*,5*R*)-5-ethyl-6-oxabicyclo[3.1.0]hexan-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
1H NMR in $CDCl_3$ (500 MHz)

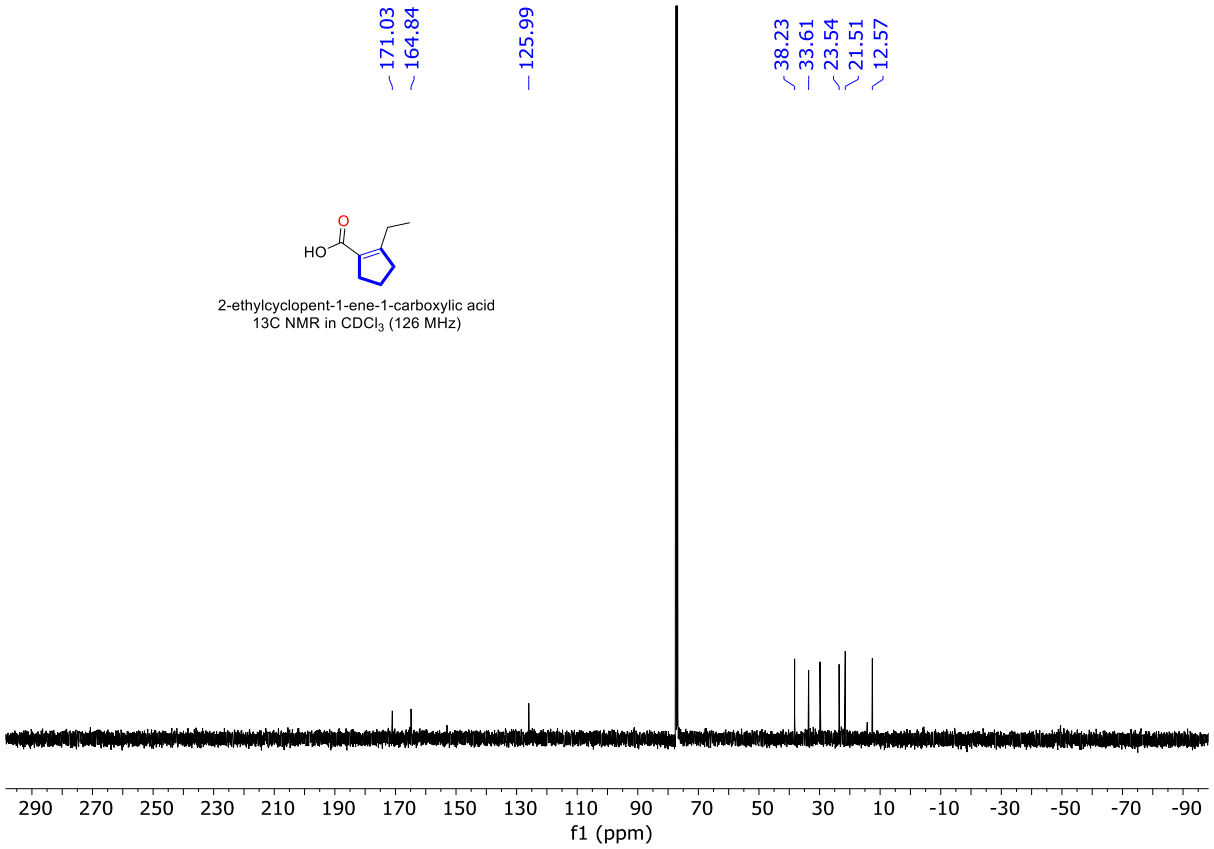


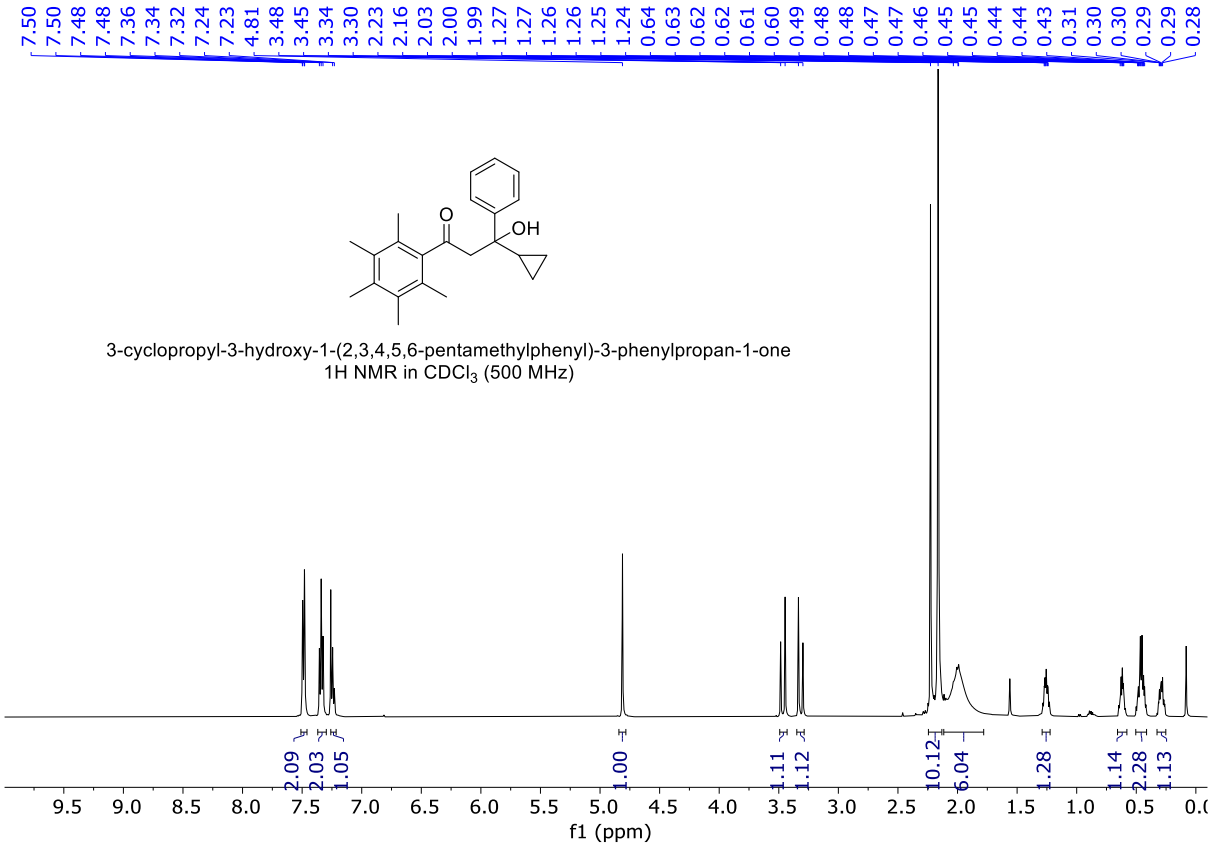


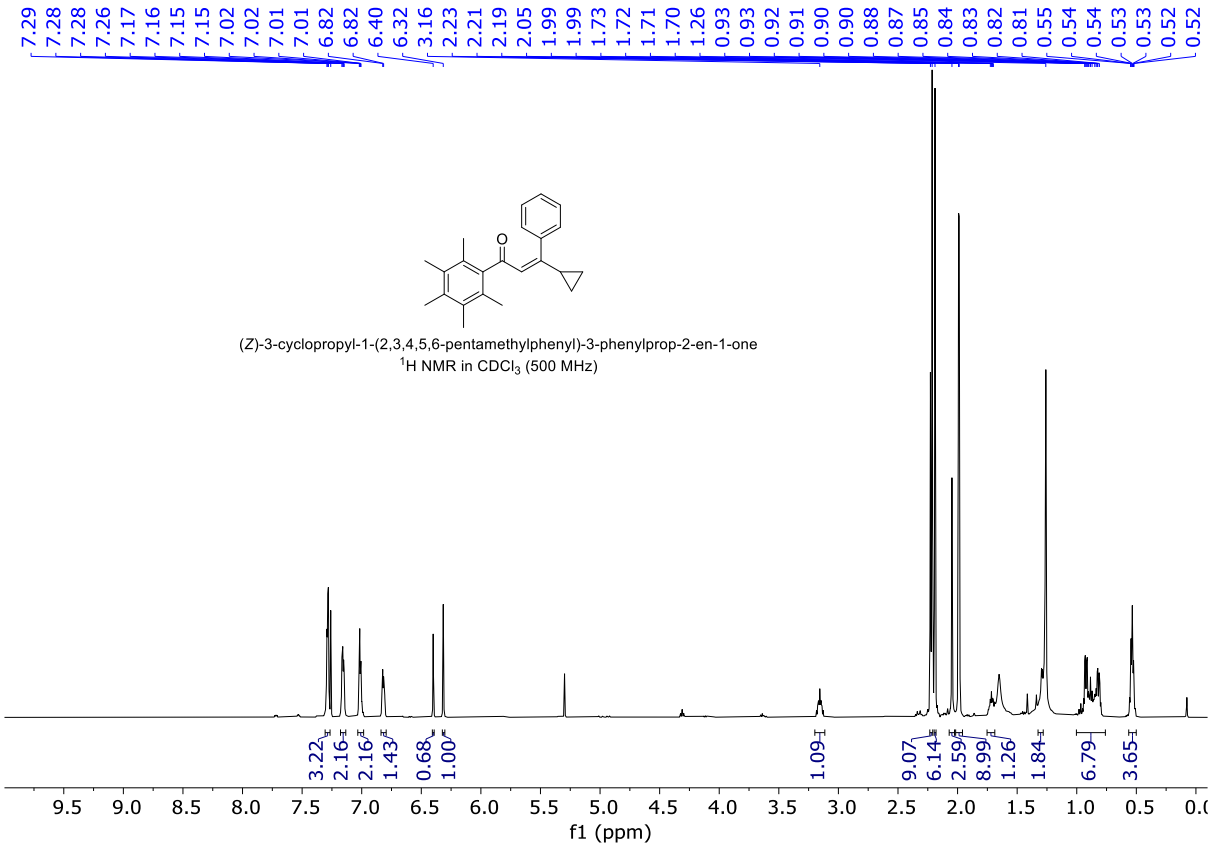
((1*S*,5*R*)-5-ethyl-6-oxabicyclo[3.1.0]hexan-1-yl)(2,3,4,5,6-pentamethylphenyl)methanone
13C NMR in $CDCl_3$ (126 MHz)

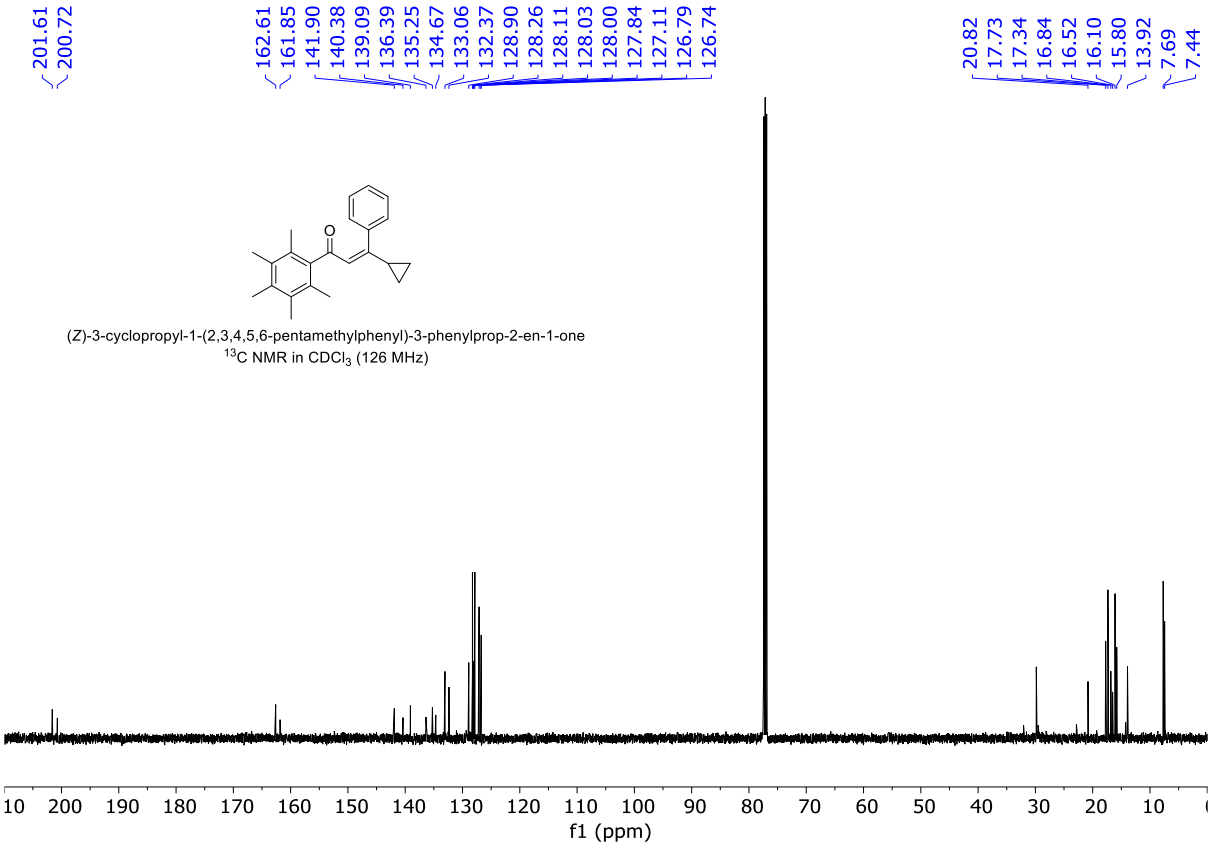


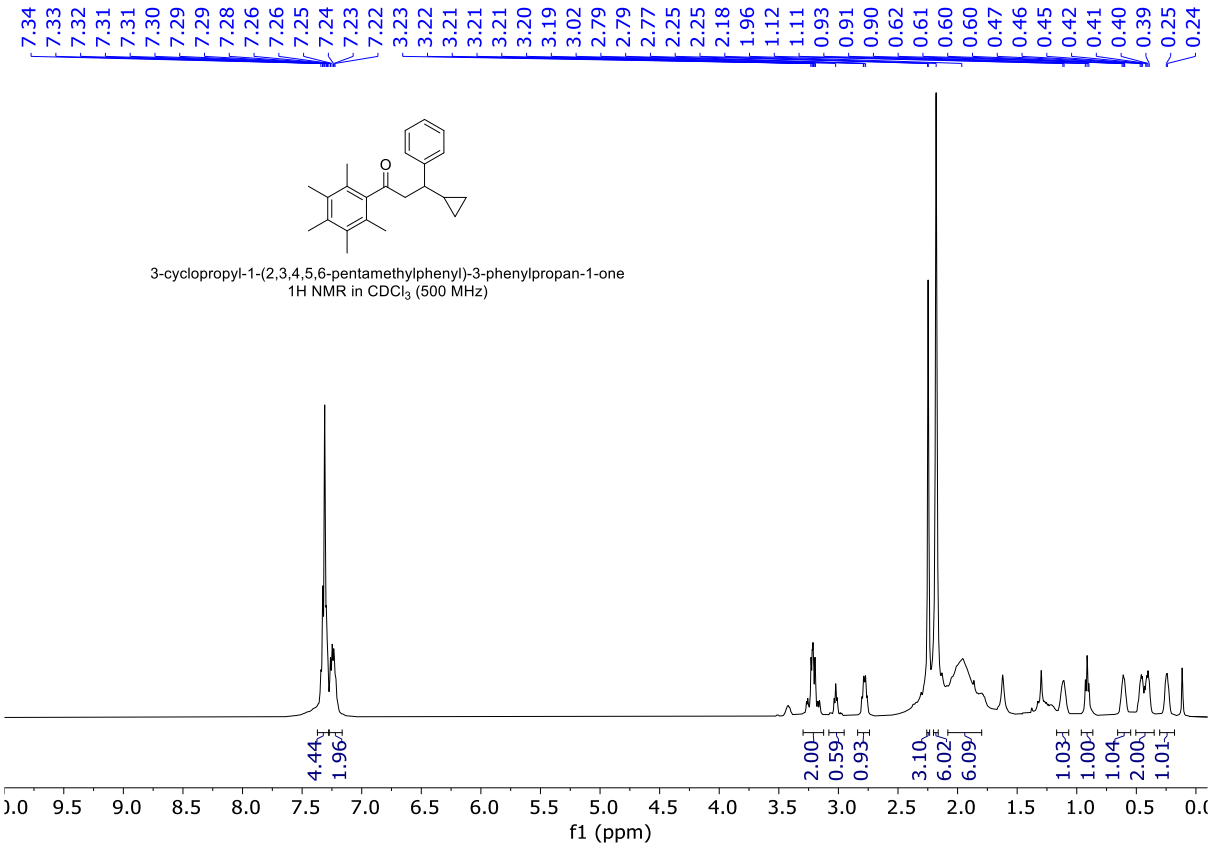

2.66
2.65
2.64
2.62
2.60
2.56
2.56
2.55
2.55
2.54
2.54
2.53
2.53
2.52
1.86
1.84
1.83
1.81
1.80
1.07
1.05
1.04
HO
O
2-ethylcyclopent-1-ene-1-carboxylic acid
^{1}H NMR in $CDCl_3$ (500 MHz)
3.94
1.95
2.23
0.57
f1 (ppm)

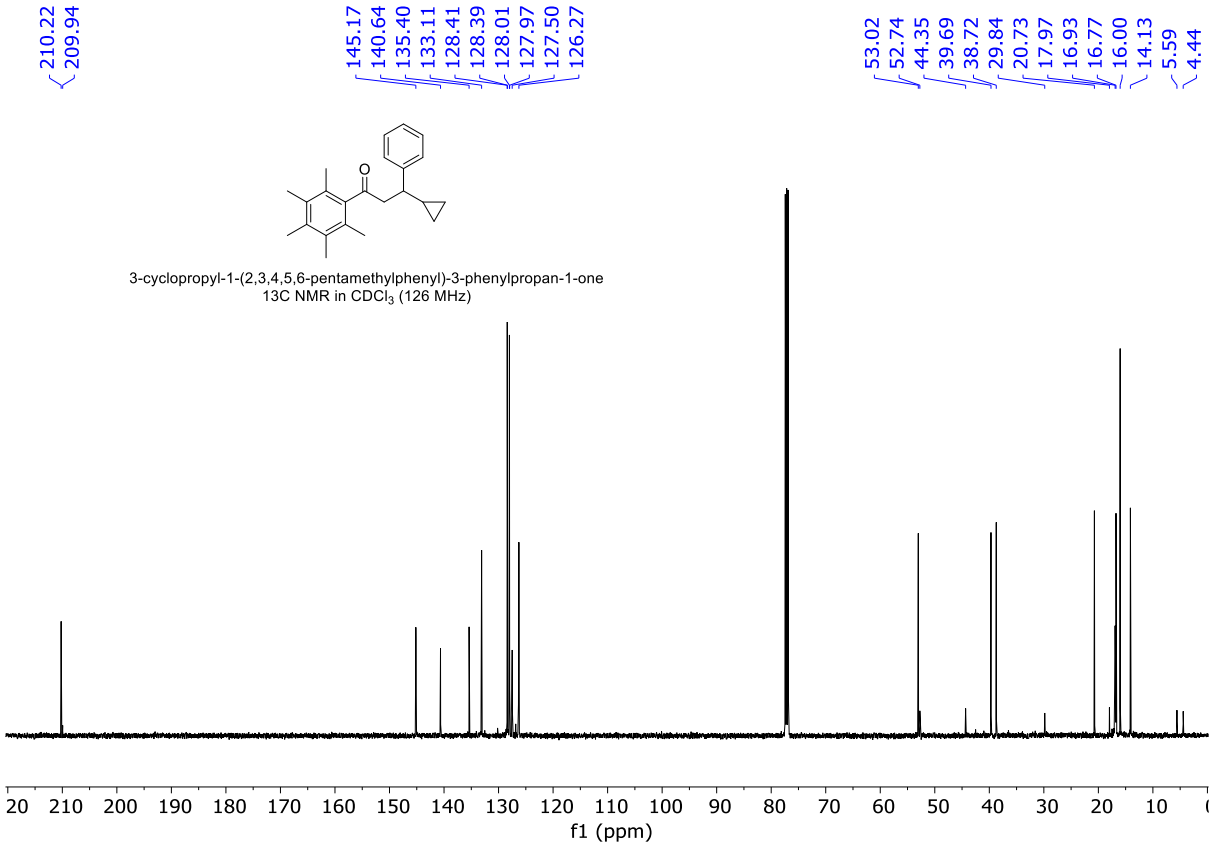

171.03
164.84
125.99
38.23
33.61
23.54
21.51
12.57
HO
O
2-ethylcyclopent-1-ene-1-carboxylic acid
13C NMR in $CDCl_3$ (126 MHz)
f1 (ppm)


O
OH
3-cyclopropyl-3-hydroxy-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one
1H NMR in CDCl3 (500 MHz)
f1 (ppm)


O
(Z)-3-cyclopropyl-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylprop-2-en-1-one
1H NMR in CDCl3 (500 MHz)
f1 (ppm)


201.61
200.72
162.61
161.85
141.90
140.38
139.09
136.39
135.25
134.67
133.06
132.37
128.90
128.26
128.11
128.03
128.00
127.84
127.11
126.79
126.74
20.82
17.73
17.34
16.84
16.52
16.10
15.80
13.92
7.69
7.44
O
(Z)-3-cyclopropyl-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylprop-2-en-1-one
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


7.34
7.33
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.26
7.26
7.25
7.24
7.23
7.22
3.23
3.22
3.21
3.21
3.21
3.20
3.19
3.02
2.79
2.79
2.77
2.25
2.25
2.18
1.96
1.12
1.11
0.93
0.91
0.90
0.62
0.61
0.60
0.60
0.47
0.46
0.45
0.42
0.41
0.40
0.39
0.25
0.24
O
3-cyclopropyl-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one
1H NMR in CDCl3 (500 MHz)
4.44
1.96
2.00
0.59
0.93
3.10
6.02
6.09
1.03
1.00
1.04
2.00
1.01
f1 (ppm)


210.22
209.94
145.17
140.64
135.40
133.11
128.41
128.39
128.01
127.97
127.50
126.27
53.02
52.74
44.35
39.69
38.72
29.84
20.73
17.97
16.93
16.77
16.00
14.13
5.59
4.44
O
3-cyclopropyl-1-(2,3,4,5,6-pentamethylphenyl)-3-phenylpropan-1-one
13C NMR in CDCl3 (126 MHz)
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

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