

Supporting Information

Photocontrolled Cobalt Catalysis for Selective Hydroboration of α,β -Unsaturated Ketones

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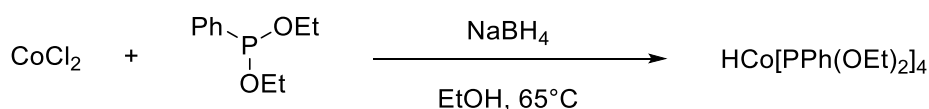
1. Materials and Methods

Unless otherwise stated, all reactions were performed utilizing standard Schlenk techniques. All reagents and starting materials were purchased at reagent grade and used as received. Anhydrous solvents were dried using an Innovative Technology PS-MD-5 solvent purification system. Thin layer chromatography (TLC) was performed on Merck Kieselgel 60 F254 aluminum plates with unmodified silica and visualized either under UV light or stained with potassium permanganate or vanillin. Column chromatography was performed with Merck silica gel 60 (35 – 70 mesh).

All ^1H , ^{13}C and ^{19}F NMR spectra were recorded at ambient temperature on either Varian V-NMRS 600, Varian V-NMRS 400, Bruker AV-600, Bruker AV-400 or Varian Mercury 300 spectrometers. Chemical shifts (δ/ppm) were referenced to the residual solvent peak in ^1H (7.26 ppm for CDCl_3) and ^{13}C spectra (77.16 ppm for CDCl_3). Coupling constants (J) are given in Hz. Signals are described as br = broad, s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, p = quintet, h = sextet and m = multiplet.

High-resolution mass spectrometry (HRMS) was performed using a Thermo Scientific LTQ Orbitrap XL spectrometer. Infrared (IR) spectra were recorded on a Perkin Elmer Spektrum 100 FT-IR spectrometer Spectrum 100 spectrometer with an UATR Diamond/KRS-5 crystal with attenuated total reflectance (ATR) and signals reported as wavenumbers in reciprocal centimeters.

2. Synthesis and Characterization Data of $\text{CoH}[\text{PPh}(\text{OEt})_2]_4$



Procedure

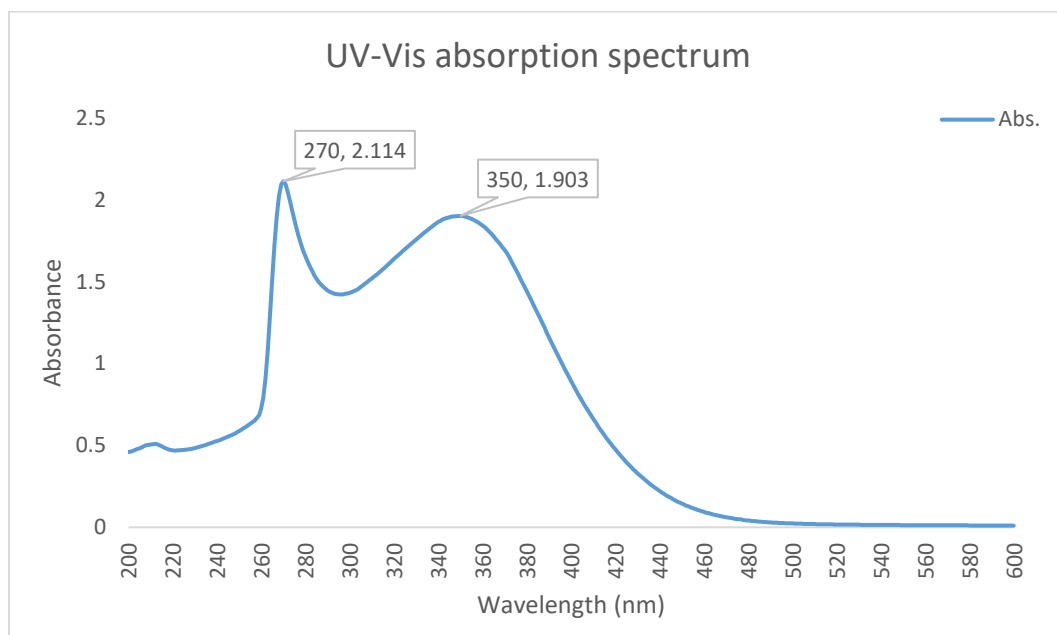
Anhydrous CoCl_2 (650 mg, 5 mmol, 1 eq) was dissolved in dry ethanol (30 ml) inside an oven dried schlenk flask under an Argon atmosphere, forming a blue solution. This solution was then heated in an oil bath at 65°C . $\text{PPh}(\text{OEt})_2$ (4.9 ml, 25 mmol, 5 eq) was added and the solution turned green. The NaBH_4 (430 mg, 11 mmol, 2.2 eq) was slowly added dropwise as suspension in dry ethanol (20 ml), during the addition the solution becomes bright yellow and H_2 is produced. Once the gas evolution has stopped, the solution was filtered under Argon into a clean Schlenk flask and around half of the solvent was removed under vacuum. The remaining solution was cooled at 0°C with an ice bath to induce the precipitation of the product. After 20 minutes the precipitate (2.25 g, 2.65 mmol, 53%), a bright yellow solid, was filtered, dried under high vacuum and weighed.

^1H NMR (400 MHz, CD_2Cl_2) δ 7.44 (s, 8H), 7.17 (s, 12H), 3.62 (s, 8H), 3.32 (s, 8H), 1.04 (s, 24H), -14.71 (q, $J = 22.7$ Hz, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 131.2 – 130.2 (m), 127.8, 127.1, 60.0, 16.5. ^{31}P NMR (162 MHz, CD_2Cl_2) $\delta = 174.32$.

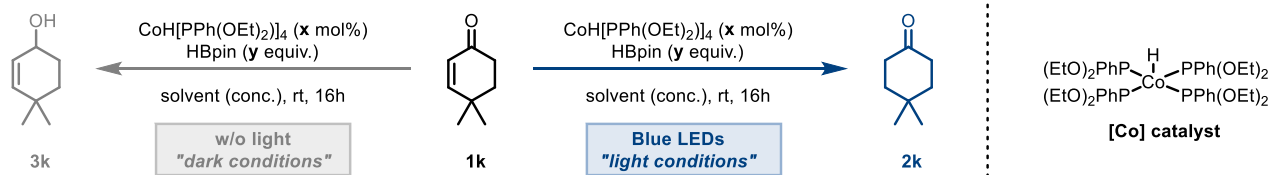
IR (neat): $\nu = 3056, 2971, 2927, 2887, 1480, 1436, 1384, 1099, 1024, 913, 726, 691$ cm^{-1}

HRMS (ESI): m/z $[\text{M}+\text{Na}]^+$ calcd. for $[\text{C}_{40}\text{H}_{61}\text{O}_8\text{P}_4\text{CoNa}]^+$: 875.2547, found: 875.2544.

Figure S1. UV-Vis absorption spectra of Cobalt catalyst CoH[PPh(OEt)₂]₄



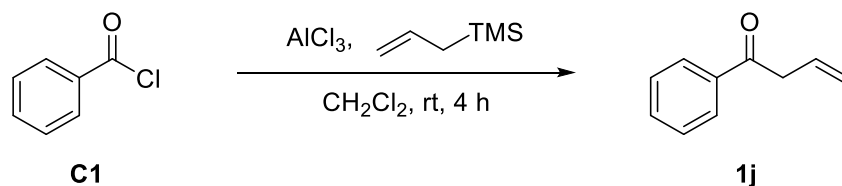
3. Selected optimization for the reduction of cyclic enones



	entry	[Co] x mol%	HBpin y equiv.	solvent (conc.)	Light source	Yield 3k (%)	Yield 2k (%)	conversion (%)
"dark conditions"	1	5	1	benzene (0.2 M)	off	33	10	100
	2	2	2	benzene (0.2 M)	off	82	7	100
	3	2	2	benzene (1 M)	off	75	12	100
	4	5	2	benzene (1 M)	off	89	5	100
	5	5	2	benzene (0.1 M)	off	77	15	100
	6	-	2	benzene (1 M)	off	0	0	0
	7	5	-	benzene (1 M)	off	0	0	0
"light conditions"	8	2	2	benzene (0.2 M)	on	0	59	100
	9	5	2	benzene (1 M)	on	18	74	100
	10	5	2	benzene (0.1 M)	on	12	77	100
	11	5	2	THF (0.2 M)	on	8	87	100
	12	5	2	THF (0.1 M)	on	0	98	100
	13	-	2	THF (0.1 M)	on	0	0	0
	14	5	-	THF (0.1 M)	on	0	5	5

4. Preparation of starting materials

4.1 Procedure for the synthesis of 1-phenylbut-3-en-1-one **1j**

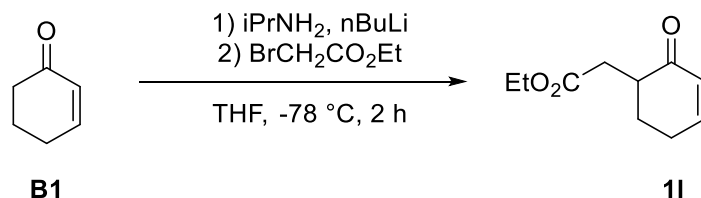


In a Schlenk tube under Argon was introduced AlCl₃ (1.1 equiv., 2.2 mmol, 293 mg), CH₂Cl₂ (C = 0.25 M, 8 mL) and benzoyl chloride (1 equiv., 2 mmol, 0.23 mL) and the resulting mixture was stirred for 20 min at room temperature. Then, a solution of allyltrimethylsilane (1.2 equiv., 2.4 mmol, 0.38 mL) in CH₂Cl₂ (1 mL) was added dropwise and the reaction mixture was stirred at room temperature for 4 h. After this time, the reaction mixture was quenched by addition of cold distilled water. The aqueous layer was extracted with Et₂O (3x) and the combined organic layers were dried (MgSO₄), filtered and concentrated under vacuum. The crude material was purified by column chromatography (0-5% Et₂O in pentane) to afford title compound **1j** as a colorless liquid (176 mg, 1,20 mmol, 60%). R_f = 0.74 (pentane/Et₂O 7:3, vanillin).

¹H NMR (400 MHz, CDCl₃) δ 8.08 – 7.88 (m, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 6.09 (ddt, *J* = 17.2, 10.5, 6.7 Hz, 1H), 5.38 – 5.14 (m, 2H), 3.77 (dt, *J* = 7.1, 1.5 Hz, 2H).
¹³C NMR (101 MHz, CDCl₃) δ 198.2, 136.7, 133.3, 131.2, 128.8 (x2), 128.4 (x2), 118.9, 43.6.

These data are in agreement with those reported previously in the literature.¹

4.2 Procedure for the synthesis of ethyl 2-(2-oxocyclohex-3-en-1-yl)acetate (**1l**)

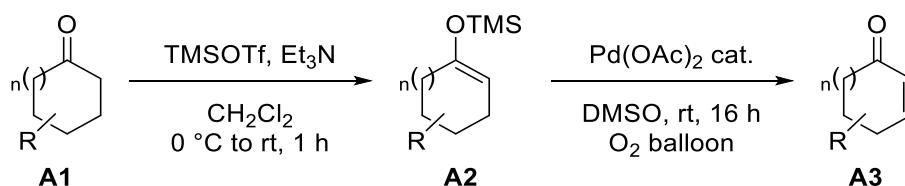


In a Schlenk tube under Argon was introduced diisopropylamine (1.1 equiv., 5.5 mmol), and THF (C = 3 M, 1.7 mL). The mixture was cooled to 0 °C and *n*-butyllithium (1.1 equiv., 5.5 mmol, 2.2 mL, 2.5 M in hexanes) was added dropwise and the resulting mixture was stirred at 0 °C for 30 min. A solution of enone **B1** (1 equiv., 5 mmol, 0.48 mL) in THF (C = 3 M, 1.7 mL) was added dropwise at -78 °C and the reaction mixture was stirred for 15 min at the same temperature. Then, a solution of ethyl bromoacetate (1.2 equiv., 6 mmol, 0.67 mL) in THF (C = 3 M, 1.7 mL) was added dropwise and the reaction mixture was stirred at -78 °C for 2 h. After this time, the reaction mixture was diluted with Et₂O and quenched at 0 °C by the addition of a saturated aqueous solution of NH₄Cl. After warming up to room temperature, the aqueous layer was extracted with Et₂O (3x). The combined organic layers were washed with a saturated aqueous solution of NH₄Cl, brine, dried (MgSO₄), filtered and concentrated under vacuum. The crude material was purified by column chromatography (0-30% Et₂O in pentane) to afford title compound **1l** as a colorless liquid (411 mg, 2.26 mmol, 45%). R_f = 0.37 (pentane/Et₂O 1:1, vanillin).

¹H NMR (400 MHz, CDCl₃) δ 7.01 – 6.91 (m, 1H), 6.02 (ddd, *J* = 10.0, 2.8, 1.2 Hz, 1H), 4.15 (qd, *J* = 7.1, 2.1 Hz, 2H), 2.94 – 2.81 (m, 2H), 2.56 – 2.40 (m, 2H), 2.31 – 2.21 (m, 1H), 2.18 – 2.07 (m, 1H), 1.90 – 1.75 (m, 1H), 1.26 (t, *J* = 7.1 Hz, 3H).
¹³C NMR (101 MHz, CDCl₃) δ 199.6, 172.7, 150.0, 129.4, 60.7, 43.8, 34.7, 28.8, 26.1, 14.3.

These data are in agreement with those reported previously in the literature.²

4.3 General procedure for the synthesis of enones: Saegusa-Ito oxidation of cycloalkanones (Procedure A)



Step 1 (Preparation of silyl enol ether): In a Schlenk tube under Argon was introduced alkanone **A1** (1 equiv, 3 mmol) and dry CH₂Cl₂ (C = 0.21 M, 14 mL). The mixture was then cooled to 0 °C before the dropwise addition of TMSOTf (1.5 equiv, 4.5 mmol, 0.82 mL) and Et₃N (3 equiv, 9 mmol, 1.25 mL). The reaction mixture was then allowed to reach room temperature and the stirring was continued for 1 h at the same temperature or until complete consumption of the starting material (monitored by TLC). The reaction mixture was quenched at 0 °C by the addition of a cold saturated aqueous solution of NaHCO₃. The aqueous layer was then extracted twice with CH₂Cl₂. The combined organic layers were dried (MgSO₄), filtered and concentrated under vacuum. The crude material **A2** was directly engaged in the next step without further purification.

Step 2 (Saegusa-Ito oxidation): In a Schlenk tube under air was introduced silyl enol ether **A2** (1 equiv, 3 mmol), DMSO (C = 0.1 M, 30 mL) and Pd(OAc)₂ (10 mol%, 0.3 mmol, 67 mg). Then, the Schlenk tube was purged with oxygen and a balloon of oxygen was placed on the top and the reaction mixture was stirred at room temperature overnight. After this time, the reaction mixture was quenched by the addition of distilled water. The aqueous layer was extracted with Et₂O (3x) and the combined organic layers were washed with brine, dried (MgSO₄), filtered and concentrated under vacuum (note: some of the synthesized enones are volatile). The crude material was purified by column chromatography to afford title compounds **A3**.

2,3-dihydro-[1,1'-biphenyl]-4(1H)-one (**1m**)

Prepared following general procedure A, **1m** was obtained after purification by column chromatography (0-20% Et₂O in pentane) as a colorless liquid (491 mg, 2.85 mmol, 95%). R_f = 0.31 (pentane/Et₂O 3:2, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 7.36 (t, J = 7.6 Hz, 2H), 7.29 (t, J = 7.4 Hz, 1H), 7.22 (dd, J = 7.0, 1.7 Hz, 2H), 6.99 (ddd, J = 10.1, 2.9, 1.3 Hz, 1H), 6.17 (dd, J = 10.1, 2.6 Hz, 1H), 3.73 (ddt, J = 10.0, 5.2, 2.7 Hz, 1H), 2.56 (dt, J = 16.7, 5.0 Hz, 1H), 2.48 (ddd, J = 16.6, 11.9, 4.7 Hz, 1H), 2.37 (dq, J = 15.2, 5.0, 1.4 Hz, 1H), 2.06 (dddd, J = 13.7, 11.8, 9.4, 4.5 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 199.4, 153.0, 143.0, 130.2, 129.0 (x2), 127.7 (x2), 127.3, 42.8, 37.1, 32.6.

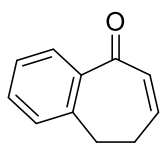
These data are in agreement with those reported previously in the literature.³

4-(tert-butyl)cyclohex-2-en-1-one (**1n**)

Prepared following general procedure A, **1n** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a colorless liquid (420 mg, 2.76 mmol, 92%). R_f = 0.41 (pentane/Et₂O 7:3, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 7.01 (dt, J = 11.0, 2.1 Hz, 1H), 6.03 (ddd, J = 11.0, 2.8, 0.9 Hz, 1H), 2.51 (dt, J = 16.7, 3.7 Hz, 1H), 2.33 (ddd, J = 16.5, 14.1, 5.1 Hz, 1H), 2.23 – 2.16 (m, 1H), 2.13 – 2.06 (m, 1H), 1.73 (ddd, J = 24.1, 13.7, 3.8 Hz, 1H), 0.97 (s, 9H). ¹³C NMR (151 MHz, CDCl₃) δ 200.2, 153.1, 130.1, 47.0, 38.0, 33.0, 27.5 (x3), 24.5.

These data are in agreement with those reported previously in the literature.⁴

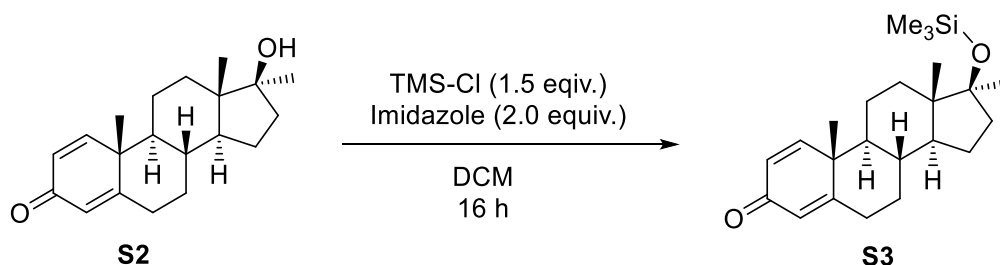
8,9-dihydro-5H-benzo[7]annulen-5-one (S1)



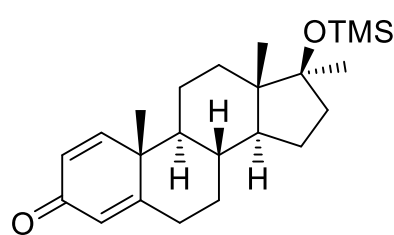
Prepared following general procedure A, **S1** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a yellow liquid (313 mg, 1.98 mmol, 66%). *R*_f = 0.44 (pentane/Et₂O 3:2, vanillin). ¹H NMR (400 MHz, CDCl₃) δ 7.75 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.42 (td, *J* = 7.4, 1.5 Hz, 1H), 7.31 (td, *J* = 7.6, 1.3 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 6.75 (dt, *J* = 12.1, 4.9 Hz, 1H), 6.28 (dt, *J* = 12.1, 1.9 Hz, 1H), 3.18 – 3.00 (m, 2H), 2.60 (dd, *J* = 8.0, 4.1 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 195.2, 151.2, 147.2, 139.9, 132.6, 132.3, 129.8, 129.0, 126.9, 34.6, 29.9.

These data are in agreement with those reported previously in the literature.⁵

4.4 Procedure for the TMS protection of the steroid **S2** to give (8R,9S,10R,13S,14S,17S)-10,13,17-trimethyl-17-((trimethylsilyl)oxy)-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-3H-cyclopenta[*a*]phenanthren-3-one (**S3**)



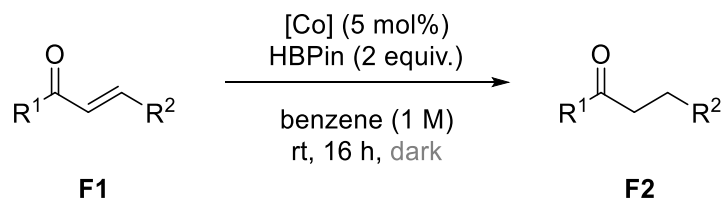
The starting material **S2** (200 mg, 0.68 mmol) was dissolved in anhydrous DCM (10 ml). Imidazole (1.36 mmol, 92 mg) was then added in one portion, followed by TMSCl (111 mg, 1.0 mmol). The resulting solution was left at stirring for 16 hours; after this time, it was quenched with a saturated aqueous solution of NaHCO₃ (10 ml). The layers were separated and the organic layer was washed with water (2x10ml) and brine, dried over MgSO₄ and evaporated. The resulting white solid (245 mg, 0.66 mmol, 97%) was used without further purification.



¹H NMR (600 MHz, Chloroform-*d*) δ 6.98 (d, *J* = 10.1 Hz, 1H), 6.14 (dd, *J* = 10.1, 1.9 Hz, 1H), 5.98 (t, *J* = 1.7 Hz, 1H), 2.38 (td, *J* = 13.4, 5.4 Hz, 1H), 2.27 (dt, *J* = 13.3, 3.5 Hz, 1H), 1.91 – 1.77 (m, 2H), 1.70 – 1.52 (m, 3H), 1.47 (s, 8H), 1.23 (tt, *J* = 12.3, 6.2 Hz, 1H), 1.16 (s, 3H), 1.07 (s, 3H), 1.00 (td, *J* = 11.4, 7.5 Hz, 1H), 0.92 (ddt, *J* = 20.3, 13.5, 6.3 Hz, 2H), 0.76 (s, 3H), 0.00 (s, 9H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 184.0, 167.0, 153.7, 125.0, 121.4, 81.3, 50.2, 46.3, 44.2, 41.3, 36.4, 34.1, 31.0, 30.5, 28.8, 23.9, 21.3, 20.27, 16.4, 11.9, 0.00. IR (neat): ν = 2943, 2868, 1664, 1623, 1247, 1169, 1091, 1018, 878, 832 cm⁻¹. HRMS (ESI): *m/z* [M+H]⁺ calcd. for [C₂₃H₃₇OSi]⁺: 373.2557, found: 373.2562.

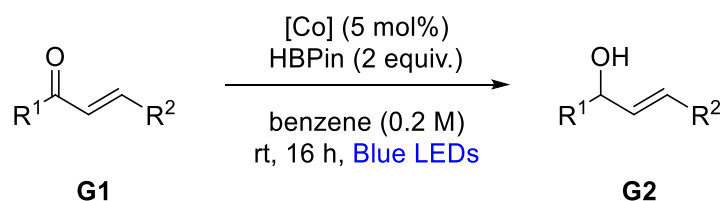
5. General procedures and characterization data of reduction products

5.1 General procedure 1



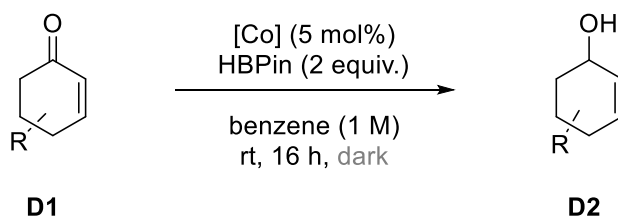
General procedure: In an oven-dried vial were introduced the cobalt catalyst (5 mol%, 10 μ mol, 8.6 mg) and a stirring bar. A cap with rubber septum was used to close the vial and the system was then purged with Argon. benzene (C = 1 M, 0.2 mL), chalcone **F1** (1 equiv, 0.2 mmol) and HBPIn (2 equiv, 0.4 mmol, 58 μ L) were then added successively and the vial was placed in the dark overnight. After this time, the solution was diluted with Et₂O and washed two times with distilled water, the combined aqueous layers were extracted two times with Et₂O and the combined organic layers were washed with brine, dried (MgSO₄), filtered and concentrated under vacuum. The crude material was purified by column chromatography to afford the corresponding ketone **F2**.

5.2 General procedure 2



General procedure: In an oven-dried vial were introduced the cobalt catalyst (5 mol%, 10 μ mol, 8.6 mg) and a stirring bar. A cap with rubber septum was used to close the vial and the system was then purged with Argon. benzene (C = 0.2 M, 1 mL), chalcone **G1** (1 equiv, 0.2 mmol) and HBPIn (2 equiv, 0.4 mmol, 58 μ L) were then added successively and the vial was placed in the dark overnight. After this time, the solution was diluted with Et₂O and washed two times with distilled water, the combined aqueous layers were extracted two times with Et₂O and the combined organic layers were washed with brine, dried (MgSO₄), filtered and concentrated under vacuum. The crude material was purified by column chromatography to afford the corresponding allylic alcohol **G2**.

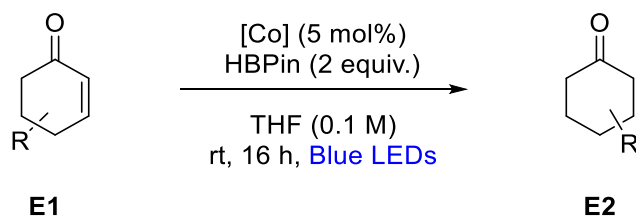
5.3 General procedure 3



General procedure: In an oven-dried vial were introduced the cobalt catalyst (5 mol%, 10 μ mol, 8.6 mg) and a stirring bar. A cap with rubber septum was used to close the vial and the system was then purged with Argon. benzene (C = 1 M, 0.2 mL), enone **D1** (1 equiv, 0.2 mmol) and HBPIn (2 equiv, 0.4 mmol, 58 μ L) were then added successively and the vial was placed

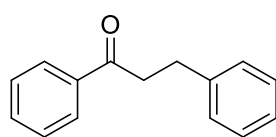
in the dark overnight. After this time, the solution was diluted with Et₂O and washed two times with distilled water, the combined aqueous layers were extracted two times with Et₂O and the combined organic layers were washed with brine, dried (MgSO₄), filtered and concentrated under vacuum. The crude material was purified by column chromatography to afford the corresponding allylic alcohol **D2**.

5.4 General procedure 4



General procedure: In an oven-dried vial were introduced the cobalt catalyst (5 mol%, 10 μmol , 8.6 mg) and a stirring bar. A cap with rubber septum was used to close the vial and the system was then purged with Argon. THF (C = 0.1 M, 2 mL), enone **E1** (1 equiv., 0.2 mmol) and HBPIn (2 equiv., 0.4 mmol, 58 μL) were then added successively and the vial was exposed to blue LEDs overnight. After this time, the solution was diluted with Et₂O and washed two times with distilled water, the combined aqueous layers were extracted two times with Et₂O and the combined organic layers were washed with brine, dried (MgSO₄), filtered and concentrated under vacuum. The crude material was purified by column chromatography to afford the corresponding ketone **E2**.

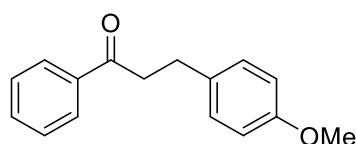
1,3-diphenylpropan-1-one (2a)



Prepared following general procedure 1, **2a** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a white solid (32.8 mg, 156 μmol , 78%). $R_f = 0.58$ (pentane/Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, CDCl₃) δ 8.01 – 7.91 (m, 2H), 7.66 – 7.51 (m, 1H), 7.45 (t, $J = 7.8$ Hz, 2H), 7.30 (t, $J = 7.5$ Hz, 2H), 7.27 – 7.24 (m, 2H), 7.23 – 7.16 (m, 1H), 3.30 (dd, $J = 8.5, 7.0$ Hz, 2H), 3.07 (t, $J = 7.7$ Hz, 2H). **¹³C NMR** (151 MHz, CDCl₃) δ 199.3, 141.4, 137.0, 133.2, 128.7 (x2), 128.7 (x2), 128.6 (x2), 128.2 (x2), 126.3, 40.6, 30.3. **IR (neat):** $\nu = 2922, 1678, 1593, 1446, 1364, 1288, 1203, 971, 743, 692$ cm⁻¹. **HRMS (ESI):** m/z [M+Na]⁺ calcd. for [C₁₅H₁₄ONa]⁺: 233.0937, found: 233.0937.

These data are in agreement with those reported previously in the literature.⁶

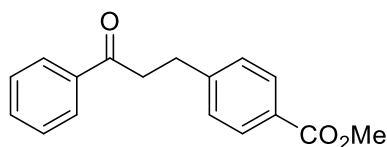
3-(4-methoxyphenyl)-1-phenylpropan-1-one (2b)



Prepared following general procedure 1, **2b** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a white solid (37 mg, 154 μmol , 77%). $R_f = 0.49$ (pentane/Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, CDCl₃) δ 8.03 – 7.91 (m, 2H), 7.63 – 7.53 (m, 1H), 7.48 – 7.42 (m, 2H), 7.18 (d, $J = 8.6$ Hz, 2H), 6.85 (d, $J = 8.6$ Hz, 2H), 3.79 (s, 3H), 3.27 (dd, $J = 8.4, 7.0$ Hz, 2H), 3.02 (t, $J = 7.7$ Hz, 2H). **¹³C NMR** (151 MHz, CDCl₃) δ 199.5, 158.1, 137.0, 133.4, 133.1, 129.5 (x2), 128.7 (x2), 128.2 (x2), 114.1 (x2), 55.4, 40.8, 29.4. **IR (neat):** $\nu = 2935, 1679, 1603, 1508, 1445, 1364, 1295, 1236, 1201, 1177, 1031, 975, 909, 822, 735, 690$ cm⁻¹. **HRMS (ESI):** m/z [M+Na]⁺ calcd. for [C₁₆H₁₆O₂Na]⁺: 263.1042, found: 163.1039.

These data are in agreement with those reported previously in the literature.⁷

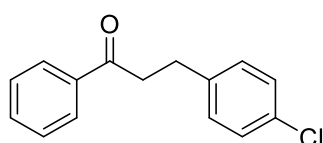
Methyl 4-(3-oxo-3-phenylpropyl)benzoate (2c)



Prepared following general procedure 1, **2c** was obtained after purification by column chromatography (0-20% Et₂O in pentane) as a white solid (45.1 mg, 168 μmol, 84%). R_f = 0.41 (pentane/Et₂O 6:4, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 7.99 – 7.90 (m, 4H), 7.59 – 7.53 (m, 1H), 7.49 – 7.42 (m, 2H), 7.32 (d, J = 8.2 Hz, 2H), 3.90 (s, 3H), 3.32 (dd, J = 8.2, 7.0 Hz, 2H), 3.13 (t, J = 7.6 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 198.8, 167.1, 146.9, 136.8, 133.3, 130.0 (x2), 128.8 (x2), 128.6 (x2), 128.3, 128.1 (x2), 52.1, 39.9, 30.1. IR (neat): ν = 2951, 1707, 1681, 1603, 1436, 1362, 1276, 1198, 1179, 1102, 969, 766, 740, 686 cm⁻¹. HRMS (ESI): m/z [M+Na]⁺ calcd. for [C₁₇H₁₆O₃Na]⁺: 291.0992, found: 291.0989.

These data are in agreement with those reported previously in the literature.⁸

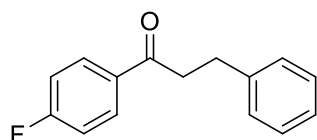
3-(4-chlorophenyl)-1-phenylpropan-1-one (2d)



Prepared following general procedure 1, **2d** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a white solid (34.7 mg, 142 μmol, 71%). R_f = 0.57 (pentane/Et₂O 6:4, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 8.08 – 7.90 (m, 2H), 7.61 – 7.53 (m, 1H), 7.50 – 7.43 (m, 2H), 7.26 (d, J = 8.4 Hz, 2H), 7.22 – 7.16 (m, 2H), 3.28 (dd, J = 8.1, 7.0 Hz, 2H), 3.05 (t, J = 7.5 Hz, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 198.9, 139.9, 136.9, 133.3, 132.0, 129.9 (x2), 128.8 (x2), 128.7 (x2), 128.1 (x2), 40.2, 29.5. IR (neat): ν = 2924, 1665, 1592, 1489, 1446, 1366, 1266, 1207, 1091, 981, 824, 772, 741, 682 cm⁻¹. HRMS (ESI): m/z [M+Na]⁺ calcd. for [C₁₅H₁₃OCINa]⁺: 267.0547, found: 267.0547.

These data are in agreement with those reported previously in the literature.⁹

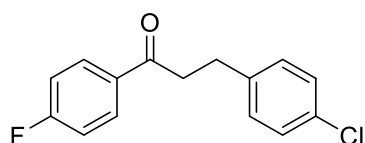
1-(4-fluorophenyl)-3-phenylpropan-1-one (2e)



Prepared following general procedure 1, **2e** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a white solid (31 mg, 136 μmol, 68%). R_f = 0.59 (pentane/Et₂O 6:4, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 8.09 – 7.95 (m, 2H), 7.37 – 7.28 (m, 2H), 7.27 – 7.24 (m, 2H), 7.24 – 7.19 (m, 1H), 7.16 – 7.07 (m, 2H), 3.28 (dd, J = 8.4, 6.9 Hz, 2H), 3.07 (t, J = 7.7 Hz, 2H). ¹⁹F NMR (565 MHz, CDCl₃) δ -105.32 (m). ¹³C NMR (151 MHz, CDCl₃) δ 197.7, 165.9 (d, ¹J_{C-F} = 254.9 Hz), 141.3, 133.4 (d, ⁴J_{C-F} = 3.2 Hz), 130.8 (d, ³J_{C-F} = 9.5 Hz, x2), 128.7 (x2), 128.5 (x2), 126.3, 115.8 (d, ²J = 21.8 Hz, x2), 40.5, 30.2. IR (neat): ν = 2927, 1678, 1593, 1499, 1449, 1410, 1364, 1294, 1236, 1203, 1155, 976, 845, 781, 746, 699 cm⁻¹. HRMS (ESI): m/z [M+Na]⁺ calcd. for [C₁₅H₁₃OFNa]⁺: 251.0843, found: 251.0842.

These data are in agreement with those reported previously in the literature.¹⁰

3-(4-chlorophenyl)-1-(4-fluorophenyl)propan-1-one (2f)

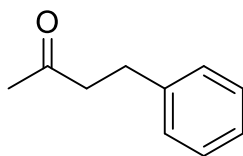


Prepared following general procedure 1, **2f** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a white solid (38.9 mg, 148 μmol, 74%). R_f = 0.56 (pentane/Et₂O 6:4, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 8.44 – 7.78 (m, 2H), 7.29 – 7.23 (m, 2H), 7.20 – 7.16 (m, 2H), 7.14 – 7.09 (m, 2H), 3.25 (dd, J = 8.0, 7.0 Hz, 2H), 3.03 (t, J = 7.5 Hz, 2H). ¹⁹F NMR (565 MHz, CDCl₃) δ -105.07 (m). ¹³C NMR (151 MHz, CDCl₃) δ 197.3, 165.9 (d, ¹J_{C-F} = 254.7 Hz), 139.7, 133.3 (d, ⁴J_{C-F} = 2.4 Hz), 132.1, 130.8 (d, ³J_{C-F} = 8.8 Hz, x2), 129.9 (x2), 128.7 (x2), 115.9 (d, ²J_{C-F} =

22.1 Hz, x2), 40.2, 29.5. **IR (neat):** $\nu = 2923, 1672, 1595, 1491, 1409, 1367, 1233, 1204, 1154, 1093, 983, 839, 812, 757 \text{ cm}^{-1}$. **HRMS (ESI):** m/z $[M+Na]^+$ calcd. for $[C_{15}H_{12}OCIFNa]^+$: 285.0453, found: 285.0454.

These data are in agreement with those reported previously in the literature.¹¹

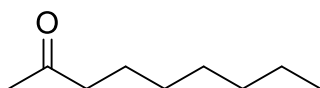
4-phenylbutan-2-one (2g)



Prepared following general procedure 2, **2g** was obtained after purification by column chromatography (0-25% Et₂O in pentane) as a colorless liquid (10.9 mg, 74 μmol , 37%). $R_f = 0.61$ (pentane/Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, Chloroform-*d*) δ 7.35 – 7.24 (m, 1H), 7.25 – 7.15 (m, 1H), 2.90 (t, $J = 7.7 \text{ Hz}$, 1H), 2.76 (t, $J = 7.7 \text{ Hz}$, 1H), 2.14 (s, 1H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 207.9, 141.0, 128.5, 128.3, 126.1, 45.2, 30.1, 29.8. **HRMS (ESI):** m/z $[M+H]^+$ calcd. for $[C_{10}H_{12}ONa]^+$: 171.0780, found: 171.0779.

These data are in agreement with those reported previously in the literature.¹²

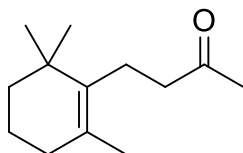
Nonan-2-one (2h)



Prepared following general procedure 4, **2h** was obtained after purification by column chromatography (10% Et₂O in pentane) as a colorless liquid (18 mg, 126 μmol , 63%). $R_f = 0.46$ (pentane/Et₂O 9:1, vanillin). **¹H NMR** (600 MHz, Chloroform-*d*) δ 2.40 (t, $J = 7.5 \text{ Hz}$, 2H), 2.12 (s, 3H), 1.56 (t, $J = 7.2 \text{ Hz}$, 2H), 1.27 (m, 8H), 0.87 (t, $J = 6.8 \text{ Hz}$, 3H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 209.4, 43.8, 31.7, 29.8, 29.1, 29.0, 23.9, 22.6, 14.0. **HRMS (ESI):** m/z $[M+H]^+$ calcd. for $[C_9H_{18}ONa]^+$: 165.1253, found: 165.1250. **IR (neat):** $\nu = 2926, 2857, 1715, 1459, 1414, 1359, 1163, 719 \text{ cm}^{-1}$

These data are in agreement with those reported previously in the literature.¹³

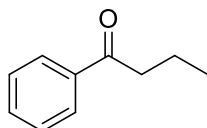
4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-one (2i)



Prepared following general procedure 1, **2i** was obtained after purification by column chromatography (0-20% Et₂O in pentane) as a colorless liquid (11 mg, 54 μmol , 27%). $R_f = 0.70$ (pentane/Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, Chloroform-*d*) δ 2.53 – 2.47 (m, 2H), 2.29 – 2.23 (m, 2H), 2.14 (s, 3H), 1.90 (t, $J = 6.3 \text{ Hz}$, 2H), 1.56 (q, $J = 6.3, 5.8 \text{ Hz}$, 6H), 1.44 – 1.38 (m, 2H), 0.97 (s, 6H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 209.0, 136.0, 127.8, 44.5, 39.7, 35.0, 32.7, 29.8, 28.4, 22.3, 19.7, 19.4. **HRMS (ESI):** m/z $[M+H]^+$ calcd. for $[C_{13}H_{22}ONa]^+$: 217.1563, found: 217.1561.

These data are in agreement with those reported previously in the literature.¹⁴

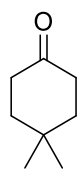
1-phenylbutan-1-one (2j)



Prepared following general procedure 4, **2j** was obtained after purification by column chromatography (% Et₂O in pentane) as a colorless liquid (19.3 mg, 130 μmol , 65%). **¹H NMR** (400 MHz, CDCl₃) δ 7.96 (dd, $J = 7.3, 1.8 \text{ Hz}$, 2H), 7.63 – 7.51 (m, 1H), 7.46 (dd, $J = 8.3, 6.8 \text{ Hz}$, 2H), 2.95 (t, $J = 7.3 \text{ Hz}$, 2H), 1.77 (h, $J = 7.4 \text{ Hz}$, 2H), 1.01 (t, $J = 7.4 \text{ Hz}$, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 200.6, 137.2, 133.0, 128.7 (x2), 128.2 (x2), 40.6, 17.9, 14.0. **IR (neat):** $\nu = 3062, 2963, 2876, 1685, 1597, 1451, 1408, 1368, 1311, 1275, 1214, 1181, 996, 897, 735, 692, 569 \text{ cm}^{-1}$. **HRMS (ESI):** m/z $[M+H]^+$ calcd. for $[C_{10}H_{13}O]^+$: 149.0961, found: 149.0960; m/z $[M+Na]^+$ calcd. for $[C_{10}H_{12}ONa]^+$: 171.0780, found: 171.0780.

These data are in agreement with those reported previously in the literature.¹⁰

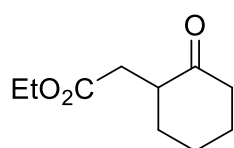
4,4-dimethylcyclohexan-1-one (2k)



Prepared following general procedure 4, **2k** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a colorless liquid (22.5 mg, 178 μmol, 89%). R_f = 0.36 (pentane/Et₂O 7:3, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 2.34 (t, J = 6.7 Hz, 4H), 1.66 (td, J = 6.8, 0.9 Hz, 4H), 1.09 (d, J = 0.9 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 212.7, 39.3 (x2), 38.1 (x2), 30.0, 27.6 (x2). IR (neat): ν = 2950, 2865, 2250, 1712, 1459, 1422, 1387, 1365, 1334, 1234, 1141, 1009, 916, 760, 734, 512 cm⁻¹. HRMS (ESI): m/z [M+Na]⁺ calcd. for [C₈H₁₄ONa]⁺: 149.0937, found: 149.0936.

These data are in agreement with those reported previously in the literature.¹⁵

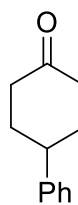
Ethyl 2-(2-oxocyclohexyl)acetate (2l)



Prepared following general procedure 4, **2l** was obtained after purification by column chromatography (0-15% Et₂O in pentane) as a colorless liquid (33.2 mg, 180 μmol, 90%). R_f = 0.43 (pentane/Et₂O 1:1, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 4.17 – 4.05 (m, 2H), 2.89 – 2.80 (m, 1H), 2.74 (dd, J = 16.5, 7.1 Hz, 1H), 2.44 – 2.38 (m, 1H), 2.34 (tdd, J = 13.5, 5.9, 1.2 Hz, 1H), 2.16 – 2.05 (m, 3H), 1.91 – 1.83 (m, 1H), 1.71 (qt, J = 12.8, 3.4 Hz, 1H), 1.62 (qdd, J = 13.1, 4.5, 3.3 Hz, 1H), 1.40 (qd, J = 12.9, 3.7 Hz, 1H), 1.24 (t, J = 7.1 Hz, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 211.1, 172.7, 60.5, 47.2, 41.9, 34.6, 34.0, 27.9, 25.3, 14.3. IR (neat): ν = 2934, 2862, 2328, 2089, 1711, 1449, 1372, 1277, 1166, 1028 cm⁻¹. HRMS (ESI): m/z [M+Na]⁺ calcd. for [C₈H₁₆O₃Na]⁺: 207.0992, found: 207.0993.

These data are in agreement with those reported previously in the literature.¹⁶

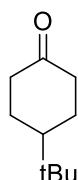
4-phenylcyclohexan-1-one (2m)



Prepared following general procedure 4, **2m** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a white solid (32.4 mg, 186 μmol, 93%). R_f = 0.33 (pentane/Et₂O 6:4, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 7.35 – 7.31 (m, 2H), 7.26 – 7.22 (m, 3H), 3.03 (tt, J = 12.1, 3.5 Hz, 1H), 2.55 – 2.44 (m, 4H), 2.29 – 2.19 (m, 2H), 2.03 – 1.90 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 211.2, 144.9, 128.7 (x2), 126.8 (x2), 126.7, 42.9, 41.5 (x2), 34.1 (x2). IR (neat): ν = 2939, 2868, 1701, 1493, 1450, 1327, 1164, 952, 757, 698 cm⁻¹. HRMS (APCI): m/z [M+H]⁺ calcd. for [C₁₂H₁₅O]⁺: 175.1123, found: 175.1116.

These data are in agreement with those reported previously in the literature.¹⁷

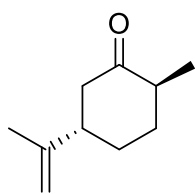
4-(tert-butyl)cyclohexan-1-one (2n)



Prepared following general procedure 4, **2n** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a white solid (25.9 mg, 168 μmol, 84%). R_f = 0.44 (pentane/Et₂O 7:3, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 2.47 – 2.35 (m, 2H), 2.34 – 2.25 (m, 2H), 2.12 – 2.02 (m, 2H), 1.54 – 1.38 (m, 3H), 0.91 (s, 9H). ¹³C NMR (151 MHz, CDCl₃) δ 212.7, 46.9, 41.4 (x2), 32.6, 27.7 (x2), 27.7 (x3). IR (neat): ν = 2948, 2868, 1720, 1462, 1421, 1364, 1332, 1219, 1161, 944, 776 cm⁻¹. HRMS (ESI): m/z [M+H]⁺ calcd. for [C₁₀H₁₉O]⁺: 155.1430, found: 155.1432.

These data are in agreement with those reported previously in the literature.¹⁸

(2R,5R)-2-methyl-5-(prop-1-en-2-yl)cyclohexan-1-one (2o)



Prepared following general procedure 4, **2o** was obtained after purification by column chromatography (0-10% Et₂O in pentane) as a colorless liquid (14.6 mg, 96 μmol, 48%). R_f = 0.53 (pentane/Et₂O 7:3, vanillin).

2o was obtained as an inseparable mixture of diastereomers: d.r. 81:19 (anti:syn).

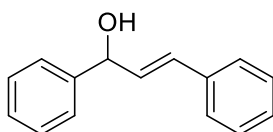
Major diastereomer (anti, fully described): ¹H NMR (600 MHz, CDCl₃) δ 4.75 (p, *J* = 1.5 Hz, 1H), 4.74 – 4.71 (m, 1H), 2.44 (dt, *J* = 11.9, 2.6 Hz, 1H), 2.40 – 2.25 (m, 3H), 2.12 (ddt, *J* = 13.1, 6.2, 3.4 Hz, 1H), 1.99 – 1.90 (m, 1H), 1.74 (s, 3H), 1.69 – 1.60 (m, 1H), 1.37 (qd, *J* = 13.1, 3.5 Hz, 1H), 1.03 (d, *J* = 6.5 Hz, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 212.8, 147.8, 109.8, 47.2, 47.0, 44.9, 35.1, 30.9, 20.6, 14.5.

Minor diastereomer (syn, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 4.86 – 4.81 (m, 1H), 4.69 (s, 1H), 2.62 – 2.53 (m, 2H), 1.90 – 1.81 (m, 3H), 1.73 (d, *J* = 1.4 Hz, 3H), 1.09 (d, *J* = 6.9 Hz, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 214.1, 147.0, 111.6, 44.7, 44.2, 44.1, 30.8, 26.5, 21.7, 15.8.

IR (neat): ν = 2965, 2930, 2862, 1710, 1645, 1449, 1373, 1217; 891, 729 cm⁻¹. **HRMS (ESI):** *m/z* [M+H]⁺ calcd. for [C₁₀H₁₇O]⁺: 153.1274, found: 153.1273.

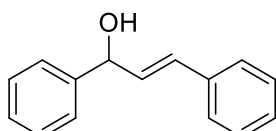
These data are in agreement with those reported previously in the literature.^{19,20}

(E)-1,3-diphenylprop-2-en-1-ol (3a)

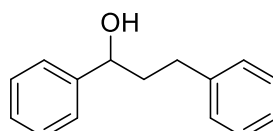


Prepared following general procedure 2, **3a** was obtained after purification by column chromatography (0-20% Et₂O in pentane) as a colorless liquid (30.7 mg, 146 μmol, 73%). R_f = 0.36 (pentane/Et₂O 6:4, vanillin).

3a was obtained as an inseparable mixture of A:B (95:5).



A



B

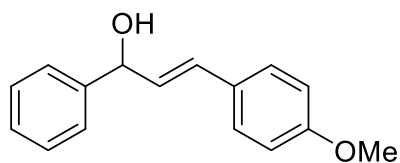
Major compound (A, fully described): ¹H NMR (600 MHz, CDCl₃) δ 7.42 – 7.33 (m, 2H), 7.32 – 7.27 (m, 4H), 7.25 – 7.19 (m, 3H), 7.18 – 7.13 (m, 1H), 6.60 (dd, *J* = 15.9, 1.3 Hz, 1H), 6.30 (dd, *J* = 15.8, 6.5 Hz, 1H), 5.30 (d, *J* = 6.5 Hz, 1H), 2.01 (s, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 142.9, 136.7, 131.7, 130.7, 128.8 (x2), 128.7 (x2), 127.9, 127.9, 126.8 (x2), 126.5 (x2), 75.3.

Minor compound (B, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 4.60 (dd, *J* = 7.9, 5.3 Hz, 1H), 2.67 (ddd, *J* = 13.9, 9.8, 5.7 Hz, 1H), 2.58 (ddd, *J* = 14.0, 9.6, 6.5 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 144.7, 128.6 (x2), 128.5 (x2), 127.6, 126.1, 74.0, 40.6, 32.2.

IR (neat): ν = 3345, 3027, 2860, 2325, 2091, 1598, 1493, 1449, 1299, 1189, 1067, 1010, 965, 745, 694 cm⁻¹. **HRMS (ESI):** *m/z* [M+Na]⁺ calcd. for [C₁₅H₁₄ONa]⁺: 233.0937, found: 233.0937.

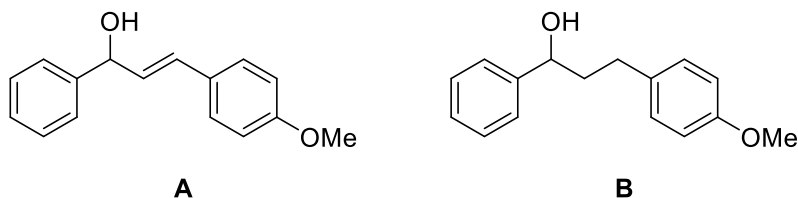
These data are in agreement with those reported previously in the literature.^{21,22}

(E)-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-ol (**3b**)



Prepared following general procedure 2, **3b** was obtained after purification by column chromatography (0-25% Et₂O in pentane) as a colorless liquid (31.7 mg, 132 μmol, 66%). R_f = 0.26 (pentane/Et₂O 6:4, vanillin).

3b was obtained as an inseparable mixture of A:B (96:4).



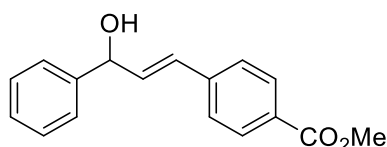
Major compound (A, fully described): ¹H NMR (600 MHz, CDCl₃) δ 7.47 – 7.42 (m, 2H), 7.41 – 7.36 (m, 2H), 7.34 – 7.28 (m, 3H), 6.85 (d, *J* = 8.8 Hz, 2H), 6.63 (dd, *J* = 15.8, 1.2 Hz, 1H), 6.26 (dd, *J* = 15.8, 6.7 Hz, 1H), 5.39 – 5.34 (m, 1H), 3.80 (s, 3H), 2.07 (d, *J* = 3.0 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 159.5, 143.1, 130.4, 129.5, 129.4, 128.7 (x2), 128.0 (x2), 127.8, 126.4 (x2), 114.1 (x2), 75.4, 55.4.

Minor compound (B, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 4.68 (t, *J* = 6.0 Hz, 1H), 3.79 (s, 3H), 2.70 (ddd, *J* = 15.1, 9.7, 5.7 Hz, 1H), 2.62 (ddd, *J* = 14.2, 9.5, 6.6 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 158.0, 144.8, 133.9, 129.4 (x2), 128.6 (x2), 127.7, 126.1 (x2), 114.0 (x2), 74.0, 40.8, 31.2.

IR (neat): ν = 3391, 3029, 2837, 1606, 1509, 1453, 1297, 1246, 1175, 1029, 967, 828, 699 cm⁻¹. **HRMS (APCI):** *m/z* [M+H]⁺ calcd. for [C₁₆H₁₇O₂]⁺: 241.1229, found: 241.1205.

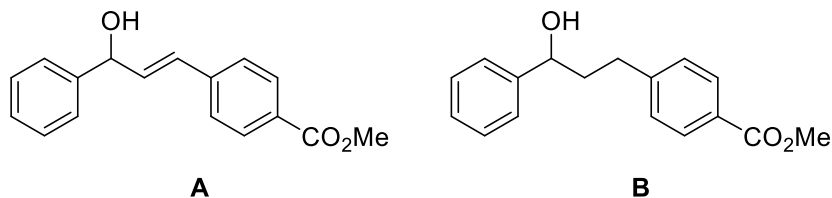
These data are in agreement with those reported previously in the literature.^{22,23}

Methyl (E)-4-(3-hydroxy-3-phenylprop-1-en-1-yl)benzoate (**3c**)



Prepared following general procedure 2, **3c** was obtained after purification by column chromatography (0-25% Et₂O in pentane) as a colorless liquid (46.7 mg, 174 μmol, 87%). R_f = 0.21 (pentane/Et₂O 6:4, vanillin).

3c was obtained as an inseparable mixture of A:B (95:5).

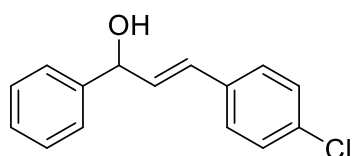


Major compound (A, fully described): ¹H NMR (600 MHz, CDCl₃) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.41 (m, 4H), 7.40 – 7.36 (m, 2H), 7.33 – 7.29 (m, 1H), 6.72 (dd, *J* = 15.9, 1.3 Hz, 1H), 6.49 (dd, *J* = 15.8, 6.2 Hz, 1H), 5.40 (d, *J* = 6.1 Hz, 1H), 3.90 (s, 3H), 2.37 (br, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 167.0, 142.6, 141.2, 134.3, 130.0 (x2), 129.4, 129.2, 128.8 (x2), 128.1, 126.6 (x2), 126.5 (x2), 75.0, 52.2.

Minor compound (B, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 4.67 (dd, *J* = 8.0, 5.3 Hz, 1H), 2.80 (ddd, *J* = 15.0, 9.9, 5.6 Hz, 1H), 2.72 (ddd, *J* = 14.4, 9.7, 6.5 Hz, 1H), 2.17 – 2.10 (m, 1H), 2.06 – 1.98 (m, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 129.9 (x2), 128.7 (x2), 128.6 (x2), 126.0 (x2), 73.8, 40.2, 32.2.

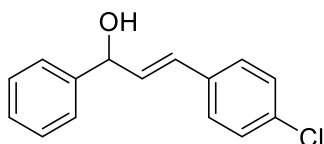
IR (neat): $\nu = 3450, 3030, 2948, 1711, 1692, 1434, 1280, 1184, 1107, 1013, 965, 757, 695$ cm^{-1} . **HRMS (ESI):** m/z $[\text{M}+\text{Na}]^+$ calcd. for $[\text{C}_{17}\text{H}_{16}\text{O}_3\text{Na}]^+$: 291.0992, found: 291.0987.

(E)-3-(4-chlorophenyl)-1-phenylprop-2-en-1-ol (**3d**)

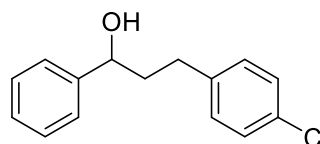


Prepared following general procedure 2, **3d** was obtained after purification by column chromatography (0-20% Et_2O in pentane) as a colorless liquid (34.7 mg, 142 μmol , 71%). $R_f = 0.32$ (pentane/ Et_2O 6:4, vanillin).

3d was obtained as an inseparable mixture of A:B (93:7).



A



B

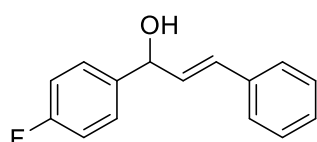
Major compound (A, fully described): $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.50 – 7.41 (m, 2H), 7.41 – 7.37 (m, 2H), 7.34 – 7.29 (m, 3H), 7.27 (d, $J = 8.6$ Hz, 2H), 6.64 (dd, $J = 15.8, 1.3$ Hz, 1H), 6.36 (dd, $J = 15.8, 6.4$ Hz, 1H), 5.38 (dd, $J = 6.0, 2.1$ Hz, 1H), 2.13 (d, $J = 3.3$ Hz, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 142.7, 135.2, 133.5, 132.3, 129.3, 128.9 (x2), 128.8 (x2), 128.1, 127.9 (x2), 126.5 (x2), 75.1.

Minor compound (B, only distinct signals): $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 4.71 – 4.64 (m, 1H), 2.79 – 2.60 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 129.9 (x2), 126.0 (x2), 40.4, 31.5.

IR (neat): $\nu = 3345, 3029, 2862, 2327, 2086, 1594, 1489, 1451, 1403, 1300, 1185, 1088, 1010, 966, 821, 698$ cm^{-1} . **HRMS (ESI):** m/z $[\text{M}+\text{H}]^+$ calcd. for $[\text{C}_{13}\text{H}_{14}\text{OCl}]^+$: 245.0733, found: 245.0733.

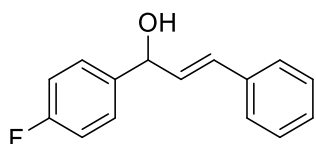
These data are in agreement with those reported previously in the literature.^{24,25}

(E)-1-(4-fluorophenyl)-3-phenylprop-2-en-1-ol (**3e**)

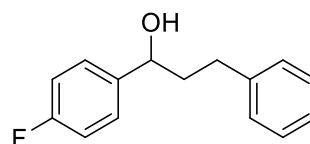


Prepared following general procedure 2, **3e** was obtained after purification by column chromatography (0-20% Et_2O in pentane) as a colorless liquid (34.2 mg, 150 μmol , 75%). $R_f = 0.31$ (pentane/ Et_2O 6:4, vanillin).

3e was obtained as an inseparable mixture of A:B (95:5).



A



B

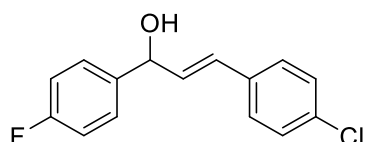
Major compound (A, fully described): $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.46 – 7.36 (m, 4H), 7.32 (dd, $J = 8.4, 6.8$ Hz, 2H), 7.28 – 7.24 (m, 1H), 7.09 – 7.03 (m, 2H), 6.68 (dd, $J = 15.8, 1.2$ Hz, 1H), 6.36 (dd, $J = 15.8, 6.6$ Hz, 1H), 5.37 (d, $J = 6.5$ Hz, 1H), 2.16 (s, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 162.5 (d, $^1J_{\text{C-F}} = 245.9$ Hz), 138.6 (d, $^4J_{\text{C-F}} = 3.3$ Hz), 136.5, 131.4, 130.9, 128.8 (x2), 128.2 (d, $^3J_{\text{C-F}} = 8.5$ Hz, x2), 128.1, 126.8 (x2), 115.6 (d, $^2J_{\text{C-F}} = 21.1$ Hz, x2), 74.6.

Minor compound (B, only distinct signals): $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 4.67 (t, $J = 6.7$ Hz, 1H), 2.74 (ddd, $J = 15.1, 9.7, 5.8$ Hz, 1H), 2.66 (ddd, $J = 13.9, 9.5, 6.5$ Hz, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 73.3, 40.7, 32.1.

IR (neat): $\nu = 3341, 3028, 2860, 2325, 2088, 1896, 1602, 1505, 1222, 1156, 1086, 1011, 966, 833, 741, 693$ cm^{-1} . **HRMS (ESI):** m/z $[\text{M}+\text{H}]^+$ calcd. for $[\text{C}_{15}\text{H}_{14}\text{FO}]^+$: 229.1023, found: 229.1020.

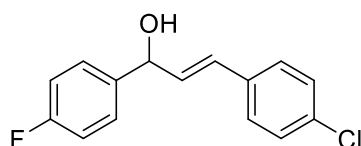
These data are in agreement with those reported previously in the literature.^{26,27}

(E)-3-(4-chlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-ol (**3f**)

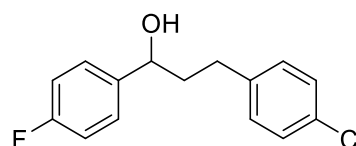


Prepared following general procedure 2, **3f** was obtained after purification by column chromatography (0-20% Et_2O in pentane) as a colorless liquid (37.3 mg, 142 μmol , 71%). $R_f = 0.29$ (pentane/ Et_2O 6:4, vanillin).

3f was obtained as an inseparable mixture of A:B (91:9).



A



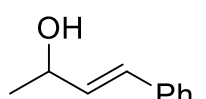
B

Major compound (A, fully described): $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.43 – 7.36 (m, 2H), 7.34 – 7.26 (m, 4H), 7.11 – 7.03 (m, 2H), 6.63 (dd, $J = 15.8, 1.3$ Hz, 1H), 6.32 (dd, $J = 15.8, 6.4$ Hz, 1H), 5.37 (dd, $J = 6.5, 3.1$ Hz, 1H), 2.07 (d, $J = 3.5$ Hz, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 162.5 (d, $^1J_{\text{C-F}} = 246.2$ Hz), 138.5 (d, $^4J_{\text{C-F}} = 2.7$ Hz), 135.0, 133.7, 132.1, 129.6, 128.9 (x2), 128.2 (d, $^3J_{\text{C-F}} = 8.2$ Hz, x2), 128.0 (x2), 115.7 (d, $^2J_{\text{C-F}} = 21.3$ Hz, x2), 74.5.

Minor compound (B, only distinct signals): $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 4.73 – 4.57 (m, 1H), 2.82 – 2.57 (m, 2H).

HRMS (ESI): m/z $[\text{M}+\text{H}]^+$ calcd. for $[\text{C}_{15}\text{H}_{13}\text{ClFO}]^+$: 263.0633, found: 263.0624. **IR (neat):** $\nu = 3340, 2864, 2325, 1896, 1601, 1504, 1406, 1223, 1156, 1085, 1011, 967, 833, 730$ cm^{-1} .

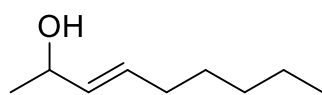
(E)-4-phenylbut-3-en-2-ol (**3g**)



Prepared following general procedure 1, **3g** was obtained after purification by column chromatography (0-25% Et_2O in pentane) as a white solid (19.9 mg, 134 μmol , 67%). $R_f = 0.34$ (pentane/ Et_2O 6:4, vanillin). $^1\text{H NMR}$ (600 MHz, Chloroform- d) δ 7.38 – 7.35 (m, 2H), 7.30 (dd, $J = 8.4, 6.8$ Hz, 2H), 7.25 – 7.21 (m, 1H), 6.67 – 6.50 (m, 1H), 6.25 (dd, $J = 15.9, 6.4$ Hz, 1H), 4.48 (td, $J = 6.4, 1.3$ Hz, 1H), 1.36 (d, $J = 6.4$ Hz, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 136.7, 133.6, 129.4, 128.6, 127.7, 126.5, 69.0, 23.4. **HRMS (ESI):** m/z $[\text{M}+\text{Na}]^+$ calcd. for $[\text{C}_{10}\text{H}_{12}\text{ONa}]^+$: 171.0780, found: 171.0779. **IR (neat):** $\nu = 3343, 3027, 2972, 1493, 1448, 1368, 1293, 1139, 1058, 965, 943, 746, 691$ cm^{-1} .

These data are in agreement with those reported previously in the literature.²⁸

(E)-non-3-en-2-ol (**3h**)

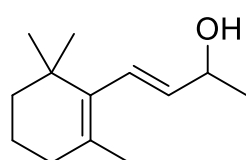


Prepared following general procedure 1, **3h** was obtained after purification by column chromatography (10% Et_2O in pentane) as a colorless oil (14 mg, 98 μmol , 49%). $R_f = 0.12$ (pentane/ Et_2O 9:1, vanillin). $^1\text{H NMR}$ (600 MHz, Chloroform- d) δ 5.63 (dd, $J = 15.3, 6.8$ Hz, 1H), 5.50 (ddt, $J = 15.4, 6.7, 1.4$ Hz, 1H), 4.25 (p, $J = 6.4$ Hz, 1H), 2.00 (q, $J = 7.2$ Hz, 2H), 1.36 (p, $J = 7.4$ Hz,

2H), 1.32 – 1.24 (m, 7H), 1.22 – 1.17 (m, 1H), 0.88 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (151 MHz, Chloroform- d) δ 134.1, 131.2, 69.0, 32.1, 31.4, 28.8, 23.4, 22.5, 14.0. **HRMS (ESI):** m/z $[\text{M}+\text{H}]^+$ calcd. for $[\text{C}_9\text{H}_{18}\text{ONa}]^+$: 165.1253, found: 165.1247. **IR (neat):** $\nu = 3339, 2959, 2857, 2325, 2109, 1884, 1456, 1370, 1370, 1146, 1123, 1059, 967, 935$ cm^{-1}

These data are in agreement with those reported previously in the literature.²⁹

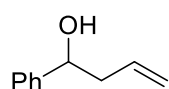
(E)-4-(2,6,6-trimethylcyclohex-1-en-1-yl)but-3-en-2-ol (3i)



Prepared following general procedure 4, **3i** was obtained after purification by column chromatography (0-20% Et_2O in pentane) as a colorless oil (33 mg, 170 μmol , 85%). $R_f = 0.44$ (pentane/ Et_2O 6:4, vanillin). ^1H NMR (600 MHz, Chloroform- d) δ 6.11 – 6.00 (m, 1H), 5.49 (dd, $J = 15.9, 6.7$ Hz, 1H), 4.36 (t, $J = 6.4$ Hz, 1H), 2.01 – 1.92 (m, 2H), 1.68 – 1.63 (m, 3H), 1.64 – 1.57 (m, 2H), 1.48 – 1.42 (m, 2H), 1.31 (d, $J = 6.3$ Hz, 3H), 0.98 (d, $J = 2.0$ Hz, 6H). ^{13}C NMR (151 MHz, Chloroform- d) δ 137.63, 136.64, 128.80, 127.52, 69.51, 39.42, 33.92, 32.70, 28.70, 28.69, 23.58, 21.35, 19.24. **IR (neat):** $\nu = 3331, 2962, 2925, 2865, 1453, 1364, 1141, 1058, 970, 941$ cm^{-1} . **HRMS (APCI):** m/z $[\text{M}+\text{H}]^+$ calcd. for $[\text{C}_{13}\text{H}_{23}\text{O}]^+$: 195.1743, found: 195.1756.

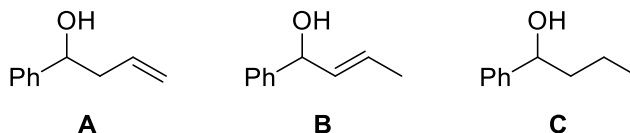
These data are in agreement with those reported previously in the literature.³⁰

1-phenylbut-3-en-1-ol (3j)



Prepared following general procedure 2, **3j** was obtained after purification by column chromatography (0-20% Et_2O in pentane) as a colorless liquid (21 mg, 142 μmol , 71%). $R_f = 0.45$ (pentane/ Et_2O 7:3, vanillin).

3j was obtained as an inseparable mixture of A:B:C (82:10:8).



Major compound (A, fully described): ^1H NMR (600 MHz, CDCl_3) δ 7.40 – 7.33 (m, 4H), 7.32 – 7.27 (m, 1H), 5.82 (ddt, $J = 17.3, 10.1, 7.1$ Hz, 1H), 5.23 – 5.11 (m, 2H), 4.74 (dd, $J = 7.8, 5.2$ Hz, 1H), 2.59 – 2.47 (m, 2H), 2.07 (s, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 144.0, 134.6, 128.6 (x2), 127.7, 126.0 (x2), 118.5, 73.4, 44.0.

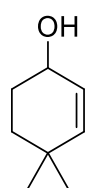
Minor compound (B, only distinct signals): ^1H NMR (600 MHz, CDCl_3) δ 5.77 – 5.63 (m, 1H), 1.73 (d, $J = 6.4$ Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 143.5, 133.8, 128.6, 126.3, 75.3, 17.8.

Minor compound (C, only distinct signals): ^1H NMR (600 MHz, CDCl_3) δ 0.94 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 145.1, 127.6, 126.0, 74.6, 41.4, 19.2, 14.1.

IR (neat): $\nu = 3369, 2927, 2333, 2091, 1641, 1492, 1450, 1311, 1199, 1035, 994, 914, 870, 756, 698$ cm^{-1} . **HRMS (ESI):** m/z $[\text{M}+\text{Na}]^+$ calcd. for $[\text{C}_{10}\text{H}_{12}\text{ONa}]^+$: 171.0780, found: 171.0782; m/z $[\text{M}+\text{Na}]^+$ calcd. for $[\text{C}_{10}\text{H}_{14}\text{ONa}]^+$: 173.0937, found: 173.0937.

These data are in agreement with those reported previously in the literature.^{31–33}

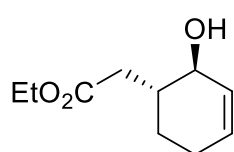
4,4-dimethylcyclohex-2-en-1-ol (**3k**)



Prepared following general procedure 3, **3k** was obtained after purification by column chromatography (0-30% Et₂O in pentane) as a colorless liquid (16.9 mg, 139 μmol, 70%). R_f = 0.25 (pentane/Et₂O 7:3, vanillin). ¹H NMR (600 MHz, CDCl₃) δ 5.58 (dd, *J* = 10.0, 3.1 Hz, 1H), 5.52 (d, *J* = 10.0 Hz, 1H), 4.17 – 4.11 (m, 1H), 1.90 (dddd, *J* = 13.4, 8.4, 5.2, 3.1 Hz, 1H), 1.62 (dddd, *J* = 13.0, 9.6, 6.4, 3.1 Hz, 1H), 1.56 (ddd, *J* = 12.2, 8.6, 3.2 Hz, 1H), 1.52 (s, 1H), 1.42 (ddd, *J* = 13.2, 9.7, 3.2 Hz, 1H), 1.01 (s, 3H), 0.96 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 140.8, 127.5, 66.0, 33.7, 32.0, 29.4, 29.3, 29.2. IR (neat): ν = 3337, 2952, 2864, 1649, 1458, 1367, 1287, 1051, 1004, 835, 742 cm⁻¹. HRMS (ESI): *m/z* [M+Na]⁺ calcd. for [C₈H₁₄ONa]⁺: 149.0937, found: 149.0937.

These data are in agreement with those reported previously in the literature.³⁴

Ethyl 2-((1R,2R)-2-hydroxycyclohex-3-en-1-yl)acetate (**3l**)



Prepared following general procedure 3, **3l** was obtained after purification by column chromatography (0-30% Et₂O in pentane) as a colorless liquid (25.8 mg, 140 μmol, 70%). R_f = 0.25 (pentane/Et₂O 1:1, vanillin).

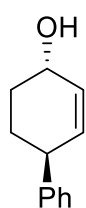
3l was obtained as an inseparable mixture of diastereomers: d.r. 73:27 (anti:syn).

Major diastereomer (anti, fully described): ¹H NMR (600 MHz, CDCl₃) δ 5.80 – 5.75 (m, 1H), 5.65 (dq, *J* = 9.9, 2.2 Hz, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 1H), 2.62 (dd, *J* = 15.4, 6.2 Hz, 1H), 2.26 (dd, *J* = 15.4, 7.2 Hz, 1H), 2.17 – 1.91 (m, 4H), 1.83 – 1.72 (m, 1H), 1.46 – 1.35 (m, 1H), 1.26 (t, *J* = 7.2 Hz, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 173.8, 130.2, 129.4, 71.6, 60.7, 39.5, 38.6, 26.7, 24.7, 14.4.

Minor diastereomer (syn, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 5.88 (ddd, *J* = 10.1, 4.6, 2.6 Hz, 1H), 5.82 (ddt, *J* = 9.8, 4.4, 2.0 Hz, 1H), 4.12 – 4.09 (m, 1H), 2.56 (dd, *J* = 15.2, 8.2 Hz, 1H), 2.31 (dd, *J* = 15.2, 6.6 Hz, 1H), 1.58 – 1.48 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 173.7, 131.2, 128.4, 65.7, 60.6, 36.5, 36.4, 25.2, 23.3, 14.4.

IR (neat): ν = 3421, 2979, 2921, 2327, 2089, 1726, 1446, 1374, 1269, 1208, 1174, 1054, 1026, 862, 678 cm⁻¹. HRMS (ESI): *m/z* [M+Na]⁺ calcd. for [C₁₀H₁₆O₃Na]⁺: 207.0992, found: 207.0993.

(1S,4S)-1,2,3,4-tetrahydro-[1,1'-biphenyl]-4-ol (**3m**)



Prepared following general procedure 3, **3m** was obtained after purification by column chromatography (0-30% Et₂O in pentane) as a colorless liquid (26.5 mg, 152 μmol, 76%). R_f = 0.11 (pentane/Et₂O 7:3, vanillin).

3m was obtained as an inseparable mixture of diastereomers: d.r. 66:34 (anti:syn).

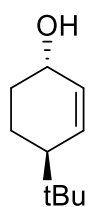
Major diastereomer (anti, fully described): ¹H NMR (600 MHz, CDCl₃) δ 7.37 – 7.28 (m, 2H), 7.25 – 7.16 (m, 3H), 5.95 – 5.88 (m, 1H), 5.84 (ddt, *J* = 10.1, 2.8, 1.3 Hz, 1H), 4.35 (ddq, *J* = 7.2, 4.7, 2.4, 1.9 Hz, 1H), 3.43 (ddq, *J* = 8.5, 5.7, 2.7 Hz, 1H), 2.16 – 2.09 (m, 1H), 1.87 – 1.80 (m, 1H), 1.68 – 1.62 (m, 1H), 1.68 – 1.54 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 145.4, 132.9, 131.7, 128.6 (x2), 127.7 (x2), 126.4, 66.7, 42.1, 32.0, 30.6.

Minor diastereomer (syn, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 6.00 (ddd, *J* = 10.0, 4.0, 2.3 Hz, 1H), 4.26 (q, *J* = 4.3 Hz, 1H), 3.35 (ddq, *J* = 8.0, 4.8, 2.3 Hz, 1H), 1.99 – 1.91 (m, 1H), 1.79 – 1.70 (m, 1H), 1.33 – 1.22 (m, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 145.3, 134.0, 130.2, 128.6, 127.8, 64.5, 30.2, 27.9.

IR (neat): $\nu = 3331, 2932, 2859, 2328, 2088, 1874, 1806, 1601, 1491, 1448, 1386, 1282, 1051, 944, 854, 756, 699 \text{ cm}^{-1}$. **HRMS (ESI):** m/z $[M+H]^+$ calcd. for $[C_{12}H_{15}O]^+$: 175.1117, found: 175.1114.

These data are in agreement with those reported previously in the literature.^{35,36}

(1R,4R)-4-(tert-butyl)cyclohex-2-en-1-ol (**3n**)



Prepared following general procedure 3, **3n** was obtained after purification by column chromatography (0-30% Et₂O in pentane) as a colorless liquid (22.8 mg, 148 μmol , 74%). $R_f = 0.19$ (pentane/Et₂O 7:3, vanillin).

3n was obtained as an inseparable mixture of diastereomers: d.r. 82:18 (anti:syn).

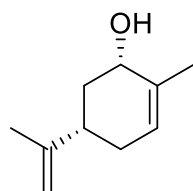
Major diastereomer (anti, fully described): ¹H NMR (600 MHz, CDCl₃) δ 5.77 (dq, $J = 10.4, 1.9 \text{ Hz}$, 1H), 5.71 (ddd, $J = 10.4, 4.5, 1.7 \text{ Hz}$, 1H), 4.20 (dddt, $J = 9.7, 5.5, 3.8, 1.8 \text{ Hz}$, 1H), 2.17 – 2.11 (m, 1H), 1.94 – 1.86 (m, 1H), 1.84 – 1.75 (m, 1H), 1.47 (br, 1H), 1.38 (dddd, $J = 14.2, 11.9, 9.7, 2.5 \text{ Hz}$, 1H), 1.29 (tdd, $J = 13.4, 10.5, 2.4 \text{ Hz}$, 1H), 0.86 (s, 9H). ¹³C NMR (151 MHz, CDCl₃) δ 132.2, 131.4, 67.8, 46.5, 33.4, 33.0, 27.3 (x3), 22.9.

Minor diastereomer (syn, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 5.92 (dt, $J = 10.4, 1.8 \text{ Hz}$, 1H), 5.87 (dddd, $J = 10.3, 4.3, 2.5, 1.5 \text{ Hz}$, 1H), 4.11 – 4.08 (m, 1H), 1.70 – 1.58 (m, 3H), 0.90 (s, 9H). ¹³C NMR (151 MHz, CDCl₃) δ 134.2, 129.1, 63.5, 46.1, 32.7, 31.3, 27.4 (x3), 18.5.

IR (neat): $\nu = 3326, 2949, 2866, 2323, 2087, 1468, 1365, 1052, 875, 730 \text{ cm}^{-1}$. **HRMS (ESI):** m/z $[M+H]^+$ calcd. for $[C_{10}H_{19}O]^+$: 155.1430, found: 155.1429.

These data are in agreement with those reported previously in the literature.³⁷

(1R,5R)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-ol (**3o**)



Prepared following general procedure 3, **3o** was obtained after purification by column chromatography (0-20% Et₂O in pentane) as a colorless liquid (19.8 mg, 130 μmol , 65%). $R_f = 0.27$ (pentane/Et₂O 7:3, vanillin).

3o was obtained as an inseparable mixture of diastereomers: d.r. 87:13 (syn:anti).

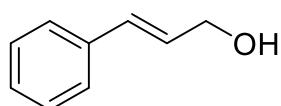
Major diastereomer (syn, fully described): ¹H NMR (600 MHz, CDCl₃) δ 5.50 (dq, $J = 5.4, 1.7 \text{ Hz}$, 1H), 4.73 (s, 2H), 4.34 – 4.13 (m, 1H), 2.40 – 2.22 (m, 1H), 2.20 – 2.13 (m, 1H), 2.11 – 2.04 (m, 1H), 2.01 – 1.91 (m, 1H), 1.76 (d, $J = 1.4 \text{ Hz}$, 3H), 1.74 (s, 3H), 1.51 (td, $J = 12.2, 9.5 \text{ Hz}$, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 149.1, 136.3, 124.0, 109.3, 71.1, 40.6, 38.2, 31.2, 20.8, 19.1.

Minor diastereomer (anti, only distinct signals): ¹H NMR (600 MHz, CDCl₃) δ 5.62 – 5.56 (m, 1H), 4.02 (s, 1H), 2.39 – 2.32 (m, 1H), 1.89 – 1.84 (m, 1H), 1.82 – 1.79 (m, 2H), 1.66 – 1.59 (m, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 149.3, 134.5, 125.5, 109.2, 68.7, 36.9, 35.4, 31.1, 21.1, 21.0.

IR (neat): $\nu = 3325, 2917, 2855, 2325, 2079, 1644, 1442, 1374, 1033, 888, 808 \text{ cm}^{-1}$. **HRMS (ESI):** m/z $[M+H]^+$ calcd. for $[C_{10}H_{17}O]^+$: 153.1274, found: 153.1272.

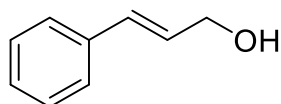
These data are in agreement with those reported previously in the literature.^{24,38}

(E)-3-phenylprop-2-en-1-ol (3p)

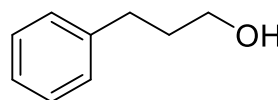


Prepared following general procedure 1, **3p** was obtained after purification by column chromatography (70:30 pentane/Et₂O) as a colorless oil. (20 mg, 147 μmol, 73%). R_f = 0.30 (pentane:Et₂O 6:4, vanillin).

3p was obtained as an inseparable mixture of A:B: (95:5).



A



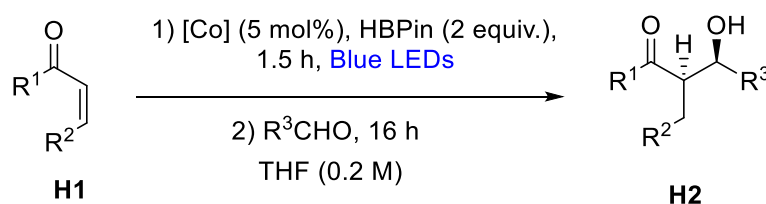
B

Major compound (A, fully described): ¹H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.36 (m, 2H), 7.34 – 7.28 (m, , 2H), 7.26 – 7.22 (m, 1H), 6.68 – 6.56 (m, 1H), 6.36 (dt, *J* = 15.9, 5.7 Hz, 1H), 4.31 (dd, *J* = 5.7, 1.5 Hz, 2H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 136.6, 131.1, 128.6, 128.5, 127.7, 126.4, 63.7. **HRMS (EI)** *m/z* [M]⁺calculated for [C₉H₁₀O]⁺: 134.0725, found: 134.0726. **IR (neat):** ν = 3290, 3028, 2896, 2856, 1492, 1448, 3172, 1274, 1213, 1090, 1010, 967, 916, 734, 688cm⁻¹.

Minor compound (B, only distinct signals): ¹H NMR (400 MHz, Chloroform-*d*) δ 3.66 (t, *J* = 6.4 Hz, 2H), 2.70 (t, *J* = 8.1 Hz, 2H), 1.94 – 1.83 (m, 2H).

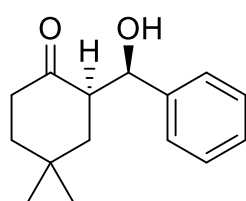
These data are in agreement with those reported previously in the literature.³⁹

5.5 General procedure for the reductive aldol reaction (Procedure 5)



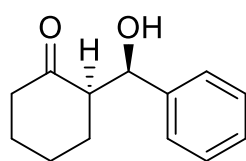
General procedure: In an oven-dried vial were introduced the cobalt catalyst (5 mol%, 10 μ mol, 8.6 mg) and a stirring bar. A cap with rubber septum was used to close the vial and the system was then purged with Argon. THF (C = 0.1 M, 2 mL), enone **H1** (1 equiv., 0.2 mmol) and HBPIn (2 equiv., 0.4 mmol, 58 μ L) were then added successively and the vial was exposed to blue LEDs for 1.5 hours. After this time, the aldehyde was added (1.5 equiv, 0.3 mmol) neat, if liquid or dissolved in THF (0.2 ml) if solid. The resulting mixture was left at stirring for 16 hours. The crude was washed twice with a buffered aqueous solution (pH=8, $\text{Na}_2\text{HPO}_4/\text{NaH}_2\text{PO}_4$) and the aqueous layer extracted twice with Et_2O . The combined organic phase was then dried over MgSO_4 and concentrated in vacuum. The resulting residue was then purified through column chromatography to afford the corresponding aldol product **H2**.

2-(hydroxy(phenyl)methyl)-4,4-dimethylcyclohexan-1-one (**4a**)



Prepared following general procedure 5, **4a** was obtained after purification by column chromatography (85:15 pentane/ Et_2O) as a white solid. (34 mg, 146 μ mol, 73%). $R_f = 0.42$ (pentane: Et_2O 6:4, vanillin). **^1H NMR** (600 MHz, Chloroform- d) δ 7.36 – 7.32 (m, 2H), 7.30 – 7.27 (m, 2H), 7.25 – 7.23 (m, 1H), 5.41 (t, $J = 3.0$ Hz, 1H), 2.97 (d, $J = 3.5$ Hz, 1H), 2.75 (dddd, $J = 13.4, 5.6, 2.6, 1.0$ Hz, 1H), 2.58 – 2.50 (m, 1H), 2.31 (ddd, $J = 14.4, 4.6, 2.8$ Hz, 1H), 1.74 – 1.62 (m, 3H), 1.34 (ddd, $J = 13.5, 5.6, 3.4$ Hz, 1H), 1.05 (s, 3H), 0.95 (s, 3H). **^{13}C NMR** (151 MHz, Chloroform- d) δ 215.3, 141.4, 128.2, 126.9, 125.6, 70.5, 52.7, 39.9, 38.7, 38.1, 31.4, 30.4, 24.3. **HRMS (ESI)** m/z $[\text{M}+\text{Na}]^+$ calculated for $[\text{C}_{15}\text{H}_{20}\text{O}_2\text{Na}]^+$: 255.1355, found: 255.1347. **IR (neat):** $\nu = 3496, 3419, 2948, 2864, 1696, 1491, 1448, 1317, 1183, 1155, 1033, 749, 698, 659$ cm^{-1} .

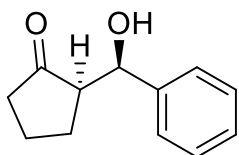
2-(hydroxy(phenyl)methyl)cyclohexan-1-one (**4b**)



Prepared following general procedure 5, **4b** was obtained after purification by column chromatography (90:9:1 pentane/ Et_2O / AcOH) as a white solid. (34 mg, 166 μ mol, 83%). $R_f = 0.31$ (pentane: Et_2O 6:4, vanillin). **^1H NMR** (600 MHz, Chloroform- d) δ 7.29 – 7.22 (m, 4H), 7.20 – 7.16 (m, 1H), 5.32 (d, $J = 2.8$ Hz, 1H), 2.94 (d, $J = 3.3$ Hz, 1H), 2.55 – 2.51 (m, 1H), 2.41 – 2.36 (m, 1H), 2.30 (tdd, $J = 13.5, 6.1, 1.3$ Hz, 1H), 2.01 (ddt, $J = 13.3, 5.9, 2.9$ Hz, 1H), 1.81 – 1.74 (m, 1H), 1.68 (dd, $J = 10.6, 3.7$ Hz, 1H), 1.61 (dtt, $J = 21.4, 13.3, 3.9$ Hz, 1H), 1.49 – 1.40 (m, 1H). **^{13}C NMR** (151 MHz, Chloroform- d) δ 214.8, 141.5, 128.2, 127.0, 125.8, 70.6, 57.2, 42.7, 28.0, 26.0, 24.9. **HRMS (ESI)** m/z $[\text{M}+\text{Na}]^+$ calculated for $[\text{C}_{13}\text{H}_{16}\text{O}_2\text{Na}]^+$: 227.1048, found: 227.1055. **IR (neat):** $\nu = 3505, 2942, 2864, 1694, 1596, 1492, 1448, 1313, 1255, 1198, 1132, 1066, 1033, 746, 697$ cm^{-1} .

These data are in agreement with those reported previously in the literature.⁴⁰

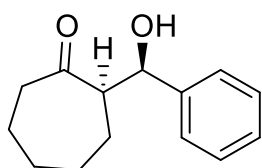
2-(hydroxy(phenyl)methyl)cyclopentan-1-one (**4c**)



Prepared following general procedure 5, **4c** was obtained after purification by column chromatography (90:9:1 pentane/Et₂O/AcOH) as a colorless oil. (28 mg, 148 μmol, 74%). *R_f* = 0.50 (pentane:Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, Chloroform-*d*) δ 7.28 – 7.24 (m, 4H), 7.18 (m, 1H), 5.22 (d, *J* = 3.1 Hz, 1H), 2.57 (s, 1H), 2.37 (ddd, *J* = 11.9, 6.2, 2.3 Hz, 1H), 2.30 – 2.23 (m, 1H), 2.06 (ddd, *J* = 19.0, 11.0, 8.6 Hz, 1H), 2.01 – 1.87 (m, 2H), 1.78 – 1.69 (m, 1H), 1.66 – 1.55 (m, 1H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 220.6, 142.8, 128.4, 127.3, 125.6, 71.5, 56.2, 39.2, 22.8, 20.5. **HRMS (ESI)** *m/z* [M+Na]⁺ calculated for [C₁₂H₁₄O₂Na]⁺: 213.0886, found: 213.0888. **IR (neat)**: *ν* = 3400, 2964, 2884, 1723, 1449, 1403, 1332, 1264, 1156, 1107, 1025, 968, 725, 698, 669 cm⁻¹.

These data are in agreement with those reported previously in the literature.⁴¹

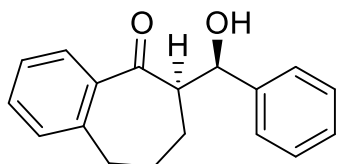
2-(hydroxy(phenyl)methyl)cycloheptan-1-one (**4d**)



Prepared following general procedure 5, **4d** was obtained after purification by column chromatography (80:20 pentane/Et₂O) as a colorless oil (28 mg, 130 μmol, 65%). *R_f* = 0.60 (pentane:Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, Chloroform-*d*) δ 7.30 – 7.23 (m, 4H), 7.21 – 7.15 (m, 1H), 5.11 (d, *J* = 3.0 Hz, 1H), 3.27 (s, 1H), 2.76 (dd, *J* = 10.9, 3.2 Hz, 1H), 2.53 – 2.46 (m, 1H), 2.38 (ddd, *J* = 15.6, 11.9, 3.5 Hz, 1H), 1.83 – 1.74 (m, 3H), 1.69 (ddd, *J* = 14.3, 6.2, 3.0 Hz, 1H), 1.55 (dd, *J* = 11.4, 3.9 Hz, 1H), 1.46 – 1.35 (m, 1H), 1.25 – 1.12 (m, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 218.2, 142.0, 128.2, 127.2, 125.9, 73.4, 57.8, 44.0, 29.2, 29.1, 24.2, 23.8. **HRMS (ESI)** *m/z* [M+Na]⁺ calculated for [C₁₄H₁₈O₂Na]⁺: 242.1199, found: 242.1191. **IR (neat)**: *ν* = 3434, 2927, 2856, 1687, 1450, 1343, 1043, 926, 763, 735, 701 cm⁻¹.

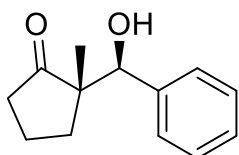
These data are in agreement with those reported previously in the literature.⁴²

6-(hydroxy(phenyl)methyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one (**4e**)



Prepared following general procedure 5, **4e** was obtained after purification by column chromatography (80:20 pentane/Et₂O) as a white solid. (37 mg, 156 μmol, 78%). *R_f* = 0.65 (pentane:Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, Chloroform-*d*) δ 7.68 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.34 (td, *J* = 7.5, 1.5 Hz, 1H), 7.32 – 7.22 (m, 4H), 7.21 – 7.13 (m, 3H), 5.34 (s, 1H), 3.84 (s, 1H), 3.11 – 3.06 (m, 1H), 2.92 – 2.77 (m, 2H), 1.95 (ddd, *J* = 24.4, 12.9, 6.0 Hz, 2H), 1.60 – 1.50 (m, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 208.8, 143.4, 141.7, 138.8, 131.9, 130.2, 128.5, 128.2, 127.1, 126.5, 125.9, 72.7, 55.6, 33.7, 25.4, 22.4. **HRMS (ESI)** *m/z* [M+Na]⁺ calculated for [C₁₈H₁₈O₂Na]⁺: 289.1199, found: 289.1204. **IR (neat)**: *ν* = 3448, 2926, 2860, 1654, 1596, 1449, 1287, 1251, 1092, 1045, 962, 762, 701 cm⁻¹.

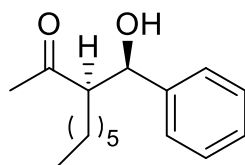
2-(hydroxy(phenyl)methyl)-2-methylcyclopentan-1-one (**4f**)



Prepared following general procedure 5, **4f** was obtained after purification by column chromatography (80:20 pentane/Et₂O) as a colorless oil. (24 mg 120 μmol, 60%). *R_f* = 0.35 (pentane:Et₂O 6:4, vanillin). **¹H NMR** (600 MHz, Chloroform-*d*) δ 7.36 – 7.30 (m, 4H), 7.29 – 7.25 (m, 1H), 4.80 (s, 1H), 4.12 (d, *J* = 1.3 Hz, 1H), 2.43 (dddd, *J* = 19.3, 8.5, 3.3, 1.8 Hz, 1H), 2.23 (dt, *J* = 19.2, 9.5 Hz, 1H), 1.97 (ddd, *J* = 12.9, 10.7, 7.2 Hz, 1H), 1.91 – 1.75 (m, 2H), 1.47 – 1.39 (m, 1H), 1.06 (s, 3H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 226.0, 139.5, 127.9, 127.2, 52.3, 38.0, 34.1, 18.5, 15.7. **HRMS (ESI)** *m/z* [M+Na]⁺ calculated for [C₁₃H₁₆O₂Na]⁺: 227.1035, found: 227.1043. **IR (neat)**: *ν* = 3457, 2963, 2875, 1720, 1452, 1404, 1197, 1163, 1043, 772, 713 cm⁻¹.

These data are in agreement with those reported previously in the literature.⁴³

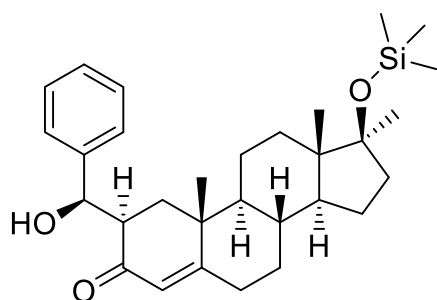
3-(hydroxy(phenyl)methyl)nonan-2-one (4g)



Prepared following general procedure 5, **4g** was obtained after purification by column chromatography (90:9:1 pentane/Et₂O/AcOH) as a colorless oil. (27 mg, 108 μmol, 54%). R_f = 0.72 (pentane:Et₂O 6:4, vanillin).

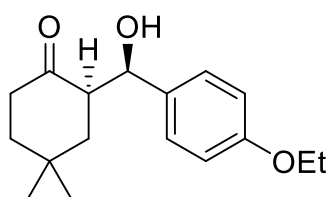
¹H NMR (600 MHz, Chloroform-*d*) δ 7.28 – 7.23 (m, 4H), 7.19 (m, 1H), 4.79 (d, *J* = 5.9 Hz, 1H), 2.80 (ddd, *J* = 9.7, 5.9, 4.0 Hz, 1H), 2.66 (s, 1H), 1.92 (s, 3H), 1.70 – 1.50 (m, 2H), 1.22 – 1.00 (m, 8H), 0.78 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 213.2, 142.0, 128.4, 127.7, 126.2, 74.1, 59.6, 31.8, 29.5, 27.8, 27.3, 22.5, 14.0. HRMS (ESI) *m/z* [M+Na]⁺ calculated for [C₁₆H₂₄O₂Na]⁺: 271.1668, found: 271.1672. IR (neat): ν = 3423, 2925, 2858, 1702, 1455, 1419, 1356, 1164, 1046, 763, 700 cm⁻¹.

(2R,8R,9S,10R,13S,14S,17S)-2-(hydroxy(phenyl)methyl)-10,13,17-trimethyl-17-((trimethylsilyl)oxy)-1,2,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3H-cyclopenta[*a*]phenanthren-3-one (4h)



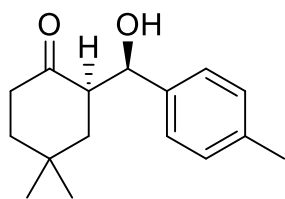
Prepared following general procedure 5, **4g** was obtained after purification by column chromatography (70:30 70:30 pentane/Et₂O) as a colorless oil. (27 mg, 102 μmol, 51%). R_f = 0.72 (pentane:Et₂O 7:3, vanillin). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.30 (m, 4H), 7.26 (m, 1H), 5.76 (d, *J* = 1.5 Hz, 1H), 5.54 (t, *J* = 3.9 Hz, 1H), 3.08 (d, *J* = 5.1 Hz, 1H), 2.74 (ddd, *J* = 10.7, 7.6, 2.9 Hz, 1H), 2.39 – 2.22 (m, 2H), 1.92 – 1.78 (m, 2H), 1.63 (dd, *J* = 10.3, 6.7 Hz, 3H), 1.60 – 1.48 (m, 2H), 1.47 – 1.36 (m, 2H), 1.33 – 1.19 (m, 3H), 1.14 (s, 3H), 1.06 (s, 3H), 0.95 (dd, *J* = 12.3, 4.5 Hz, 1H), 0.91 – 0.78 (m, 2H), 0.75 (s, 3H), 0.07 (s, 9H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 201.0, 172.2, 141.7, 128.2, 126.9, 125.8, 123.7, 83.7, 71.3, 54.2, 49.0, 48.7, 46.2, 39.0, 38.9, 36.4, 34.9, 32.6, 31.6, 31.1, 26.2, 23.4, 20.5, 17.5, 14.1, 2.4. HRMS (ESI) *m/z* [M+Na]⁺ calculated for [C₃₀H₄₄O₃SiNa]⁺: 503.2952, found: 503.2958. IR (neat): ν = 3442, 2948, 1660, 1450, 1249, 1168, 1092, 1065, 1019, 877, 836, 730, 699 cm⁻¹.

2-((4-ethoxyphenyl)(hydroxy)methyl)-4,4-dimethylcyclohexan-1-one (4i)



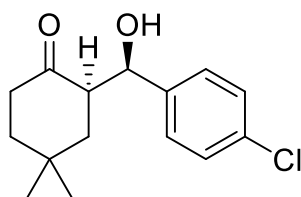
Prepared following general procedure 5, **4i** was obtained after purification by column chromatography (90:9:1 pentane/Et₂O/AcOH) as a white solid. (45 mg, 162 μmol 81%). R_f = 0.63 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.19 (m, 2H), 6.94 – 6.72 (m, 2H), 5.34 (t, *J* = 3.1 Hz, 1H), 4.03 (q, *J* = 7.0 Hz, 2H), 2.94 (d, *J* = 3.5 Hz, 1H), 2.71 (ddd, *J* = 13.8, 6.0, 2.8 Hz, 1H), 2.53 (td, *J* = 14.0, 6.4 Hz, 1H), 2.30 (ddd, *J* = 14.3, 4.6, 2.8 Hz, 1H), 1.76 – 1.63 (m, 3H), 1.45 – 1.35 (m, 4H), 1.06 (s, 3H), 0.96 (s, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 215.4, 157.9, 133.3, 126.7, 114.2, 70.3, 63.4, 52.7, 39.9, 38.7, 38.2, 31.4, 30.4, 24.3, 14.9. HRMS (ESI) *m/z* [M+Na]⁺ calculated for [C₁₇H₂₄O₃Na]⁺: 299.1618, found: 299.1623. IR (neat): ν = 3433, 2927, 2870, 1700, 1610, 1511, 1473, 1244, 1175, 1115, 1091, 1049, 845, 816, 659 cm⁻¹.

2-(hydroxy(*p*-tolyl)methyl)-4,4-dimethylcyclohexan-1-one (4j)



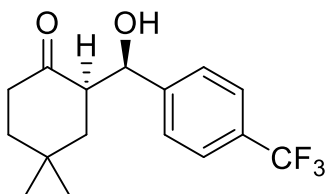
Prepared following general procedure 5, **4j** was obtained after purification by column chromatography (90:9:1 pentane/Et₂O/AcOH) as a white solid. (27 mg, 110 μmol, 55%). *R_f* = 0.59 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.17 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 5.39 – 5.36 (m, 1H), 2.96 (s, 1H), 2.74 (ddd, *J* = 13.4, 5.6, 2.5 Hz, 1H), 2.53 (td, *J* = 14.0, 6.5 Hz, 1H), 2.34 (s, 3H), 2.31 (ddd, *J* = 14.4, 4.5, 2.9 Hz, 1H), 1.74 – 1.62 (m, 3H), 1.38 (ddd, *J* = 13.5, 5.7, 3.4 Hz, 1H), 1.06 (s, 3H), 0.96 (s, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 215.3, 138.4, 136.4, 128.9, 125.5, 70.4, 52.7, 39.9, 38.7, 38.1, 31.4, 30.4, 24.3, 21.1. HRMS (ESI) *m/z* [M+Na]⁺ calculated for [C₁₆H₂₂O₂Na]⁺: 269.1512, found: 269.1503. IR (neat): ν = 3419, 2947, 2865, 1700, 1512, 1643, 1399, 1368, 1154, 1092, 1043, 836, 784, 659 cm⁻¹.

2-((4-chlorophenyl)(hydroxy)methyl)-4,4-dimethylcyclohexan-1-one (4k)



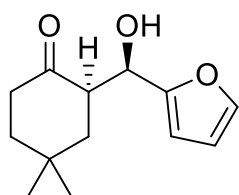
Prepared following general procedure 5, **4k** was obtained after purification by column chromatography (70:30 pentane/Et₂O) as a white solid. (29 mg, 156 μmol, 78%). *R_f* = 0.41 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.31 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 5.38 (t, *J* = 3.0 Hz, 1H), 3.00 (d, *J* = 3.4 Hz, 1H), 2.71 (ddd, *J* = 13.5, 5.7, 2.4 Hz, 1H), 2.54 (td, *J* = 14.1, 6.4 Hz, 1H), 2.32 (dt, *J* = 14.4, 3.7 Hz, 1H), 1.80 – 1.60 (m, 3H), 1.28 (ddd, *J* = 13.5, 5.6, 3.6 Hz, 1H), 1.06 (s, 3H), 0.96 (s, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 215.1, 139.9, 132.6, 128.4, 127.0, 70.0, 52.6, 39.9, 38.6, 38.1, 31.4, 30.4, 24.3. HRMS (ESI) *m/z* [M+Na]⁺ calculated for [C₁₅H₁₉O₂ClNa]⁺: 289.0966, found: 289.0970. IR (neat): ν = 3470, 2953, 2925, 1690, 1490, 197, 1311, 1257, 1212, 1185, 1161, 1088, 1043, 1011, 838, 802 cm⁻¹.

2-(-hydroxy(4-(trifluoromethyl)phenyl)methyl)-4,4-dimethylcyclohexan-1-one (4l)



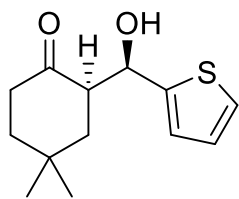
Prepared following general procedure 5, **4l** was obtained after purification by column chromatography (70:30 pentane/Et₂O) as a white solid. (41 mg, 136 μmol, 68%). *R_f* = 0.45 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 8.1 Hz, 2H), 5.47 (s, 1H), 3.04 (s, 1H), 2.83 – 2.70 (m, 1H), 2.56 (td, *J* = 14.1, 6.4 Hz, 1H), 2.34 (ddd, *J* = 14.4, 4.6, 2.8 Hz, 1H), 1.79 – 1.61 (m, 3H), 1.06 (s, 3H), 0.96 (s, 3H). ¹⁹F NMR (565 MHz, Chloroform-*d*) δ -62.39. HRMS (ESI) *m/z* [M+Na]⁺ calculated for [C₁₆H₁₉O₂F₃Na]⁺: 323.1229, found: 323.1235. IR (neat): ν = 3414, 2951, 2929, 1699, 1329, 1154, 1123, 1095, 1068, 1015, 849, 659 cm⁻¹.

2-(furan-2-yl(hydroxy)methyl)-4,4-dimethylcyclohexan-1-one (4m)



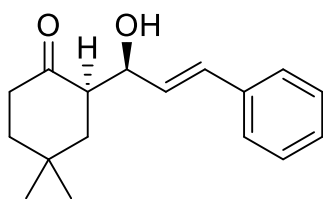
Prepared following general procedure 5, **4m** was obtained after purification by column chromatography (85:15 pentane/Et₂O) as a white solid. (39 mg, 168 μmol, 84%). *R_f* = 0.62 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.41 – 7.30 (m, 1H), 6.33 (dd, *J* = 3.2, 1.8 Hz, 1H), 6.25 (dd, *J* = 3.2, 1.0 Hz, 1H), 5.34 – 5.20 (m, 1H), 3.07 (d, *J* = 5.2 Hz, 1H), 3.03 – 2.85 (m, 1H), 2.61 – 2.46 (m, 1H), 2.31 (ddd, *J* = 14.7, 4.7, 2.8 Hz, 1H), 1.77 – 1.61 (m, 3H), 1.54 (ddd, *J* = 13.5, 5.7, 3.4 Hz, 1H), 1.16 (s, 3H), 1.00 (s, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 214.1, 154.6, 141.5, 110.2, 106.6, 66.7, 50.1, 39.5, 39.4, 38.5, 31.4, 30.4, 24.4. HRMS (ESI) *m/z* [M+Na]⁺ calculated for [C₁₃H₁₈O₃Na]⁺: 245.1154, found: 245.1154. IR (neat): ν = 3417, 2945, 2865, 1698, 1365, 1254, 1148, 1116, 1002, 953, 816, 795, 733 cm⁻¹.

2-(hydroxy(thiophen-2-yl)methyl)-4,4-dimethylcyclohexan-1-one (4n)



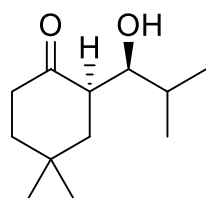
Prepared following general procedure 5, **4n** was obtained after purification by column chromatography (50:50 pentane/Et₂O) as a white solid. (29 mg, 122 μmol, 61%). *R_f* = 0.63 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.15 (d, *J* = 5.0 Hz, 1H), 6.91 (t, *J* = 4.2 Hz, 1H), 6.83 (d, *J* = 3.6 Hz, 1H), 5.49 (d, *J* = 3.6 Hz, 1H), 3.08 (d, *J* = 4.3 Hz, 1H), 2.80 (ddd, *J* = 13.5, 5.8, 2.8 Hz, 1H), 2.48 (td, *J* = 14.1, 6.4 Hz, 1H), 2.25 (dt, *J* = 14.3, 3.9 Hz, 1H), 1.72 – 1.44 (m, 4H), 1.08 (s, 3H), 0.93 (s, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 214.5, 145.3, 126.7, 124.1, 123.1, 68.5, 52.7, 39.7, 38.8, 38.6, 31.4, 30.5, 24.3. **HRMS (ESI)** *m/z* [M+Na]⁺ calculated for [C₁₃H₁₈O₂SNa]⁺: 261.0920, found:261.0923. **IR (neat)**: ν = 3410, 2956, 2928, 1695, 1443, 1365, 1310, 1216, 1156, 1121, 1094, 1039, 837, 704 cm⁻¹.

2-(E-1-hydroxy-3-phenylallyl)-4,4-dimethylcyclohexan-1-one (4o)



Prepared following general procedure 5, **4o** was obtained after purification by column chromatography (90:9:1 pentane/Et₂O/AcOH) as a white solid. (22 mg, 86 μmol, 43%). *R_f* = 0.54 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.41 – 7.38 (m, 2H), 7.32 (m, 2H), 7.26 – 7.22 (m, 1H). 6.62 (dd, *J* = 16.0, 1.6 Hz, 1H), 6.19 (dd, *J* = 15.9, 5.9 Hz, 1H). 4.82 – 4.70 (m, 1H), 2.95 (d, *J* = 5.2 Hz, 1H), 2.71 (ddd, *J* = 12.2, 6.6, 2.9 Hz, 1H), 2.51 (td, *J* = 14.2, 6.2 Hz, 1H), 2.30 (ddd, *J* = 14.7, 4.7, 2.6 Hz, 1H), 1.77 – 1.61 (m, 4H), 1.19 (s, 3H), 1.03 (s, 3H).. ¹³C NMR (151 MHz, Chloroform-*d*) δ 214.8, 136.8, 131.0, 128.9, 128.6, 127.6, 126.5, 70.7, 51.2, 39.6, 39.5, 38.6, 31.5, 30.5, 24.4. **HRMS (ESI)** *m/z* [M+Na]⁺ calculated for [C₁₇H₂₂O₂Na]⁺: 281.1512, found: 281.1517. **IR (neat)**: ν = 3433, 3056, 3027, 2927, 2859, 1701, 1447, 1327, 1154, 1127, 967, 742, 693 cm⁻¹.

2-(1-hydroxy-2-methylpropyl)-4,4-dimethylcyclohexan-1-one (4p)

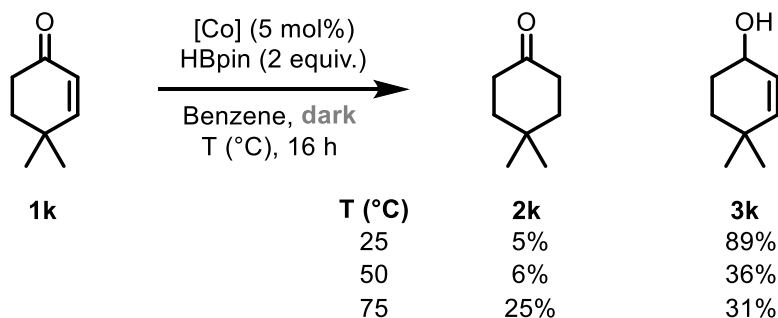


Prepared following general procedure 5, **4p** was obtained after purification by column chromatography (85:15 pentane/Et₂O) as a colorless oil. (26 mg, 132 μmol, 66%). *R_f* = 0.71 (pentane:Et₂O 6:4, vanillin). ¹H NMR (600 MHz, Chloroform-*d*) δ 3.52 (dd, *J* = 7.6, 3.6 Hz, 1H), 2.65 – 2.54 (m, 1H), 2.48 (tdd, *J* = 14.1, 6.2, 1.2 Hz, 1H), 2.25 (ddd, *J* = 14.2, 4.7, 2.6 Hz, 1H), 1.80 – 1.69 (m, 3H), 1.69 – 1.58 (m, 3H), 1.40 (t, *J* = 13.4 Hz, 1H), 1.21 (s, 3H), 1.01 (s, 3H), 0.98 (d, *J* = 6.8 Hz, 3H), 0.86 (d, *J* = 6.8 Hz, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 216.8, 75.4, 49.4, 43.0, 39.7, 39.0, 31.4, 30.6, 28.9, 24.5, 20.1, 14.8. **HRMS (ESI)** *m/z* [M+Na]⁺ calculated for [C₁₂H₂₂O₂Na]⁺: 221.1512, found: 221.1502. **IR (neat)**: ν = 3377, 2955, 2869, 1688, 1617, 1463, 1365, 1303, 1176, 1142, 857, 834 cm⁻¹.

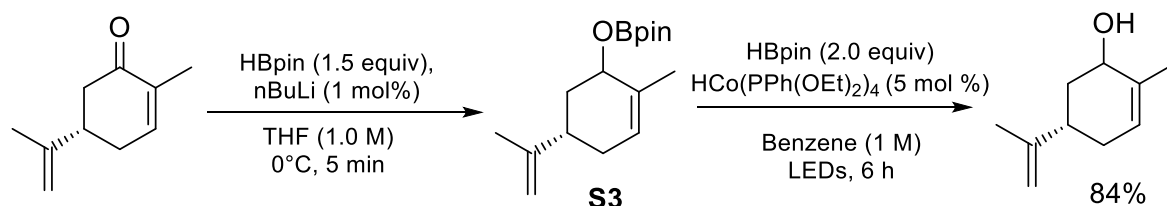
6. Mechanistic Experiments

6.1 Temperature dependence of the reaction in the dark

The hydroboration of 4,4-dimethylcyclohexenone has been carried out following the general procedure 3 with the difference that the reaction vial has been kept for the whole reaction time in an heated oil bath at the given temperature.

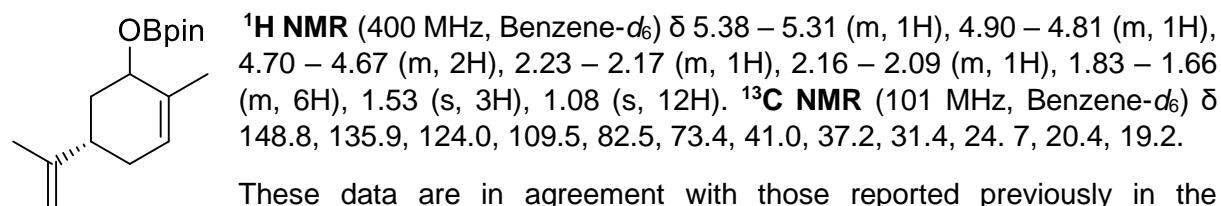


6.2 1,2 hydroboration of carvone and attempted isomerization



In a schlenk tube under argon carvone (1 equiv, 0.1 mmol) was dissolved in dry THF ($c = 1\text{ M}$, 1.0 ml) and the resulting solution was cooled at 0°C . HBpin (1.5 equiv, 1.5 mmol) was added followed by nBuLi (1 mol%, 0.001 mmol, 2.5 M in hexane). After 5 minutes the volatiles were removed under high vacuum. The colorless oil obtained was used without further purification. Dry benzene ($c = 1\text{ M}$, 0.1 ml) was added under Ar; the cobalt catalyst (5 mol %, 0.005 mmol) was then quickly added as a solid followed by HBpin (2 equiv, 0.2 mmol). The reaction mixture has been irradiated with Blue LEDs for 6 hours. After this time, the solution was diluted with Et_2O and washed two times with distilled water, the combined aqueous layers were extracted two times with Et_2O and the combined organic layers were washed with brine, dried (MgSO_4), filtered and concentrated under vacuum. ^1H NMR analysis of the residue revealed that only the 1,2 reduced product was formed (84%, CH_2Br_2 as internal standard)

4,4,5,5-tetramethyl-2-(((5S)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-yl)oxy)-1,3,2-dioxaborolane (S3)



These data are in agreement with those reported previously in the literature.⁴⁴

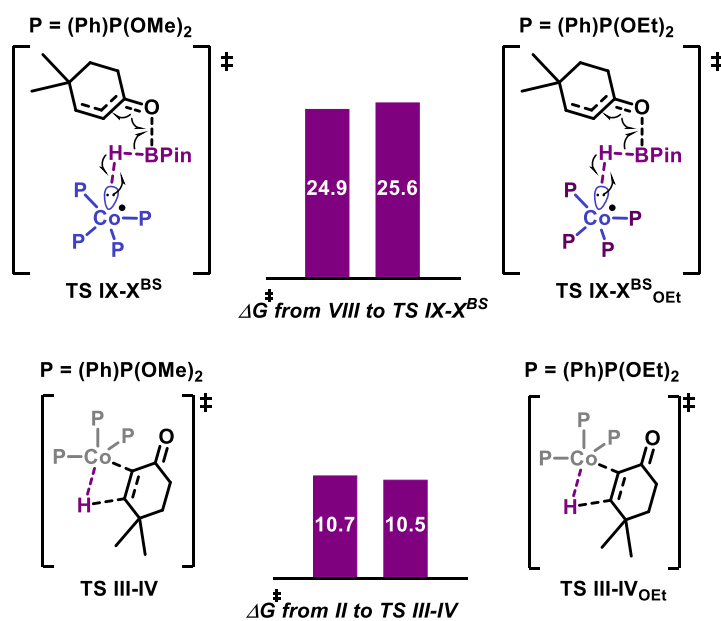
7. Computational details

7.1 General computational details

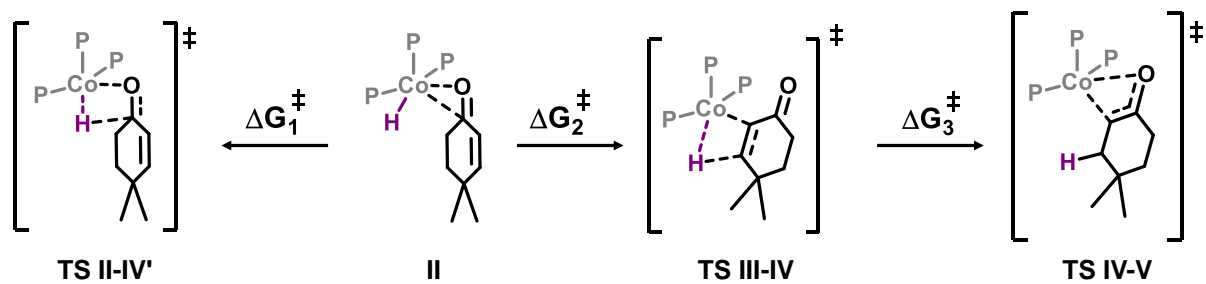
The computational study was carried out using Gaussian16 program package(A.03)⁴⁵ at the B3LYP-D3 level of theory⁴⁶ (this functional has been successfully used for low-valent cobalt homogeneous catalysis,⁴⁷ other functionals were also tested for the light-selectivity determining step but not significant differences were found, see below). The combination of LANL2DZ basis set (for Co) and 6-31G(d) was used for optimization and frequency calculations. In addition, potential energies were further refined using the larger basis set Def2TZVPP for all atoms. All the calculations (optimizations and single points) were computed using the CPCM implicit solvation model with benzene as solvent. Minima and transition states were analyzed by frequency calculation to check the nature of stationary points (zero imaginary frequencies for minima and one for transition states). Thermochemistry corrections were added at standard conditions (298.15 K). Additionally, 1M standard state correction was applied by adding 1.89 kcal/mol when needed. Spin state was checked for all the relevant steps (singlet or triplet for Co(I) species and doublet or quartet for Co(0) species), finding low spin state more stable. The Minimum Energy Crossing Point (MECP) to study the inner-sphere single electron transfer (see below, Figure S3) was calculated using the EasyMECP tool^{48,49}

3D structures were prepared using CYLview.⁵⁰

Ethyl groups on the phosphonite ligand were replaced by methyl groups to reduce the conformational space of the system. We validated that simplification by comparing the highest barrier of the mechanism using the real ligand and the simplified one, being both free energy barriers very similar.



7.2 Benchmark of the computational method:



Functional	ΔG_1^\ddagger	ΔG_2^\ddagger	ΔG_3^\ddagger	$\Delta\Delta G^\ddagger$
B3LYP-D3	18.4	10.7	13.5	4.9
M06	17.2	11.4	11.1	5.8
M06L	19.9	13.5	15.3	4.6
wB97xD	14.5	8.2	9.9	4.6

Table S3. Functional benchmarking of the light mediated Co(I) hydroboration. Energies in kcal/mol. $\Delta\Delta G^\ddagger$ refers to the difference between 1,2 free energy barrier (ΔG_1^\ddagger) and the highest of 1,4 hydroboration pathway (ΔG_2^\ddagger or ΔG_3^\ddagger)

7.3 Complementary pathways:

'Light' Pathways:

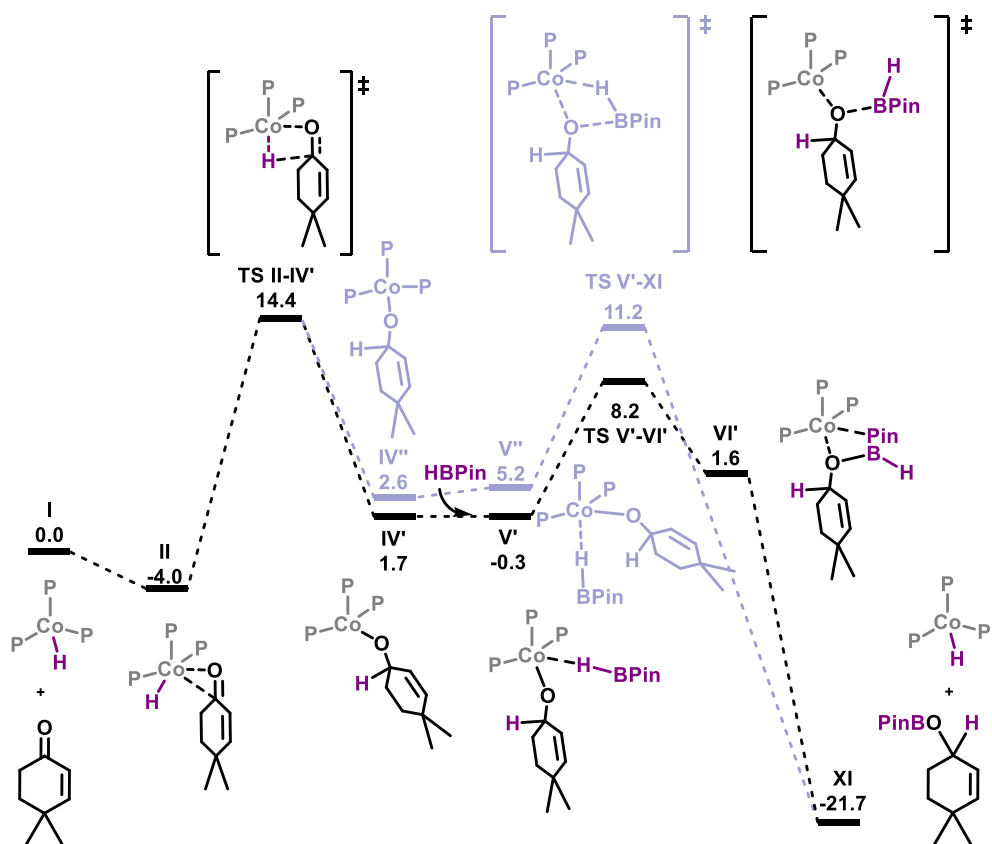


Figure S1. Free energy profile of light-mediated 1,2 hydroboration of cyclohexenone catalysed by Co(I). Energies in kcal/mol. P = P(Ph)(OMe)₂

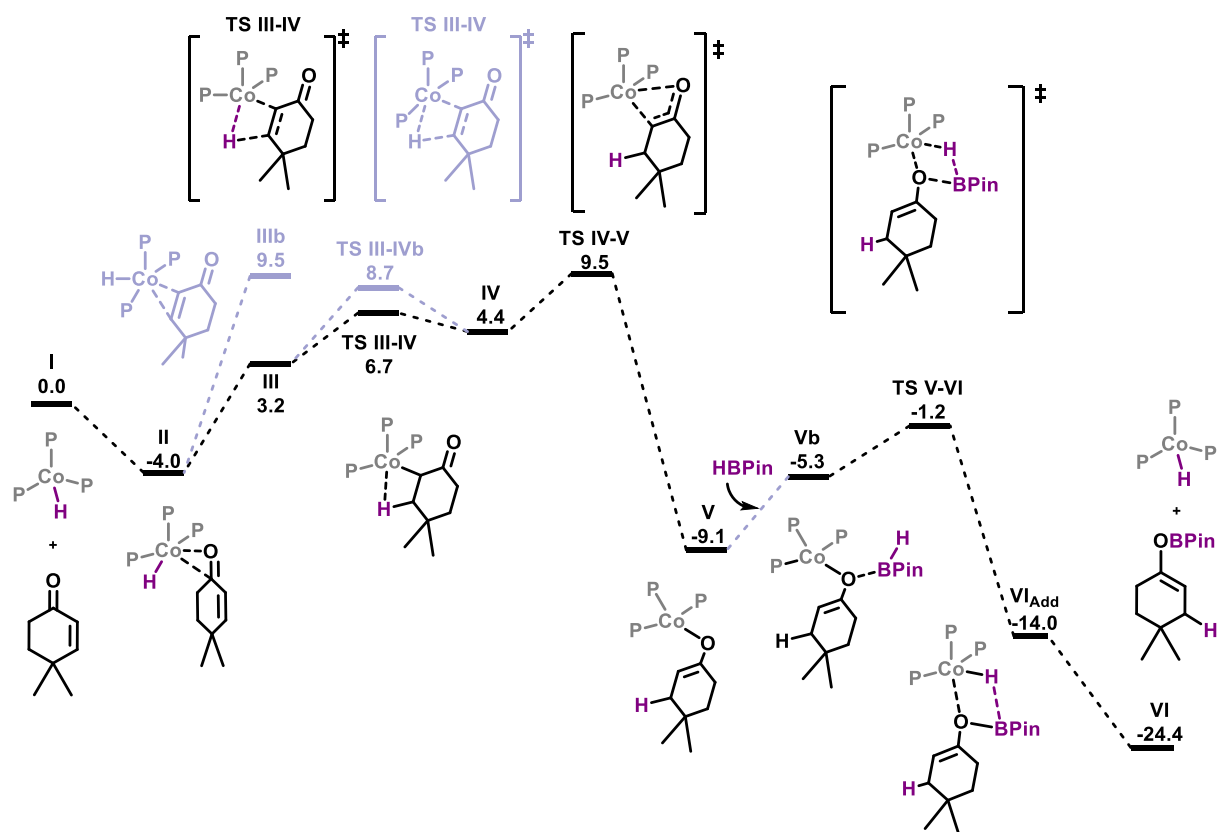


Figure S2. Detailed free energy profile of light-mediated 1,4 hydroboration of cyclohexenone catalysed by Co(I). Energies in kcal/mol. P = (P(Ph)(OMe)₂

'Dark' pathways:

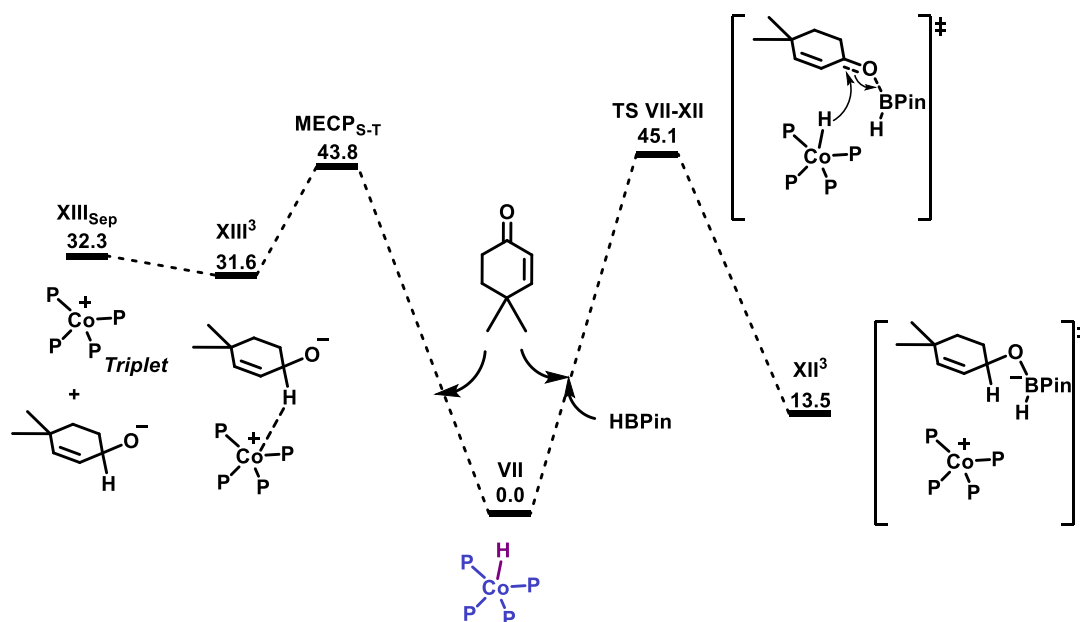


Figure S3. Hydrogen transfer pathways from Co(I)-H. Free energies in kcal/mol. ³ superscript means triplet state. P = (P(Ph)(OMe)₂)

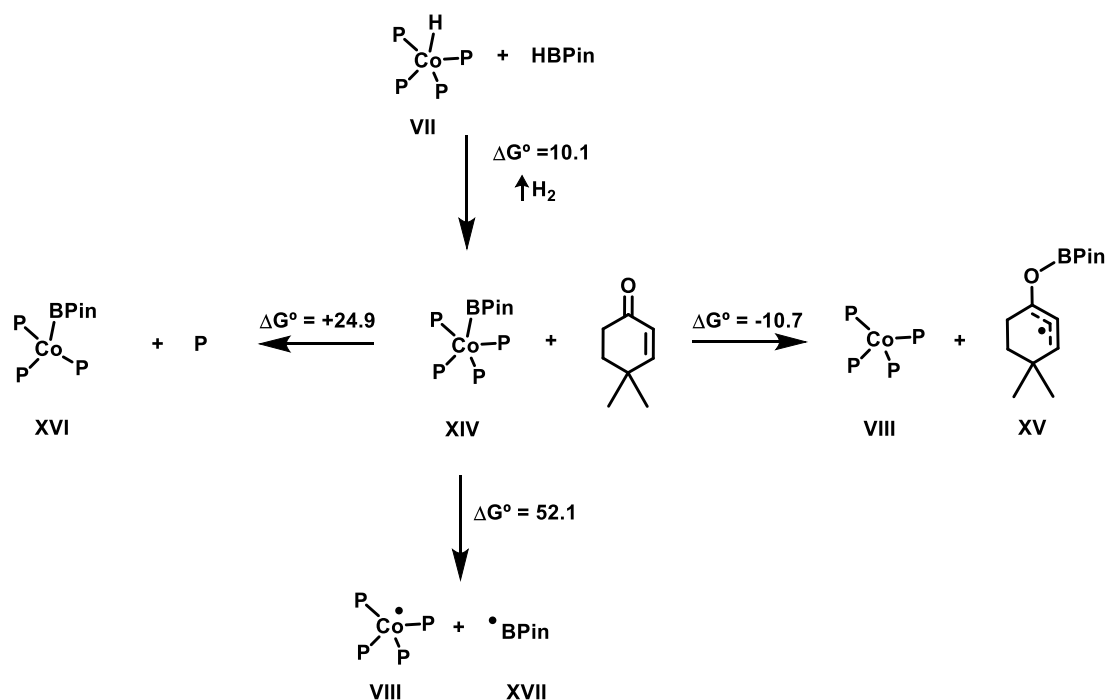


Figure S4. Alternative pathway for Co(0) formation via catalyst reduction with HBPin. Energies in kcal/mol. P = (P(Ph)(OMe)₂)

Due to the experimental detection of H₂, we explored the formation of Co-Bpin species. According to the mechanism proposed in our previous manuscript on cobalt catalysis⁵¹ we calculated the dissociation of a phosphine ligand after CoBPin formation but it is endergonic by 24.9 kcal/mol. However, the formation of P₄-Co(0) species is much more favored, through a single electron transfer from the cyclohexenone substrate to Co-Bpin species. The homolytic

Co-B bond cleavage was also explored and was found highly endergonic, discarding the formation of free BPin radical in solution.

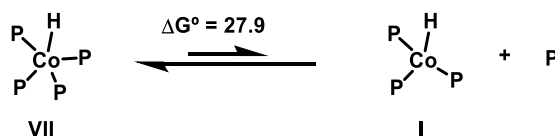


Figure S5. Thermal ligand dissociation in P₄Co(I)-H catalyst. Energies in kcal/mol. P = (P(Ph)(OMe)₂)

The high energy of ligand dissociation excludes this pathway under thermal conditions, since the overall barrier of light mechanism would be added to that equilibrium, yielding an energy span of more than 35 kcal/mol.

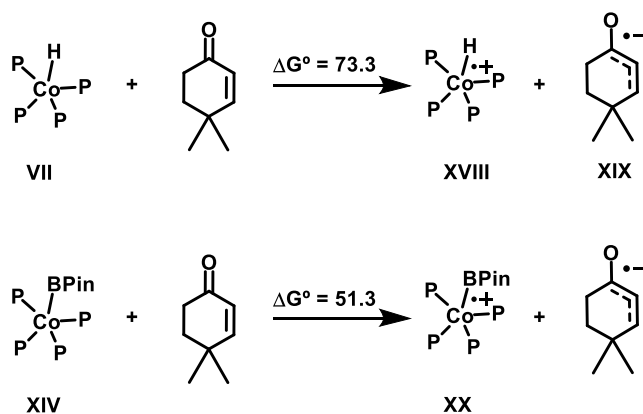


Figure S6. Co(II) formation through Single Electron Transfer from Co(I)-H to the substrate. Energies in kcal/mol. P = (P(Ph)(OMe)₂)

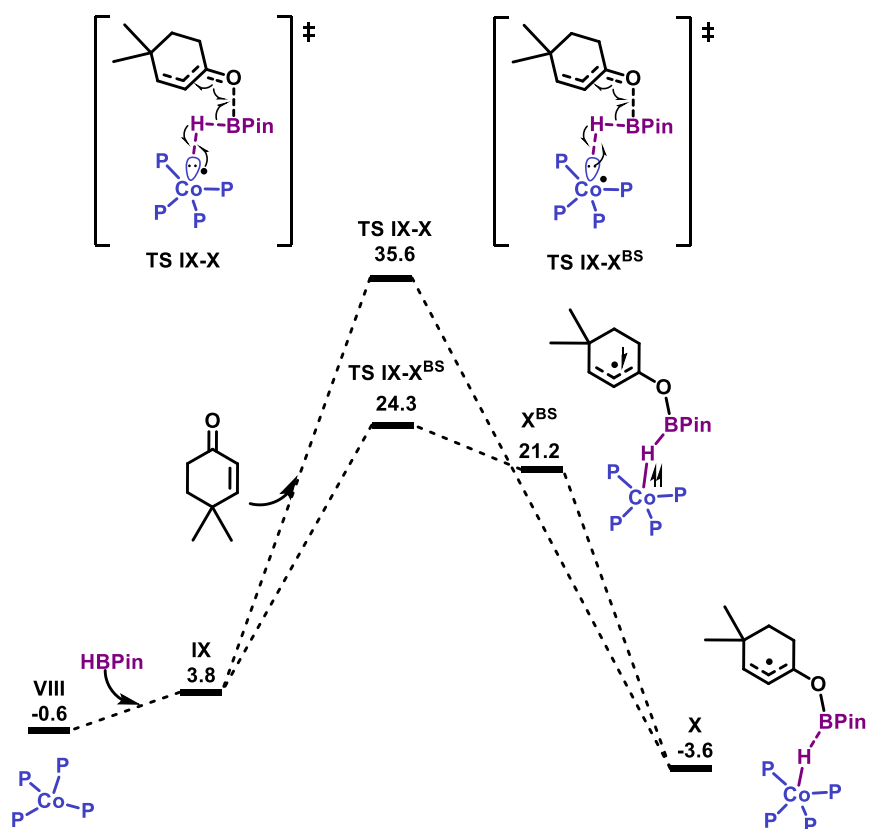


Figure S7. Hydrogen atom abstraction of HBPIn by Co(0) – broken symmetry vs standard pathway. Energies in kcal/mol. P = (P(Ph)(OMe)₂)

Optimized cartesian coordinates and energies of all calculated compounds.

G_{Corr} stands for the thermochemistry correction calculated at low level and E stands for single point energy calculated at high level.

HBPin

$E = -412.0613643$

$G_{\text{Corr}} = 0.159625$

C	0.00000000	0.78782700	-0.19232100
C	0.00000000	-0.78782700	-0.19232100
O	0.32085400	1.10147600	1.19963800
O	-0.32085400	-1.10147600	1.19963800
C	1.05109500	1.43415000	-1.08959000
H	0.88428200	1.15716600	-2.13635400
H	0.98320700	2.52368000	-1.00954300
H	2.06237200	1.13589200	-0.80495700
C	-1.38026100	1.39628500	-0.46564300
H	-1.34331700	2.46924800	-0.25436400
H	-1.67865700	1.25734500	-1.50955700
H	-2.14316700	0.94913600	0.17926800
C	-1.05109500	-1.43415000	-1.08959000
H	-0.88428200	-1.15716600	-2.13635400
H	-0.98320700	-2.52368000	-1.00954300
H	-2.06237200	-1.13589200	-0.80495700
C	1.38026100	-1.39628500	-0.46564300
H	1.34331700	-2.46924800	-0.25436400
H	1.67865700	-1.25734500	-1.50955700
H	2.14316700	-0.94913600	0.17926800
B	0.00000000	0.00000000	1.94269700
H	0.00000000	0.00000000	3.13398600

Cyclohexenone

$E = -387.4700977$

$G_{\text{Corr}} = 0.151558$

C	-2.40112800	0.29066000	-0.93402400
H	-3.03332800	1.09095000	-0.53093900
H	-2.07965700	0.58407700	-1.93996400
H	-3.01566800	-0.61303700	-1.02332200
C	-1.18994800	0.02313600	-0.01762600
C	-0.34688500	-1.13308600	-0.60399100
C	-0.34459000	1.27545900	0.07096100
C	1.04336500	-1.24986400	0.03489000
H	-0.22179600	-0.95695000	-1.68071600
H	-0.89459100	-2.07755500	-0.49975900
C	0.99950700	1.29717200	0.05129300
H	-0.89018400	2.21443400	0.17191300
C	1.81078500	0.06436200	-0.01356000
H	1.65009100	-2.02267500	-0.44710300
H	0.95790000	-1.53184800	1.09423600
H	1.55579600	2.22957600	0.10800000
C	-1.70315100	-0.32047000	1.40213000
H	-2.27474500	0.51498000	1.82264300
H	-2.36238600	-1.19597700	1.36261400
H	-0.87926600	-0.53934100	2.08896100
O	3.03501300	0.10239400	-0.05837500

H₂

$E = -1.180095054$

$G_{\text{Corr}} = -0.001349$

H	0.00000000	0.00000000	0.37146800
H	0.00000000	0.00000000	-0.37146800

I

$E = -3794.102427$

$G_{\text{Corr}} = 0.470988$

Co	0.18635900	-0.16768100	-0.74349300
H	0.70447800	-1.21389800	-1.72805400
P	-0.54008300	1.44765800	0.45136300
O	-0.28716800	1.26125200	2.07026300
O	-2.16813800	1.79992000	0.54245200
C	0.09109900	3.13517300	0.04664200
C	-0.76851600	2.19328600	3.04937700
C	-2.88553400	2.04385000	-0.66794000
C	1.28041000	3.27241200	-0.68577200
C	-0.60785100	4.29433800	0.42927800
H	-0.49840400	1.78090400	4.02417200
H	-0.29146100	3.17244500	2.92630600
H	-1.85470300	2.30285200	2.98316000
H	-3.94720900	2.04130900	-0.41126400
H	-2.61351400	3.01723600	-1.09607900
H	-2.70216900	1.25938600	-1.41052700
C	1.77245200	4.53842100	-1.01044700
H	1.82142400	2.38747800	-1.00185000
C	-0.11380300	5.55893400	0.10850400
H	-1.54651200	4.19844900	0.96617500
C	1.07963000	5.68295400	-0.60972300
H	2.69532100	4.62875300	-1.57693400
H	-0.66156200	6.44709600	0.41240400
H	1.46266000	6.66823800	-0.86180000
P	-1.56353600	-1.30990600	-1.05674000
O	-1.19758000	-2.92723700	-1.13400600
O	-2.45373000	-1.07170800	-2.43919100
C	-2.94720300	-1.29300300	0.14770800
C	-2.23359000	-3.90963000	-1.27572700
C	-1.73224800	-0.62415200	-3.59700800
C	-2.59717500	-1.29437900	1.50647000
C	-4.30073600	-1.26596000	-0.21395400
H	-1.73256700	-4.86912900	-1.42247500
H	-2.85960500	-3.95696000	-0.37748800
H	-2.86394200	-3.68957500	-2.14420700
H	-1.15214600	-1.44363500	-4.03601200
H	-2.47505400	-0.27377800	-4.31782000
H	-1.04884900	0.19294000	-3.33476200
C	-3.58536400	-1.27482400	2.49016900
H	-1.54737400	-1.27518700	1.78922900
C	-5.28967000	-1.23874700	0.77245500
H	-4.57519400	-1.25573900	-1.26376200
C	-4.93425100	-1.24547500	2.12389300
H	-3.30415700	-1.27053000	3.53984100
H	-6.33776000	-1.21229400	0.48551300
H	-5.70566700	-1.22212600	2.88914100
P	2.28425800	-0.26612600	-0.43172900
O	3.24449200	0.80731200	0.42237900
O	3.16723100	-0.20475700	-1.82474900
C	2.78263200	-1.83911200	0.39658000
C	2.87221800	1.19095900	1.74883600
C	4.59918000	-0.30209200	-1.81870100
C	1.96823000	-2.97743500	0.27416000
C	3.95636200	-1.92020800	1.16545500
H	2.23665600	2.08042500	1.72365600
H	2.33651200	0.39382100	2.27506200
H	3.79660200	1.41737400	2.28853600
H	4.91187200	-0.28103700	-2.86506700
H	5.04830000	0.53812200	-1.28096900
H	4.92756200	-1.24338900	-1.36254700
C	2.32662000	-4.17093300	0.90384600

H	1.05285800	-2.92304000	-0.30594200
C	4.31333300	-3.11609300	1.79075900
H	4.58611800	-1.04310100	1.27488000
C	3.49862000	-4.24404300	1.66129900
H	1.68675400	-5.04387400	0.80388900
H	5.22505300	-3.16636200	2.38044500
H	3.77447600	-5.17389300	2.15188600

II

E = -4181.600021

G_{Corr} = 0.646686

Co	0.26314400	-0.17622200	0.13502200
H	1.38899600	-0.28170800	1.12789400
P	-1.37872200	-0.04139500	-1.30187900
O	-1.71336300	-1.40083400	-2.18916300
O	-1.14866400	1.12288100	-2.45409000
C	-3.09876200	0.26679500	-0.74972700
C	-0.61315100	-2.18011300	-2.68612900
C	-2.04813100	1.25642300	-3.56351300
C	-3.51033100	1.58377500	-0.49600100
C	-3.97726500	-0.79061400	-0.47460600
H	-0.94413400	-3.22036200	-2.71710100
H	-0.34409600	-1.84131900	-3.69358200
H	0.25620200	-2.09351200	-2.02954800
H	-1.64125100	2.04584400	-4.19971900
H	-2.11135700	0.32142900	-4.12996700
H	-3.05100900	1.54145600	-3.22639300
C	-4.77219500	1.83742100	0.04318000
H	-2.84971600	2.41069100	-0.72662900
C	-5.23980800	-0.53502300	0.06321800
H	-3.67057000	-1.80808100	-0.68466900
C	-5.63739300	0.77840600	0.33086600
H	-5.07426300	2.86313200	0.23709700
H	-5.91313600	-1.36183000	0.27431600
H	-6.61860200	0.97495700	0.75507600
P	0.51787900	1.78648100	0.85123200
O	2.04117200	2.40528200	0.51058400
O	0.41413900	2.04444300	2.49363000
C	-0.54676700	3.22032200	0.39943900
C	2.42761600	3.69464700	1.00652700
C	0.98476400	1.10271300	3.40597200
C	-0.46987100	3.69957700	-0.91846200
C	-1.49493900	3.77356900	1.27175600
H	3.50131700	3.79516800	0.82813300
H	1.89583700	4.49442300	0.47830300
H	2.22683400	3.77891900	2.07970400
H	2.07451700	1.05388700	3.28905100
H	0.74643000	1.46479300	4.41012300
H	0.57273000	0.10107700	3.25835400
C	-1.32673300	4.70986000	-1.35557400
H	0.24592400	3.26187300	-1.60739500
C	-2.35713000	4.78127800	0.83159900
H	-1.55692000	3.41108100	2.29207300
C	-2.27794000	5.24901600	-0.48250500
H	-1.25935900	5.07108300	-2.37848700
H	-3.09228200	5.19891700	1.51485100
H	-2.95268200	6.02876400	-0.82591600
P	-0.45600500	-1.85196700	1.19060200
O	-1.98599300	-1.77808400	1.85199100
O	0.47746700	-2.27480000	2.50863000
C	-0.68082400	-3.49862200	0.38939400
C	-2.38188800	-0.56155800	2.49617400
C	0.04573900	-3.32276500	3.38639700
C	0.47647700	-4.17066500	-0.03673000
C	-1.93320200	-4.03887600	0.06855800
H	-1.93901000	0.30649200	1.99600800
H	-3.47051200	-0.50225600	2.43309400
H	-2.06863400	-0.57100600	3.54771100

H	0.73549300	-3.32506400	4.23411500
H	-0.97395700	-3.14322700	3.74387500
H	0.08194000	-4.29741600	2.88539000
C	0.38526100	-5.35481800	-0.76735300
H	1.45515700	-3.75916300	0.19965900
C	-2.02667800	-5.21804000	-0.67561200
H	-2.83178500	-3.53721100	0.40934700
C	-0.86972400	-5.87762800	-1.09740200
H	1.28990300	-5.86655500	-1.08555600
H	-3.00473100	-5.62324200	-0.92268200
H	-0.94371800	-6.79369300	-1.67742000
C	7.18760900	-0.39932100	-0.37957200
H	7.52197500	-0.66141200	0.63152700
H	7.28066900	-1.29128200	-1.01033800
H	7.86732300	0.36630200	-0.77194000
C	5.73986100	0.12467800	-0.36486700
C	5.30492800	0.48498500	-1.80480500
C	4.80920400	-0.93869300	0.17720700
C	3.80984500	0.80336600	-1.91663400
H	5.53752900	-0.36843900	-2.45566900
H	5.89935400	1.33268300	-2.16742300
C	3.52552100	-1.07531500	-0.20644600
H	5.20393900	-1.58712500	0.95950000
C	2.92464300	-0.19857000	-1.20882900
H	3.48618600	0.88152500	-2.96045300
H	3.56905200	1.76604300	-1.44490000
H	2.85762400	-1.79762700	0.25167800
C	5.64873800	1.35705400	0.56971400
H	5.97237000	1.09754900	1.58449900
H	6.29823700	2.16142100	0.20198000
H	4.62194300	1.72917900	0.63214700
O	1.70614300	-0.21208000	-1.44858600

III

E = -4181.596399

G_{Corr} = 0.654547

Co	0.23967900	-0.64293900	-0.01756500
H	0.65486100	-1.63261400	-1.04111200
P	-0.60260900	0.98961900	1.21148900
O	0.30003000	2.01556600	2.15420000
O	-1.67398400	0.37233900	2.30980900
C	-1.50564600	2.34363900	0.34499100
C	0.82095500	1.61037700	3.43245600
C	-2.63225300	1.15698100	3.02946700
C	-1.87162500	2.18403900	-0.99701900
C	-1.83565400	3.54492500	0.99722800
H	1.34611800	2.48252000	3.82951500
H	0.00726500	1.33935600	4.11407100
H	1.51714000	0.77194800	3.35331600
H	-3.13003300	0.47468600	3.72160700
H	-2.15147500	1.96311200	3.59452000
H	-3.37515800	1.58122900	2.34714900
C	-2.57708100	3.18381800	-1.66877600
H	-1.57288700	1.29122300	-1.52998600
C	-2.53803300	4.54598500	0.32684600
H	-1.52061000	3.70237100	2.02279100
C	-2.91721000	4.36458200	-1.00714500
H	-2.85063400	3.04033800	-2.71070700
H	-2.78577500	5.46959100	0.84313200
H	-3.46364000	5.14578400	-1.52889100
P	-1.62789300	-1.29441900	-0.87411200
O	-1.74517800	-2.94802100	-0.89835800
O	-1.95818900	-0.91193100	-2.45815600
C	-3.29983300	-0.86971900	-0.22496500
C	-2.83964200	-3.60693500	-1.54708100
C	-0.89531400	-0.88153000	-3.42352500
C	-3.65298600	-1.40530700	1.02377600
C	-4.21287100	-0.04520600	-0.89423300

H	-2.58236400	-4.66852300	-1.58233900	C	-2.22121500	-0.39584300	-2.84856300
H	-3.76910300	-3.47320300	-0.98210300	C	-1.38488600	-2.65008900	1.05875500
H	-2.97908500	-3.22850600	-2.56479700	C	-2.43896100	-3.21380800	-1.04301700
H	-0.37517000	0.07873300	-3.38713700	H	1.75818000	-3.88616400	-2.46766100
H	-0.16953200	-1.68204200	-3.25351300	H	0.14169000	-4.19048800	-1.76730400
H	-1.36566600	-1.01539000	-4.40148400	H	0.29448700	-3.27395400	-3.29432000
C	-4.89314500	-1.12009300	1.59307000	H	-1.98729600	0.66671700	-2.77734600
H	-2.94877400	-2.03816400	1.55594900	H	-2.57465300	-0.62982600	-3.85624400
C	-5.45062000	0.25252700	-0.31766100	H	-2.99783300	-0.66442000	-2.12565500
H	-3.95597200	0.35958700	-1.86605000	C	-2.22936200	-3.54017900	1.72291500
C	-5.79317800	-0.28297900	0.92545300	H	-0.65651800	-2.07604000	1.61752600
H	-5.15550900	-1.54422200	2.55870900	C	-3.29508700	-4.09262600	-0.37699900
H	-6.14761700	0.89970600	-0.84366900	H	-2.51659900	-3.09267500	-2.11865300
H	-6.75675200	-0.05244100	1.37222000	C	-3.19293200	-4.25623300	1.00736400
P	1.66125600	0.46833200	-1.23417600	H	-2.14415900	-3.66261200	2.79933200
O	1.07523300	1.64839100	-2.28017100	H	-4.04113600	-4.64936100	-0.93781000
O	2.29858000	-0.52774500	-2.39402200	H	-3.86130700	-4.93884000	1.52542200
C	3.12063600	1.36902900	-0.53994400	P	-1.44566300	0.94172200	1.13008400
C	1.04443000	3.03479000	-1.92391700	O	-1.51075900	2.52152400	1.66396000
C	3.10912700	-0.10280800	-3.49267700	O	-1.77175500	0.12719500	2.55270300
C	3.25763200	1.34682700	0.85089700	C	-3.13154000	0.73085000	0.41749200
C	4.07416200	2.07439800	-1.29948300	C	-2.59300200	2.99014400	2.48128100
H	0.85745400	3.18640900	-0.85594600	C	-0.72314400	0.02776800	3.52021400
H	1.98819000	3.52291300	-2.18888900	C	-3.57703800	1.67616700	-0.52113600
H	0.22347500	3.48856500	-2.48270600	C	-3.93431300	-0.38628800	0.69058300
H	3.05081900	-0.89546100	-4.24337400	H	-2.31819300	3.99455700	2.81242800
H	2.73607400	0.83117900	-3.92417900	H	-3.52570900	3.03501900	1.90876400
H	4.15276100	0.01903800	-3.18243100	H	-2.73610000	2.34070800	3.35063400
C	4.33344300	1.97345000	1.48293300	H	-1.12925100	-0.53728500	4.36331400
H	2.50872800	0.83518900	1.43342700	H	0.14996300	-0.49209100	3.11554100
C	5.14859300	2.70482100	-0.67262200	H	-0.41140100	1.02077400	3.86684900
C	3.97329100	2.15390900	-2.37594100	C	-4.79678800	1.50531400	-1.17551200
C	5.28522400	2.64966600	0.71965300	H	-2.96425100	2.53704400	-0.76394400
H	4.42211900	1.92228300	2.56419600	C	-5.14912500	-0.56268500	0.02403800
H	5.87961800	3.24414000	-1.26941400	H	-3.60670100	-1.12043300	1.41620300
H	6.12750400	3.13857900	1.20204400	C	-5.58330800	0.38012300	-0.91078200
C	0.94987500	-4.31823800	-0.90319900	H	-5.12569900	2.24477400	-1.90068300
H	-0.01132100	-4.80071100	-0.70297500	H	-5.75289500	-1.44125900	0.23608300
H	0.78760400	-3.57367600	-1.68685100	H	-6.52755500	0.23982300	-1.43041800
H	1.65009900	-5.07641300	-1.27639100	P	1.96978100	-0.60238400	0.92619100
C	1.52041800	-3.66518400	0.36476600	O	1.81493100	-2.01939600	1.79859900
C	2.87108700	-3.00125400	0.03140300	O	2.52407800	0.34009800	2.16589800
C	0.57469600	-2.63761700	0.99019000	C	3.49001000	-0.98029800	-0.06729200
C	3.48866000	-2.24995600	1.21710000	C	1.90652200	-3.33931900	1.25169100
H	2.70542300	-2.30374900	-0.79266400	C	3.56154200	-0.02478000	3.08228300
H	3.57283700	-3.76594600	-0.32694700	C	3.48643600	-0.64410000	-1.42866500
C	1.06489900	-1.65084900	1.84490700	C	4.63467600	-1.59551000	0.46974800
H	-0.43929800	-2.99321300	1.14267100	H	1.00810400	-3.59511900	0.68603700
C	2.49821900	-1.51076100	2.10593200	H	2.77955200	-3.44677000	0.60119900
H	4.22831900	-1.51505000	0.87710800	H	2.00337300	-4.01669300	2.10442200
H	4.03148800	-2.93327500	1.88365100	H	3.46074600	0.64338500	3.94108400
H	0.41603300	-1.24239400	2.61344100	H	3.45137200	-1.06158800	3.41469100
C	1.70616300	-4.77772500	1.43062600	H	4.54881400	0.11910000	2.62977000
H	0.74551300	-5.24907500	1.67138600	C	4.60782900	-0.87460800	-2.22719500
H	2.37900100	-5.55712400	1.05181200	H	2.58274500	-0.23117800	-1.86301000
H	2.12633500	-4.38521700	2.36251500	C	5.75677100	-1.82978900	-0.32701000
O	2.92437100	-0.86006900	3.06847800	H	4.64488600	-1.92165300	1.50425000
				C	5.74904400	-1.46058900	-1.67515400
				H	4.58586600	-0.60569300	-3.27983400
				H	6.63358900	-2.30721400	0.10239400
				H	6.62350700	-1.64226500	-2.29421100
				C	3.29073200	3.96666500	-0.53403700
				H	3.99944400	3.31715600	-0.00548100
				H	3.46671900	3.85904400	-1.61123900
				H	3.51032500	5.00498900	-0.25733100
				C	1.83361400	3.61018300	-0.16595000
				C	0.88500400	4.61964500	-0.85454800
				C	1.58064300	2.18469700	-0.73385900
				C	-0.53766400	4.07139500	-1.01365500
				H	1.27993300	4.86196200	-1.85106400
				H	0.87549200	5.55710800	-0.28448300
				C	0.57522000	1.89828600	-1.69252300

TS III-IV

E = -4181.591504

G_{Corr} = 0.655203

Co	0.31919700	0.44072200	-0.01791500
H	0.95408900	1.60833400	0.70974600
P	-0.34054700	-1.28705100	-1.15969300
O	0.92923800	-2.25815500	-1.58152500
O	-1.03031500	-1.18803600	-2.65481500
C	-1.48208800	-2.47602300	-0.32955200
C	0.75700600	-3.47388900	-2.32375300

H	2.51078900	1.63824300	-0.84618500
C	-0.52482500	2.83930800	-1.90774200
H	-1.20816600	4.80677100	-1.46967200
H	-0.94606000	3.79748100	-0.03562900
H	0.75583800	1.18279500	-2.49071800
C	1.68661100	3.69468000	1.36550600
H	2.30944700	2.93853700	1.85501400
H	2.00058800	4.68647100	1.71514800
H	0.65196600	3.52456100	1.67449800
O	-1.37544300	2.69965100	-2.79432500

IV

E = -4181.599567

G_{Corr} = 0.65966

A Co	0.32862700	0.41135600	-0.20373900
H	1.89703700	1.34163600	-0.46623100
P	-0.14321800	-1.30366600	-1.41110800
O	1.11474400	-2.37291200	-1.58059200
O	-0.52330400	-1.19070100	-3.03186400
C	-1.52029100	-2.40200000	-0.83627500
C	1.01938000	-3.61074700	-2.29593800
C	-1.73210800	-0.58567900	-3.51744000
C	-1.89638600	-2.35447900	0.51258900
C	-2.20655100	-3.27420700	-1.69714700
H	2.02938100	-4.02666700	-2.32545500
H	0.35168300	-4.31119400	-1.78081000
H	0.65874000	-3.44692000	-3.31581200
H	-1.76207900	0.48887800	-3.31146700
H	-1.73993600	-0.75080200	-4.59796400
H	-2.61723600	-1.05973900	-3.07824400
C	-2.93486300	-3.14888700	0.99675600
H	-1.36548800	-1.68466500	1.17768400
C	-3.25254200	-4.06574900	-1.21825700
H	-1.92719000	-3.32698800	-2.74489700
C	-3.62093500	-4.00183900	0.12846500
H	-3.21621100	-3.09145500	2.04478600
H	-3.78131100	-4.73019900	-1.89657000
H	-4.44001900	-4.61294200	0.49799800
P	-1.10727600	1.30075900	1.18398700
O	-1.17212400	2.95318700	1.24963700
O	-1.09282400	1.08584900	2.84476500
C	-2.87193700	0.85666300	0.83882000
C	-2.14041000	3.67473000	2.02161900
C	-1.15582600	-0.18981400	3.47751400
C	-3.23958200	0.57794900	-0.48355500
C	-3.84722400	0.77110200	1.84540700
H	-1.92243400	4.73499700	1.87122000
H	-3.15725800	3.46051800	1.67493400
H	-2.05569500	3.42601400	3.08353000
H	-0.29415500	-0.81268900	3.23236000
H	-1.16315700	-0.00031900	4.55479800
H	-2.07612200	-0.72599800	3.21193700
C	-4.54472200	0.20082700	-0.79697500
H	-2.49618600	0.68183400	-1.26189900
C	-5.15180100	0.37903700	1.53643300
H	-3.58607600	1.01226700	2.87094600
C	-5.50115100	0.08601900	0.21535700
H	-4.81269200	-0.00828600	-1.82937200
H	-5.89515800	0.30488500	2.32614800
H	-6.51538000	-0.22312400	-0.02374200
P	1.63911900	-0.65059500	1.18679200
O	1.24981300	-2.01859300	2.05019000
O	1.94170100	0.34113700	2.45885300
C	3.30490000	-1.12770700	0.55238600
C	1.27270300	-3.34385800	1.50252000
C	2.74207300	0.01519000	3.60307900
C	3.65985000	-0.83104600	-0.77077100
C	4.23178000	-1.80418400	1.36574800

H	0.42523900	-3.50673500	0.83377200
H	2.20272300	-3.53561700	0.95916300
H	1.20061600	-4.02433800	2.35454300
H	2.51116100	0.76841200	4.35934300
H	2.49205000	-0.97791800	3.98829500
H	3.80818800	0.06256600	3.35675100
C	4.92663000	-1.15594400	-1.25835200
H	2.92765100	-0.37696800	-1.42493500
C	5.49756500	-2.13173300	0.87841400
H	3.95700600	-2.10114700	2.37239900
C	5.85133800	-1.79825500	-0.43206000
H	5.18531700	-0.91739000	-2.28638300
H	6.20417700	-2.65269800	1.51881200
H	6.83747800	-2.05285400	-0.81093200
C	3.55147800	3.57275200	-1.43500500
H	4.18347100	2.80978000	-0.96249400
H	3.65522200	3.47084300	-2.52260400
H	3.94138500	4.55753400	-1.14898200
C	2.08448200	3.41385900	-0.99454700
C	1.20657300	4.43976500	-1.74024600
C	1.61653000	1.97421300	-1.37421700
C	-0.29156300	4.24539500	-1.46889100
H	1.39011600	4.34578000	-2.82074000
H	1.51160800	5.45649500	-1.45853800
C	0.17035200	1.72748700	-1.75328100
H	2.26279100	1.57221200	-2.16124500
C	-0.76832300	2.85632700	-1.87309300
H	-0.89864900	4.97351200	-2.01734800
H	-0.50689600	4.37445900	-0.40426200
H	0.08515700	1.12590100	-2.65506700
C	2.00992400	3.63122100	0.52817200
H	2.68940000	2.94208700	1.04439600
H	2.30639100	4.65700400	0.78302900
H	1.00840400	3.45135300	0.92051900
O	-1.89443500	2.70905600	-2.36210000

TS IV-V

E = -4181.588622

G_{Corr} = 0.656733

Co	0.06178500	0.20560900	0.15499200
H	-0.65940800	3.19944000	-0.63503100
P	1.17579500	-1.40454500	-0.93405700
O	2.48222200	-1.90110000	-0.04540600
O	1.99639700	-1.22534200	-2.35552000
C	0.25796400	-2.97895800	-1.14452800
C	3.42082700	-2.89397200	-0.46417300
C	1.42585200	-1.10756700	-3.66550300
C	-0.85488300	-3.22060000	-0.32854500
C	0.67069500	-3.96764300	-2.04921300
H	4.23809100	-2.86757100	0.26086400
H	2.96115900	-3.88968700	-0.46527600
H	3.81004100	-2.66972700	-1.46137800
H	0.59526600	-1.80146500	-3.80689900
H	1.07080900	-0.08976400	-3.84011900
H	2.23559600	-1.34439100	-4.36210400
C	-1.55358600	-4.42419200	-0.41910600
H	-1.18172000	-2.45027200	0.36250300
C	-0.02743000	-5.17463100	-2.13936000
H	1.53343400	-3.79396200	-2.68506300
C	-1.14071700	-5.40405100	-1.32677600
H	-2.42436500	-4.59026500	0.20956100
H	0.29668100	-5.93364200	-2.84648300
H	-1.68520800	-6.34149500	-1.40245100
P	-1.67731800	0.93050200	1.29310500
O	-2.17401700	2.46428000	0.95657800
O	-1.75114800	1.07236300	2.94532300
C	-3.17465500	-0.11958000	1.01721900
C	-3.35218000	3.05929400	1.52053200
C	-1.44453100	-0.03449300	3.79436100

C	-3.29945100	-0.90421800	-0.14040400
C	-4.20879700	-0.14650400	1.97171000
H	-3.39687900	4.07710800	1.12675200
H	-4.25011100	2.51027500	1.21606300
H	-3.28965200	3.08607400	2.61217000
H	-1.89914100	-0.96401900	3.42996800
H	-0.36410700	-0.16362800	3.88659600
H	-1.86529000	0.20009300	4.77580800
C	-4.43387200	-1.69545600	-0.33660400
H	-2.51156300	-0.91404600	-0.88758200
C	-5.34199000	-0.93481100	1.76945600
H	-4.12036900	0.44670200	2.87623400
C	-5.45676500	-1.71296100	0.61379600
H	-4.51031700	-2.30339000	-1.23418700
H	-6.13259900	-0.94447400	2.51520800
H	-6.33681200	-2.33176400	0.45921100
P	1.45444600	0.29801300	1.72989700
O	1.80741200	-0.87397100	2.84953900
O	1.12259200	1.57713700	2.71452300
C	3.14527700	0.71971900	1.15275600
C	1.19755500	-2.16570100	2.76170500
C	1.98949300	1.91742700	3.80574900
C	3.27639000	1.78171000	0.24659200
C	4.28618500	0.02050300	1.56671600
H	0.26513600	-2.11740900	2.18817800
H	1.87814300	-2.86350600	2.26772400
H	0.98620800	-2.50031200	3.78130700
H	1.56040100	2.80468100	4.27544800
H	2.03401400	1.09956000	4.53255900
H	3.00146200	2.14306900	3.45007700
C	4.53385300	2.13687400	-0.24463500
H	2.39053800	2.31691400	-0.07990900
C	5.54294700	0.37767000	1.07571800
H	4.18139300	-0.80458500	2.26305000
C	5.66871800	1.43317800	0.16729300
H	4.62616900	2.95900200	-0.94938000
H	6.42465600	-0.16968900	1.39906600
H	6.64785400	1.70587300	-0.21752700
C	0.33278900	3.83474000	-3.86272200
H	1.07908300	4.57358600	-3.54291000
H	0.85912700	2.90011800	-4.09447800
H	-0.12855800	4.20056000	-4.78917900
C	-0.72102700	3.60129400	-2.76656700
C	-1.82089200	2.63002300	-3.30540700
C	-0.03235000	2.98453300	-1.50529200
C	-2.18697600	1.51070100	-2.30764000
H	-1.46926200	2.15149300	-4.22889000
H	-2.72107100	3.19518600	-3.57817400
C	0.19468700	1.48972700	-1.61393300
H	0.91789400	3.50611500	-1.33203800
C	-0.91758400	0.71782500	-2.00745100
H	-2.94206800	0.83597000	-2.72242700
H	-2.59638200	1.95187700	-1.39306200
H	1.18657500	1.15734100	-1.90915600
C	-1.35631500	4.94379000	-2.36531000
H	-0.61211100	5.61060400	-1.91076800
H	-1.78580800	5.45906400	-3.23409400
H	-2.15881100	4.79074900	-1.63209200
O	-0.91040000	-0.56154400	-2.18869200

V

E = -4181.613207

G_{corr} = 0.651753

Co	-0.08067800	0.17680500	-0.30127000
H	-5.00592500	-1.52203400	1.95511900
P	1.88863500	0.87199500	-0.75151000
O	1.80889400	2.42659900	-1.32193200
O	2.66401000	0.09706000	-1.98362000

C	3.25615500	0.86993000	0.45575200
C	2.98012000	3.08709500	-1.82489400
C	1.86825800	-0.26740800	-3.12216200
C	2.90360700	0.97585400	1.80987500
C	4.60339700	0.70516800	0.10078100
H	2.65342600	4.06066100	-2.19570000
H	3.72118700	3.22812700	-1.02926700
H	3.43134100	2.51359900	-2.64097800
H	0.91532500	-0.71012900	-2.80561000
H	1.67023100	0.60903100	-3.75003600
H	2.44206200	-1.00678500	-3.68291300
C	3.88742900	0.92030500	2.79842100
H	1.85890300	1.09351200	2.08300500
C	5.58409900	0.64627100	1.09122200
H	4.87287400	0.58919500	-0.94352800
C	5.22754200	0.75139800	2.43953200
H	3.60772400	0.99883700	3.84532000
H	6.62547200	0.50860100	0.81302800
H	5.99314500	0.69701200	3.20878700
P	0.55064600	-1.87039400	0.20295600
O	-0.52264200	-3.06683000	-0.16029400
O	0.87857800	-2.06282600	1.81336600
C	2.12256800	-2.61445800	-0.39239900
C	-0.38998400	-4.36667300	0.43674300
C	0.13023000	-1.35449100	2.81129400
C	2.12884800	-3.26706800	-1.63522500
C	3.32879300	-2.45473700	0.30282600
H	-1.15153600	-4.99852000	-0.02313300
H	0.60312200	-4.79138000	0.25128600
H	-0.56533300	-4.31087600	1.51570800
H	-0.74943600	-1.93706700	3.10510900
H	0.79191000	-1.23058300	3.67281400
H	-0.19447800	-0.37461500	2.44855400
C	3.32198500	-3.74621800	-2.17626700
H	1.19523300	-3.40404500	-2.17472900
C	4.52308100	-2.92995200	-0.24221500
H	3.33382700	-1.95298700	1.26405700
C	4.52366000	-3.57224800	-1.48241500
H	3.31496900	-4.25545300	-3.13645100
H	5.45333400	-2.79219100	0.30236700
H	5.45470000	-3.93937800	-1.90616800
P	-0.80287000	2.02219900	0.64547700
O	0.12818500	3.03342500	1.58470200
O	-1.78636200	1.52033400	1.85792400
C	-1.79854500	3.22201400	-0.32556300
C	1.06224000	3.99970700	1.09494700
C	-2.53479600	2.42788200	2.67831100
C	-2.32582400	2.78824000	-1.55292200
C	-2.03265100	4.53942900	0.10044900
H	2.05775900	3.55576000	1.01152700
H	0.76765700	4.40007900	0.12108600
H	1.08580000	4.81121100	1.82857000
H	-3.06919600	1.81112400	3.40375600
H	-1.86980900	3.12333600	3.20014800
H	-3.25799600	2.99099000	2.07832700
C	-3.08044300	3.66207500	-2.33760400
H	-2.15847200	1.75943600	-1.85838000
C	-2.78366000	5.41142000	-0.68964000
H	-1.62466300	4.88158900	1.04707900
C	-3.30785600	4.97318300	-1.90918400
H	-3.49170600	3.31971800	-3.28356400
H	-2.95947500	6.43043200	-0.35507600
H	-3.89185600	5.65309700	-2.52393100
C	-6.31001500	-3.41888800	0.73891800
H	-6.19073100	-4.08781900	1.60124200
H	-6.97822500	-2.60137400	1.03846100
H	-6.80809200	-3.98555900	-0.05860000
C	-4.94970500	-2.88080500	0.26874400
C	-5.15870900	-1.87454100	-0.88342600
C	-4.24967000	-2.13090500	1.42762400
C	-3.83703500	-1.29836600	-1.40860500
H	-5.78821300	-1.05292100	-0.51212000

H	-5.71477900	-2.35145200	-1.70306100
C	-3.08871400	-1.27632700	0.97912800
H	-3.90926700	-2.87024500	2.17142300
C	-2.87819400	-0.90498000	-0.30177700
H	-4.02552400	-0.41578100	-2.03487100
H	-3.32888300	-2.02391100	-2.06175300
H	-2.38420100	-0.93556600	1.72856900
C	-4.07483600	-4.05929900	-0.20059700
H	-3.99277700	-4.81521100	0.59120900
H	-4.50896700	-4.54458400	-1.08460300
H	-3.06497500	-3.72182000	-0.44807300
O	-1.85086400	-0.18643800	-0.75159300

TS V-VI

E = -4593.6834

G_{Corr} = 0.83575

Co	-0.33683500	0.35768200	-0.02077100
H	3.67004700	0.37461500	-3.93083900
P	-2.14431800	0.87572900	1.03584000
O	-1.94483300	2.28224000	1.87056800
O	-2.65921100	-0.02911900	2.31521100
C	-3.69007200	1.12334500	0.08741000
C	-2.98102700	2.81770600	2.70832400
C	-2.72534400	-1.46222900	2.27502200
C	-3.57613000	1.63461300	-1.21533200
C	-4.94981500	0.75209100	0.57765000
H	-2.61983000	3.78529900	3.06275600
H	-3.90939100	2.95944900	2.14253300
H	-3.16735400	2.15618000	3.55848400
H	-1.79595300	-1.89120400	1.89733500
H	-2.88303900	-1.78805200	3.30606000
H	-3.56320800	-1.79388800	1.65465000
C	-4.70940000	1.77250100	-2.01661200
H	-2.59689700	1.90838200	-1.59666500
C	-6.08193100	0.88222900	-0.22887700
H	-5.03474400	0.34552200	1.58064600
C	-5.96204800	1.38842000	-1.52640800
H	-4.61492700	2.16492600	-3.02540000
H	-7.05502900	0.58283000	0.15091600
H	-6.84285500	1.48125400	-2.15600400
P	-1.13847000	-1.25544100	-1.28818200
O	-0.01333900	-2.36381100	-1.75517000
O	-1.74300800	-0.67781100	-2.72444500
C	-2.56868500	-2.35041900	-0.92253400
C	-0.23564900	-3.23010200	-2.87358300
C	-1.02146500	0.34075900	-3.43221000
C	-2.32438200	-3.54630600	-0.22633100
C	-3.88994600	-1.98227300	-1.21094500
H	0.63250600	-3.89108500	-2.92642400
H	-1.14434100	-3.82922500	-2.74495300
H	-0.31392900	-2.65481200	-3.80211900
H	-0.40649700	0.94462100	-2.75874100
H	-0.37343200	-0.12035900	-4.18660100
H	-1.76014900	0.97677200	-3.92850200
C	-3.38459800	-4.35790000	0.17549200
H	-1.30264800	-3.82096100	0.02015200
C	-4.95098200	-2.79276100	-0.79884600
H	-4.09015600	-1.06439000	-1.75182400
C	-4.70214800	-3.97935800	-0.10498400
H	-3.18527100	-5.28150800	0.71264100
H	-5.97163600	-2.49143500	-1.01914300
H	-5.52916600	-4.60715600	0.21611500
P	0.27192500	2.45173800	-0.33148400
O	-0.72893500	3.67870500	-0.85212000
O	1.24341600	2.46066800	-1.64924400
C	1.25301800	3.27132100	0.98827300
C	-1.63817300	4.44818200	-0.06270300

C	1.98556700	3.60679000	-2.07645900
C	1.80371500	2.43887500	1.97501300
C	1.47570300	4.65552600	1.05042400
H	-2.61099200	3.95275400	-0.00487300
H	-1.26186200	4.61426000	0.95014300
H	-1.75043800	5.41061000	-0.57138300
H	2.49633100	3.31231500	-2.99573900
H	1.32156900	4.45455800	-2.27608400
H	2.73001900	3.89166200	-1.32473500
C	2.56882100	2.98330600	3.00726500
H	1.64703900	1.36726200	1.90780500
C	2.23532500	5.19928200	2.08824600
H	1.05553200	5.30610300	0.28879000
C	2.78159800	4.36366000	3.06709400
H	2.99789500	2.32977000	3.76193800
H	2.40202300	6.27235300	2.13296300
H	3.37254000	4.78866300	3.87417100
C	6.20365300	0.01797300	-3.40711300
H	6.30157200	-0.73175800	-4.20305900
H	6.02167400	0.99025100	-3.88278400
H	7.16528500	0.07596000	-2.88067500
C	5.06571200	-0.34869500	-2.44166000
C	4.89518500	0.76969700	-1.39261700
C	3.73205900	-0.46655200	-3.21644800
C	3.76410500	0.48809200	-0.39562700
H	4.67369700	1.70532700	-1.92709900
H	5.84173400	0.93178800	-0.85713400
C	2.51605200	-0.50195100	-2.32241800
H	3.76424700	-1.37204700	-3.84392800
C	2.50963700	-0.07265500	-1.04188600
H	3.48951900	1.41017100	0.12977900
H	4.09270200	-0.20605200	0.39030400
H	1.59237500	-0.88263500	-2.74213600
C	5.39982400	-1.68851800	-1.75754200
H	5.62189900	-2.45901800	-2.50690700
H	6.27733300	-1.59091600	-1.10524200
H	4.55908000	-2.04539400	-1.15547700
O	1.47476800	-0.12442600	-0.20341100
C	2.73821400	-2.69926300	2.69258400
C	1.73852500	-3.47500200	1.75087100
O	2.24291800	-1.32799800	2.62827900
O	0.53813600	-2.64294200	1.82423400
C	2.64009800	-3.12080100	4.16393100
H	3.03999100	-4.12753600	4.32247600
H	3.21660600	-2.41797700	4.77343300
H	1.60176300	-3.09715900	4.50972400
C	4.19304000	-2.71579100	2.23475600
H	4.80237400	-2.12453200	2.92613300
H	4.58129000	-3.74048300	2.22675800
H	4.30475600	-2.29275900	1.23537300
C	2.17735700	-3.50060200	0.28451500
H	3.07587000	-4.11308800	0.15353000
H	1.37132800	-3.92307400	-0.31989600
H	2.35614800	-2.49230700	-0.09220300
C	1.37057700	-4.87923100	2.22187000
H	0.65794900	-5.32387300	1.51922900
H	2.25941500	-5.51915400	2.25479600
H	0.90903500	-4.86888900	3.21201000
B	0.94576600	-1.38924300	2.19758200
H	0.19402200	-0.47032600	2.27839000

VI

E = -799.5914689

G_{Corr} = 0.33539

C	-5.17342300	0.70709600	0.17918500
H	-5.53141000	1.26764900	-0.69356300
H	-5.76090100	-0.21691200	0.24989900
H	-5.38199100	1.30840700	1.07286300

C	-3.67179300	0.40391700	0.05930200
C	-3.22091900	-0.45661000	1.26136900
C	-1.72562700	-0.80718600	1.21139500
H	-3.80806900	-1.38523800	1.26203900
H	-3.44872800	0.06279700	2.20103500
C	-2.03214100	-1.02345100	-1.27365300
H	-1.50092900	-1.64117400	1.88958300
H	-1.11048500	0.03651000	1.55330300
H	-1.62410900	-1.33281800	-2.23320000
C	-2.88810400	1.73180200	0.02110900
H	-3.25917100	2.37228300	-0.78855400
H	-3.00885400	2.27973100	0.96409100
H	-1.81807600	1.56981900	-0.14457500
O	-0.01189700	-1.73241500	-0.26186800
C	2.34766000	0.96303200	-0.12408400
C	3.23560400	-0.31150700	0.14342400
O	1.00136900	0.44335700	0.07463400
O	2.35266400	-1.39661500	-0.26539100
C	2.57009200	2.12040600	0.84360100
H	3.60383100	2.47813200	0.78349400
H	1.90544500	2.95062700	0.58384600
H	2.35933700	1.82718600	1.87438700
C	2.42043600	1.45415300	-1.57437100
H	1.62904600	2.19194600	-1.73798000
H	3.38503100	1.92359200	-1.79162300
H	2.26721700	0.62853100	-2.27668400
C	4.51617100	-0.38742300	-0.68125600
H	5.16551500	0.46697300	-0.46059800
H	5.06094900	-1.30385600	-0.43301100
H	4.30305400	-0.39927700	-1.75238700
C	3.54168300	-0.52662700	1.63026000
C	3.97262100	-1.52358600	1.76257200
H	4.25549500	0.21400500	2.00443900
H	2.62885000	-0.46725000	2.23179300
B	1.07263700	-0.91371100	-0.15357600
C	-1.28933500	-1.17990800	-0.17717000
C	-3.40848400	-0.40603000	-1.23417100
H	-3.54117600	0.24806100	-2.10759800
H	-4.17368900	-1.19218600	-1.33434600

TS II-IV'

E = -4181.575283

G_{Corr} = 0.651225

Co	0.13244500	0.02619600	0.07791100
H	1.35647700	-0.12209900	-0.84141500
P	-1.01297400	-0.73458700	-1.66118300
O	-0.40268600	-2.18787600	-2.16435600
O	-0.86351100	0.05183100	-3.13320500
C	-2.84613000	-1.00926200	-1.66523300
C	-0.89684900	-2.88238000	-3.31685900
C	-1.32300300	1.40431400	-3.26066100
C	-3.49320000	-1.16533400	-0.43322400
C	-3.61777700	-1.01748700	-2.83887700
H	-0.26680000	-3.76699400	-3.43619100
H	-1.93753700	-3.19492200	-3.17251900
H	-0.82576000	-2.25710600	-4.21200700
H	-1.15213700	1.69296500	-4.30128400
H	-2.39675400	1.47926000	-3.04452400
H	-0.76386400	2.06230900	-2.59159000
C	-4.87524000	-1.34185600	-0.36411800
H	-2.90585800	-1.12002900	0.47659600
C	-5.00188100	-1.18821900	-2.77534400
H	-3.13029500	-0.87669000	-3.79904000
C	-5.63252200	-1.35252100	-1.53807900
H	-5.36047000	-1.44984600	0.60214100
H	-5.58976700	-1.18924000	-3.68961900
H	-6.71095500	-1.47796600	-1.48990600
P	-0.99829400	0.84806400	1.76847200

O	-0.15486300	2.05137900	2.50598000
O	-1.43847000	0.03125800	3.14623600
C	-2.60984600	1.63623800	1.33162600
C	-0.73122000	2.84799300	3.55195400
C	-2.05037300	-1.25159700	3.08812800
C	-2.76349100	2.19567300	0.05352800
C	-3.70831500	1.61860900	2.20448900
H	0.02479700	3.58684800	3.82637600
H	-1.63402700	3.36249600	3.20385000
H	-0.97594200	2.22978100	4.42128200
H	-1.52484000	-1.91620200	2.39955100
H	-1.99792400	-1.67598200	4.09393300
H	-3.10380700	-1.17283300	2.78844500
C	-3.99149600	2.72246400	-0.34471600
H	-1.91528100	2.20816700	-0.61946400
C	-4.94160100	2.13644600	1.80042900
H	-3.59768800	1.19588500	3.19834100
C	-5.08612700	2.68608200	0.52444100
H	-4.09809100	3.15129700	-1.33782000
H	-5.78819900	2.10995500	2.48171800
H	-6.04714200	3.08314700	0.20832200
P	1.10542100	-1.61361700	1.03189800
O	0.74188900	-3.18730400	0.63339500
O	1.05219700	-1.64732500	2.68775100
C	2.89673500	-1.79001300	0.67855500
C	-0.60542200	-3.64580000	0.53897100
C	1.41813500	-2.83014600	3.41551800
C	3.86699100	-1.41396800	1.61634600
C	3.29824800	-2.22841800	-0.59275600
H	-1.28987100	-2.84524600	0.24808000
H	-0.63514900	-4.42219900	-0.22909600
H	-0.92743600	-4.07159600	1.49809700
H	1.50598500	-2.53364100	4.46321000
H	0.64320500	-3.59778600	3.31800800
H	2.37260500	-3.24155000	3.07104700
C	5.22507200	-1.49936500	1.29660200
H	3.55954700	-1.05040300	2.59260700
C	4.65355300	-2.31001400	-0.91033600
H	2.54515800	-2.50150800	-1.32671400
C	5.61990500	-1.95139900	0.03583500
H	5.97172300	-1.20801200	2.03039400
H	4.95791700	-2.65304900	-1.89556300
H	6.67551400	-2.01272700	-0.21442600
C	4.84194800	3.96340800	-1.87177900
H	5.43306900	3.76454500	-2.77455700
H	4.04908800	4.67347200	-2.13504400
H	5.49994000	4.44426800	-1.13730000
C	4.25197600	2.66020000	-1.29533400
C	3.45156800	2.98442300	-0.01187100
C	3.33136500	2.03564800	-2.32638100
C	2.54003100	1.82404000	0.42561700
H	2.83044900	3.87192500	-0.19653200
H	4.14528200	3.24441000	0.79840000
C	2.11872800	1.53089700	-2.06470300
H	3.70373900	2.01865500	-3.35173900
C	1.54093300	1.51893200	-0.68338200
H	1.97862300	2.06355200	1.33072800
H	3.14898200	0.94067700	0.63091900
H	1.48543900	1.12920500	-2.85053800
C	5.40835500	1.67981300	-0.99411400
H	5.95362200	1.42904400	-1.91240600
H	6.12080800	2.13169400	-0.29172400
H	5.04446100	0.74455000	-0.56078400
O	0.29626300	1.90427700	-0.56421100

IV'

E = -4181.596814

G_{Corr} = 0.652491

Co	-0.00822600	-0.43826700	0.23767100
H	1.90129100	0.76579100	1.62897600
P	-0.24571100	-0.51006800	-1.94658000
O	0.08580300	-1.93091100	-2.71432900
O	0.53880100	0.49112900	-3.00328800
C	-2.00755700	-0.16993500	-2.38355900
C	-0.16517100	-2.13685800	-4.11203700
C	0.49845000	1.91732000	-2.78475600
C	-3.00279300	-0.41818900	-1.42646500
C	-2.38022200	0.35428700	-3.63211300
H	0.20166900	-3.13902400	-4.34469300
H	-1.23818900	-2.08211500	-4.32809100
H	0.36785700	-1.39792000	-4.71734000
H	1.32282500	2.34062400	-3.36268400
H	-0.45194000	2.32528700	-3.15243000
H	0.62408500	2.13485700	-1.72297300
C	-4.34337200	-0.15373100	-1.70718400
H	-2.71083300	-0.79195100	-0.44971100
C	-3.72153100	0.61941600	-3.91481500
H	-1.61618700	0.56167800	-4.37545400
C	-4.70424600	0.36615000	-2.95290700
H	-5.10036100	-0.33545000	-0.94914000
H	-3.99973300	1.02836600	-4.88256900
H	-5.74671100	0.58143000	-3.17189900
P	-1.04644700	0.13492200	2.04232200
O	-0.14902500	0.81516000	3.23608800
O	-1.88911500	-0.95189000	2.98461700
C	-2.40059500	1.34570300	1.68984000
C	-0.75160300	1.43761300	4.38081200
C	-2.77091900	-1.87782100	2.35267400
C	-2.29350500	2.23246400	0.60501000
C	-3.58108200	1.34472800	2.45330100
H	0.07073200	1.79796600	5.00242900
H	-1.38048300	2.28327900	4.08142300
H	-1.35180100	0.71692800	4.94541300
H	-2.27215800	-2.41637600	1.54133800
H	-3.07934400	-2.59619900	3.11606600
H	-3.65988200	-1.36997400	1.95544200
C	-3.34826200	3.08952100	0.28918600
H	-1.37198500	2.23995700	0.03475800
C	-4.63449600	2.20378300	2.13385500
H	-3.67478100	0.66895600	3.29761500
C	-4.52198600	3.07488500	1.04716300
H	-3.25498200	3.76669700	-0.55603200
H	-5.54187300	2.19121900	2.73226900
H	-5.34479100	3.73852600	0.79391500
P	0.40986100	-2.48967900	0.57124900
O	0.07784400	-3.80464400	-0.37200600
O	0.18408600	-3.06608100	2.10148200
C	2.22260800	-2.44186500	0.37842900
C	-1.27348700	-4.00552200	-0.80338900
C	0.67434600	-4.36433800	2.47596500
C	3.01361800	-2.03948300	1.46665200
C	2.81333600	-2.62371400	-0.88216600
H	-1.73609100	-3.06432300	-1.11630900
H	-1.23702100	-4.68455700	-1.65799400
H	-1.87053100	-4.46071200	-0.00338100
H	0.40493400	-4.50556800	3.52461100
H	0.21116900	-5.14592200	1.86544500
H	1.76319100	-4.42021300	2.36665700
C	4.38327700	-1.83467200	1.29870700
H	2.55062700	-1.87887800	2.43622400
C	4.18406200	-2.41729100	-1.04389500
H	2.19276400	-2.90475900	-1.72627100
C	4.96914800	-2.02189800	0.04362100
H	4.99087200	-1.52187900	2.14330500
H	4.63912700	-2.55692800	-2.02080800
H	6.03449200	-1.85374900	-0.08832300
C	3.52560900	4.44541000	-1.79073000
H	4.43080000	4.26008900	-2.38317400
H	2.65855900	4.17988900	-2.40659500
H	3.47561900	5.52138000	-1.57981500

C	3.54126400	3.63370000	-0.47952900
C	2.25849400	3.94235300	0.32991800
C	3.60037900	2.15235700	-0.80861000
C	1.99001200	2.90227400	1.42142500
H	1.39997200	3.94760000	-0.35419600
H	2.33053000	4.95226700	0.75645900
C	2.84234200	1.21249200	-0.23500200
H	4.32848100	1.86814200	-1.57155300
C	1.78785300	1.50380200	0.81375900
H	1.09220700	3.15617500	1.99477000
H	2.83053500	2.87062700	2.12835100
H	2.92739500	0.17519000	-0.55111500
C	4.80460900	4.02320500	0.32262500
H	5.71403000	3.76911800	-0.23608200
H	4.82142000	5.10287800	0.52174800
H	4.84710700	3.49687500	1.28200300
O	0.49066300	1.41141400	0.25027700

V'

E = -4593.680624

G_{Corr} = 0.8345

Co	0.61942500	0.55934700	0.26013500
H	1.28485300	-2.49409900	1.22312100
P	0.91979300	0.65092500	-1.91979300
O	1.16822400	2.15073400	-2.57838900
O	-0.24234100	-0.00220100	-2.88584200
C	2.38671500	-0.24953300	-2.54752700
C	1.29553200	2.33894400	-3.99285900
C	-1.53148500	-0.25985100	-2.28722700
C	3.65410400	0.21106800	-2.16257600
C	2.28716100	-1.39312500	-3.34845200
H	1.36421800	3.41643200	-4.16022300
H	2.20020700	1.84856300	-4.37164000
H	0.42008200	1.94274100	-4.51678700
H	-1.99422700	0.66241400	-1.92564100
H	-2.15011100	-0.69509300	-3.07604700
H	-1.41748200	-0.96167600	-1.45899400
C	4.80535600	-0.47137300	-2.55873300
H	3.74134500	1.09593100	-1.53847900
C	3.43851300	-2.07643400	-3.74458300
H	1.30820400	-1.74627900	-3.64996100
C	4.69869800	-1.62124100	-3.34674900
H	5.78206500	-0.10953000	-2.24875200
H	3.35093400	-2.96804600	-4.35991800
H	5.59340600	-2.15804400	-3.65072500
P	1.30004600	0.16511100	2.28871400
O	0.39046700	-0.93845400	3.10025900
O	1.44524400	1.25458500	3.53606900
C	3.01804000	-0.52397400	2.27758400
C	0.77679700	-1.51280600	4.35671000
C	2.27561600	2.41197000	3.42872000
C	3.55312300	-1.02085100	1.07805500
C	3.81797500	-0.52973200	3.43363600
H	-0.04947200	-2.15665900	4.66544100
H	1.68610600	-2.11436700	4.24694300
H	0.93923300	-0.73486500	5.10901600
H	1.86152100	3.13201800	2.71990600
H	2.30373000	2.86584500	4.42269100
H	3.29795800	2.14682200	3.13194000
C	4.85515200	-1.52171100	1.03767100
H	2.93693200	-1.01853600	0.18465200
C	5.11994700	-1.03189400	3.39177100
H	3.42288500	-0.13028100	4.36292200
C	5.64089100	-1.52878500	2.19315100
H	5.25211200	-1.89759000	0.09845500
H	5.72887800	-1.03082000	4.29213400
H	6.65667800	-1.91436800	2.16091700
P	0.12927300	2.63002400	0.48740900

O	1.31995300	3.77891900	0.33825100	Co	-0.31620000	-0.09538100	-0.30089900
O	-0.52211600	2.99079000	1.95950800	P	-2.36783400	0.72217200	-0.47469300
C	-1.11781000	3.37042800	-0.64021100	O	-3.57345800	-0.24105400	0.06878800
C	2.66600000	3.37873200	0.05029800	O	-2.89506600	1.00168000	-2.01889500
C	-0.86286400	4.33854900	2.31542600	C	-2.80652100	2.33070800	0.30907100
C	-2.45989600	2.99597800	-0.48235500	C	-4.95755000	0.07192300	-0.14568900
C	-0.76527100	4.23520900	-1.68525800	C	-1.98018700	1.35971700	-3.06484800
H	2.84892600	2.34973300	0.38199400	C	-2.89602400	2.41916000	1.70721600
H	2.84206900	3.43802000	-1.02763700	C	-3.08799200	3.46437300	-0.46593500
H	3.33386300	4.06398100	0.57980200	H	-5.52687800	-0.68464600	0.39729500
H	-1.23988500	4.30209700	3.33961200	H	-5.20119900	1.06842200	0.23955200
H	0.02029000	4.98475800	2.27142900	H	-5.19744100	0.01553800	-1.21081500
H	-1.63875200	4.73784100	1.65279400	H	-2.20810000	0.74127000	-3.93539400
C	-3.43353600	3.46314400	-1.36652700	H	-2.10853000	2.41857800	-3.31373300
H	-2.74828500	4.31604300	0.32109400	H	-0.94628300	1.19096300	-2.76176900
C	-1.74047400	4.70625300	-2.56590900	C	-3.25929000	3.62209500	2.31458000
H	0.27055100	4.52837100	-1.80779300	H	-2.66958800	1.55412000	2.32049800
C	-3.07470600	4.31695800	-2.41264500	C	-3.43958900	4.67025100	0.14474600
H	-4.46736600	3.15379600	-1.23763900	H	-3.04643700	3.40633200	-1.54705700
H	-1.45879500	5.37654900	-3.37399000	C	-3.52705500	4.75167900	1.53657900
H	-3.83029700	4.67978500	-3.10466900	H	-3.32679400	3.67837200	3.39785900
C	-2.24125600	-4.30332900	-2.25608600	H	-3.65011900	5.54303200	-0.46758000
H	-3.19850100	-4.69608500	-1.88930200	H	-3.80275700	5.68942500	2.01150200
H	-2.39093600	-3.25513500	-2.53787200	P	-0.67348900	-1.67859700	-1.74656300
H	-1.97273900	-4.86275800	-3.16144400	O	0.48379700	-2.85967300	-1.61197200
C	-1.13573200	-4.43520800	-1.18879600	O	-0.85981800	-1.58802900	-3.40768200
C	0.18387500	-3.85348100	-1.74763100	C	-2.22436900	-2.60623200	-1.43492600
C	-1.54301100	-3.67207000	0.05887000	C	0.37436300	-4.10308200	-2.31937100
C	1.20672300	-3.55841700	-0.64708800	C	0.22681700	-1.03186300	-4.15598500
H	-0.03780400	-2.90662100	-2.25290400	C	-2.29407700	-3.39626200	-0.27726200
H	0.59631000	-4.53585800	-2.50358300	C	-3.36333700	-2.45785000	-2.23613300
C	-0.75532400	-2.82400000	0.73048600	H	1.34515800	-4.59627700	-2.23146400
H	-2.55265600	-3.86775200	0.42519500	H	-0.40241600	-4.73440100	-1.87463300
C	0.66012100	-2.49103500	0.31535700	H	0.13977100	-3.93548600	-3.37536300
H	2.14207100	-3.18953700	-1.08151200	H	0.69442800	-0.19666400	-3.62578000
H	1.44067500	-4.47336000	-0.08498700	H	0.98913600	-1.79605200	-4.34998100
H	-1.12826200	-2.30684600	1.60854100	H	-0.18027800	-0.67836100	-5.10696500
C	-0.97498700	-5.93063700	-0.83083200	C	-3.48537100	-4.03274200	0.07105600
H	-1.90207400	-6.33085000	-0.40149500	H	-1.41676300	-3.50714800	0.35487500
H	-0.73549600	-6.52009500	-1.72558000	C	-4.55687200	-3.09025500	-1.88224400
H	-0.17674700	-6.08236800	-0.09665200	H	-3.31687500	-1.83988400	-3.12620100
O	0.71046500	-1.23313200	-0.31870700	C	-4.62167000	-3.87592300	-0.72866700
C	-4.94038200	-1.28444300	1.53704300	H	-3.52837000	-4.64693200	0.96682600
C	-4.90209300	-0.62282000	0.10634400	H	-5.43775100	-2.96793200	-2.50725700
O	-3.53710600	-1.25305700	1.93996700	H	-5.55222200	-4.36604100	-0.45461700
O	-3.70003300	0.19986500	0.17677700	P	-0.23208800	-0.33168000	1.89434700
C	-5.70292200	-0.44913000	2.57199300	O	-1.57201800	-0.24131000	2.89664700
H	-6.78031400	-0.45495100	2.37827500	O	0.66489600	0.84138600	2.61579200
H	-5.52542900	-0.86888800	3.56673800	C	0.46212200	-1.92333500	2.53125600
H	-5.35205800	0.58770500	2.57448800	C	-2.56114000	-1.28095700	2.84054700
C	-5.42200300	-2.73154600	1.56514400	C	0.98562600	0.92386400	4.00812900
H	-5.38319600	-3.11136500	2.59095600	C	0.98360200	-2.85779500	1.62813700
H	-6.45750400	-2.79894200	1.21347800	C	0.41757700	-2.25501400	3.89796400
H	-4.79866300	-3.37557700	0.94158600	H	-3.48059500	-0.85975500	3.25531900
C	-4.67086000	-1.62737300	-1.02623500	H	-2.75506700	-1.60131600	1.81425400
H	-5.54153400	-2.27359700	-1.17636000	H	-2.24641200	-2.13980700	3.44400000
H	-4.48289200	-1.07837500	-1.95419800	H	1.45311200	1.90055700	4.15314200
H	-3.79782400	-2.25071600	-0.82092400	H	0.08424300	0.85401600	4.62532700
C	-6.08308900	0.28626200	-0.22124700	H	1.69314400	0.13770200	4.29267300
H	-5.94501500	0.71671500	-1.21848400	C	1.48485800	-4.08172200	2.07762400
H	-7.02036100	-0.28092200	-0.22012000	H	0.98013000	-2.63497200	0.57037300
H	-6.16940400	1.10808300	0.49313300	C	0.92252500	-3.47493200	4.34852400
B	-2.91675700	-0.29370300	1.18722500	H	-0.03632700	-1.57055700	4.60713400
H	-1.81729400	0.10088600	1.39680500	C	1.46429700	-4.38912000	3.43911800

TS V'-VI'

E = -4593.668967

G_{corr} = 0.836273

C	4.80316900	-1.25000900	-1.78416800	O	-0.99757600	-0.64779200	3.12129500
C	4.88924600	-0.69157000	0.65431800	O	0.55775200	-2.55957600	3.13195500
C	3.45344100	-0.52373800	-1.80509100	C	-1.61658300	-2.89334000	1.60008400
H	4.62618500	-2.33081200	-1.67617000	C	-1.76858200	-1.08893900	4.24564400
H	5.33383100	-1.11420800	-2.73671100	C	1.25152300	-3.75392100	2.77496600
C	3.55365700	-0.71879900	0.69319400	C	-2.13530000	-2.86158300	0.30010200
H	5.45848300	-0.57784000	1.57931800	C	-2.08665500	-3.86601900	2.49854000
H	2.86252300	-0.82634900	-2.67778200	H	-2.00287100	-0.19357800	4.82511600
H	3.60446700	0.55577400	-1.87602000	H	-2.70012300	-1.56284400	3.91592500
H	3.02830100	-0.63322500	1.64235100	H	-1.19718200	-1.78852100	4.86373500
C	6.31458600	0.61020200	-0.92378300	H	2.14163800	-3.53070800	2.18264600
H	6.92067000	0.96177500	-0.07931300	H	1.55718300	-4.22750900	3.71160000
H	6.96338900	0.56782200	-1.80870200	H	0.60452400	-4.44781600	2.22384900
H	5.53230400	1.35454600	-1.10442200	C	-3.12491100	-3.76066700	-0.09765900
O	1.55504800	0.03759500	-0.37327400	H	-1.74961000	-2.12422600	-0.39425100
C	2.65479500	-0.82150900	-0.52500200	C	-3.07368600	-4.77019500	2.10243900
H	2.31349200	-1.86232100	-0.60832600	H	-1.67053100	-3.92175300	3.50001000
C	0.87442200	3.79760800	-0.22910500	C	-3.59760400	-4.71548600	0.80623600
C	2.42741600	3.54967000	-0.23175000	H	-3.51710700	-3.71303300	-1.10979400
O	0.35990800	2.61291900	-0.92296200	H	-3.43261000	-5.51992000	2.80266900
O	2.60709500	2.73205100	-1.42311100	H	-4.36616500	-5.42117800	0.50205200
C	0.26419100	3.89682200	1.16236600	P	2.53456500	-1.18609100	0.46378500
H	0.76989300	4.68615100	1.73193800	O	2.99039100	-2.68609100	-0.05024800
H	-0.79337900	4.15511500	1.09325400	O	3.02277300	-1.17296800	2.03636600
H	0.35790300	2.95338900	1.70029200	C	3.84318200	-0.17100000	-0.31985400
C	0.44717900	4.99761000	-1.08349100	C	2.02536600	-3.60889500	-0.57429700
H	-0.64221100	4.98232900	-1.18459100	C	4.35256700	-1.56689400	2.40799300
H	0.73877700	5.94541300	-0.61879200	C	4.02856200	1.13708400	0.15245000
H	0.88845000	4.94727100	-2.08420600	C	4.60534300	-0.62973800	-1.40163700
C	3.27282800	4.81099200	-0.38900000	H	1.00512100	-3.27746200	-0.35133200
H	3.09511100	5.49923300	0.44522800	H	2.14707300	-3.67488000	-1.65765900
H	4.33405300	4.54110100	-0.38749100	H	2.20797800	-4.58298600	-0.11207300
H	3.05628900	5.33133000	-1.32513500	H	4.39412700	-1.52127700	3.49793900
C	2.90997400	2.72596200	0.96555000	H	4.56072400	-2.58919800	2.07459100
H	3.94933800	2.42918700	0.79386600	H	5.09751200	-0.88564500	1.98244600
H	2.86238900	3.30991700	1.89152800	C	4.96215800	1.97679200	-0.45537700
H	2.31598600	1.81843100	1.07325400	H	3.41918300	1.51265700	0.96742200
B	1.41158100	2.10355300	-1.66596800	C	5.53866100	0.21273200	-2.00876500
H	1.25195400	1.43747800	-2.63314900	H	4.45733500	-1.64010900	-1.76558500

TS V'-XI

E = -4593.669231

G_{corr} = 0.841354

Co	0.49155500	-0.45824900	0.30859100	H	-4.81649100	3.89554100	-2.20597900
H	-2.43162500	-0.29038900	1.24497000	C	-4.43531700	2.52269200	-0.54967100
P	0.59084600	-0.31135400	-1.86978900	C	-3.62898700	1.52628500	-1.41224800
O	1.81430900	-1.26320600	-2.47566900	C	-3.82664200	2.59260500	0.83832500
O	0.78249900	1.09464500	-2.72214700	C	-3.27959300	0.25344600	-0.64060600
C	-0.82534000	-0.91308300	-2.87463000	H	-2.68971900	2.00118300	-1.72266900
C	2.06635200	-1.36568700	-3.88199100	H	-4.18497200	1.29269100	-2.33002700
C	1.96377300	1.88853000	-2.50514900	C	-2.90100400	1.75363700	1.31783800
C	-1.08927900	-2.29110500	-2.86896900	H	-4.18869700	3.40940200	1.46714800
C	-1.63939000	-0.06436100	-3.63612700	C	-2.36333600	0.56068200	0.55684300
H	3.10896000	-1.67418200	-3.99352400	H	-2.79252900	-0.46774000	-1.29637400
H	1.40678300	-2.11484800	-4.33387200	H	-4.19564900	-0.22584400	-0.26691900
H	1.91520900	-0.40503000	-4.38367800	H	-2.47510700	1.91366300	2.30282800
H	2.86479800	1.32372200	-2.76882700	C	-5.91378200	2.08508100	-0.43627300
H	1.87152100	2.75319900	-3.16796000	H	-6.47452500	2.77061200	0.21138900
H	2.01882900	2.21772400	-1.46886200	H	-6.39418500	2.08493400	-1.42353300
C	-2.16612200	-2.80994300	-3.58899200	H	-6.00348500	1.07957500	-0.01185200
H	-0.45093600	-2.95961600	-2.29807300	O	-1.01325600	0.77358500	0.16849400
C	-2.72012200	-0.58297800	-4.35205600	C	0.11052600	4.04644100	2.01387200
H	-1.43159400	0.99887900	-3.65535700	C	0.60903400	4.02538200	0.52209400
C	-2.99082100	-1.95327100	-4.32457300	O	-0.14898100	2.64204400	2.28579200
H	-2.35977300	-3.87923500	-3.57692300	O	1.20307500	2.70496600	0.43164400
H	-3.35372500	0.08572000	-4.92844600	C	1.20053500	4.48286300	3.00199100
H	-3.83546500	-2.35357000	-4.87875000	H	1.42520100	5.55117200	2.91389500
P	-0.30992400	-1.66151200	2.02886300	H	0.85367900	4.28335500	4.02072500
				H	2.12216300	3.91463800	2.83965600

C	-1.16702300	4.84690000	2.24703700
H	-1.44697300	4.79511300	3.30481800
H	-1.01178500	5.90037800	1.98650200
H	-1.99316100	4.45141200	1.65590600
C	-0.52949100	4.08321600	-0.50211500
H	-1.00387200	5.07038300	-0.51997900
H	-0.12138600	3.87383800	-1.49617800
H	-1.27811900	3.32227400	-0.27875500
C	1.68518700	5.05392200	0.18346000
H	1.97368400	4.94891300	-0.86783300
H	1.30938800	6.07228200	0.33360000
H	2.58040300	4.91626300	0.79491400
B	0.56480700	1.90284700	1.36108700
H	1.03075300	0.82780800	1.64487700

VI'

E = -4593.683488

G_{Corr} = 0.840412

Co	-0.31707500	0.11122300	-0.30864400
P	-2.47235400	0.54053300	-0.46403000
O	-3.47966100	-0.65549100	0.00513800
O	-3.00214900	0.78566900	-2.00542800
C	-3.20001500	1.99617500	0.38316300
C	-4.89548700	-0.59525700	-0.22552400
C	-2.16113700	1.37572300	-3.01655900
C	-3.23211200	2.03256000	1.78610200
C	-3.73290300	3.06842600	-0.34561200
H	-5.31935500	-1.47045900	0.26955500
H	-5.32414100	0.31898500	0.19976700
H	-5.10641300	-0.64274400	-1.29702800
H	-2.19457900	0.72641200	-3.89272800
H	-2.55854900	2.36441200	-3.26910500
H	-1.13293400	1.48278100	-2.66765800
C	-3.77759000	3.13428900	2.44499800
H	-2.81504700	1.21231500	2.36055400
C	-4.26819700	4.17471300	0.31795600
H	-3.73659200	3.03844200	-1.42899100
C	-4.28835900	4.21080300	1.71392600
H	-3.79583300	3.15673900	3.53137400
H	-4.67011700	5.00528300	-0.25590100
H	-4.70261700	5.07269200	2.23006500
P	-0.51024400	-1.54976000	-1.74445500
O	0.84376000	-2.50693100	-1.67537400
O	-0.75513900	-1.45460100	-3.39347300
C	-1.85946700	-2.75523400	-1.44166400
C	0.93029600	-3.74316100	-2.40058100
C	0.23057300	-0.77899700	-4.18703100
C	-1.76314100	-3.57492000	-0.30772500
C	-3.00668200	-2.82004100	-2.24245300
H	1.98951300	-4.00821100	-2.43684100
H	0.36898300	-4.52910000	-1.88464600
H	0.54209900	-3.63218900	-3.41763900
H	0.55826000	0.15107600	-3.71413000
H	1.10317500	-1.42498900	-4.34358200
H	-0.23378300	-0.56237400	-5.15244700
C	-2.80031800	-4.44821100	0.02130900
H	-0.87871700	-3.52600700	0.32177900
C	-4.04703200	-3.68878700	-1.90757700
H	-3.08684800	-2.18416900	-3.11727300
C	-3.94815700	-4.50163000	-0.77511600
H	-2.71444900	-5.08273000	0.89958500
H	-4.93668300	-3.72997300	-2.53069100
H	-4.75976800	-5.17644600	-0.51613900
P	-0.18998200	-0.38006000	1.88197700
O	-1.54925500	-0.50613000	2.85470100
O	0.54939000	0.83595700	2.71077800
C	0.69432700	-1.90368500	2.45175500
C	-2.41001800	-1.64979000	2.74255600

C	0.81926800	0.86138700	4.11713300
C	1.41153100	-2.66545400	1.52127800
C	0.64152700	-2.34212400	3.78772400
H	-3.36705400	-1.36216500	3.18551900
H	-2.57517600	-1.93047300	1.70088100
H	-1.99238100	-2.49947700	3.29420400
H	1.18236400	1.86794200	4.33667900
H	-0.08933600	0.66368000	4.69427200
H	1.59202800	0.13111600	4.37989800
C	2.08852700	-3.82247400	1.91451500
H	1.41515800	-2.36945300	0.48131700
C	1.31808200	-3.49642700	4.18250800
H	0.05282600	-1.79146200	4.51444300
C	2.04939500	-4.23604000	3.24712500
H	2.64025100	-4.39969200	1.17728200
H	1.26989400	-3.82340400	5.21785100
H	2.57461600	-5.13582300	3.55612500
C	7.03511300	-1.06392600	-0.17965400
H	7.61434300	-0.69143600	0.67465900
H	6.68027500	-2.07199300	0.06654900
H	7.71421000	-1.14196500	-1.03832000
C	5.85618800	-0.12498200	-0.50288700
C	5.08186800	-0.67358400	-1.72584100
C	4.92495500	-0.04873600	0.69220500
C	3.70746600	-0.01456200	-1.89761000
H	4.94810000	-1.75829400	-1.59918100
H	5.68566900	-0.53657400	-2.63256500
C	3.59434900	-0.12991600	0.61426700
H	5.40086100	0.10614100	1.66191900
H	3.20941800	-0.37820200	-2.80349100
H	3.81836600	1.06676200	-1.99862200
H	2.98040800	-0.05505800	1.50799800
C	6.40843200	1.29100600	-0.79031600
H	6.93385100	1.68637400	0.08781200
H	7.11946600	1.26846500	-1.62643900
H	5.60302900	1.99003400	-1.03709800
O	1.62724600	0.44727300	-0.62762000
C	2.83425700	-0.32316900	-0.67611100
H	2.52895500	-1.36859900	-0.75450800
C	0.35652600	3.54601400	-0.28055000
C	1.92351100	3.61932600	-0.14551800
O	0.13164700	2.21011000	-0.80957200
O	2.38213000	2.77562600	-1.20076100
C	-0.36683900	3.75524600	1.04580700
H	0.01508400	4.65995300	1.53458100
H	-1.43722900	3.89125900	0.89103000
H	-0.21334100	2.90397400	1.71033400
C	-0.19698400	4.51066300	-1.33949600
H	-1.25063500	4.26886300	-1.51320500
H	-0.13340100	5.55520400	-1.01455400
H	0.34414900	4.40007000	-2.28411700
C	2.49810700	5.02103400	-0.36869000
H	2.08371500	5.73803700	0.35019900
H	3.58506000	4.99360200	-0.23270800
H	2.29487000	5.37909700	-1.38098300
C	2.43128000	3.06873000	1.19649000
H	3.51493200	2.93116600	1.12505200
H	2.22008400	3.75310000	2.02692700
H	1.97856400	2.10320400	1.41296200
B	1.40662100	1.74283500	-1.42632200
H	1.30844900	1.47663000	-2.61087600

IV''

E = -4181.595696

G_{Corr} = 0.65285

Co	0.03268000	-0.13443000	-0.04970800
P	-0.03251500	-2.29331200	0.09949700
O	-1.18229200	-3.18941400	-0.64754500

O	0.01215700	-3.17107200	1.51155100
C	1.56065500	-2.79909800	-0.67991500
C	-1.09482200	-4.61987600	-0.74867600
C	0.94264200	-2.84423700	2.55097000
C	2.08889400	-2.02383900	-1.72772000
C	2.26880400	-3.93237000	-0.24530900
H	-1.96526200	-4.93839300	-1.32578300
H	-0.18001700	-4.91889800	-1.27243800
H	-1.11659000	-5.08089700	0.24299900
H	1.23845500	-3.78357400	3.02657500
H	1.83957000	-2.35305400	2.15725800
H	0.46660600	-2.19132400	3.28456800
C	3.30598700	-2.37118600	-2.31583000
H	1.55681500	-1.14388500	-2.07652400
C	3.48309100	-4.27936700	-0.83938400
H	1.86775600	-4.54107100	0.55901700
C	4.00546400	-3.49658700	-1.87288000
H	3.70763200	-1.75901500	-3.11862100
H	4.02142500	-5.15847500	-0.49523000
H	4.95365600	-3.76416700	-2.33143400
P	-0.66914900	0.47923900	1.87294500
O	-0.78340400	2.12716700	1.93674000
O	-0.17010500	0.10773400	3.42910400
C	-2.41049900	-0.05793800	2.06291100
C	-1.30142800	2.79628100	3.09553000
C	1.20662400	0.35804700	3.73877400
C	-3.43254300	0.74704100	1.53445400
C	-2.72612200	-1.32782700	2.56871400
H	-1.42631600	3.84434400	2.81425800
H	-2.26917900	2.38412300	3.40071400
H	-0.60213600	2.72350300	3.93474200
H	1.86859900	-0.03604900	2.95974300
H	1.39587700	1.43233400	3.84874800
H	1.41786400	-0.14436400	4.68582400
C	-4.75249000	0.29485900	1.53033300
H	-3.18933000	1.71586800	1.10873700
C	-4.04639900	-1.78095300	2.55223100
H	-1.94131100	-1.96998500	2.95483200
C	-5.06212500	-0.97077700	2.03568500
H	-5.53631200	0.92653000	1.12089200
H	-4.28213900	-2.76770000	2.94188400
H	-6.08873600	-1.32669000	2.02287700
P	-1.16706900	0.12354300	-1.86892800
O	-2.36439200	-0.93491500	-2.30490300
O	-0.32611500	0.11624400	-3.28226800
C	-2.11322200	1.70842300	-1.86952800
C	-3.38250100	-1.26891600	-1.35171200
C	-0.94750500	0.39330200	-4.54747600
C	-1.66101000	2.78452000	-1.08948600
C	-3.31802300	1.83319700	-2.58250300
H	-3.86892000	-2.17542700	-1.71804800
H	-2.96107000	-1.46591100	-0.36395300
H	-4.11691100	-0.45996800	-1.27519600
H	-0.16187400	0.30961800	-5.30137800
H	-1.74006000	-0.33152500	-4.75783900
H	-1.36273500	1.40703400	-4.56469900
C	-2.40714800	3.96308800	-1.02432500
H	-0.73261400	2.67133700	-0.53997300
C	-4.06031800	3.01334500	-2.51396500
H	-3.67700900	1.00179200	-3.18168900
C	-3.60725600	4.07940600	-1.73118600
H	-2.05209400	4.79018400	-0.41456900
H	-4.99229800	3.09930100	-3.06671400
H	-4.18956100	4.99543900	-1.67179700
C	5.91403600	3.26248700	1.26130900
H	6.41067200	4.08282500	0.72780700
H	5.33554200	3.69676000	2.08535900
H	6.69334100	2.62084700	1.69251200
C	5.00527900	2.45194000	0.31481100
C	4.35904600	1.28000800	1.09610800
C	3.92437800	3.36175400	-0.24381900
C	3.12528600	0.72044800	0.38367900

H	4.05621600	1.64306100	2.08977800
H	5.10942900	0.49600200	1.26518700
C	2.61863000	3.07495900	-0.25971400
H	4.27573000	4.30723400	-0.66133400
H	2.71974200	-0.15835900	0.90231600
H	3.37445000	0.38645100	-0.63043200
H	1.90022100	3.78025400	-0.67640800
C	5.86352100	1.91498400	-0.85412100
H	6.27484000	2.74064800	-1.44775100
H	6.70466800	1.31962800	-0.47574800
H	5.27122400	1.28506100	-1.52608600
O	0.97227300	1.38145600	-0.56880300
C	2.02424000	1.78641900	0.26858900
H	1.63679900	1.98929100	1.28611300

V''

E = -4593.671826

G_{Corr} = 0.834365

Co	-0.56723100	0.08624200	0.03819000
P	-0.48325000	-2.05200200	0.50732300
O	-1.87350000	-2.91124900	0.39590200
O	-0.11131000	-2.41919900	2.08409000
C	0.73883800	-3.09844500	-0.38750200
C	-1.99656500	-4.26340900	0.85650700
C	1.01394100	-1.77216800	2.69327000
C	1.01866400	-2.85505400	-1.74049000
C	1.39889000	-4.14991500	0.26803400
H	-3.01234200	-4.57681000	0.60745100
H	-1.27534700	-4.91923900	0.35572700
H	-1.85272600	-4.31258200	1.93922500
H	0.76242800	-1.60497000	3.74283600
H	1.90084600	-2.40792900	2.60984600
H	1.23014600	-0.81676200	2.20758600
C	1.94355100	-3.64785900	-2.42238100
H	0.53830900	-2.03491100	-2.26026100
C	2.32407100	-4.94144800	-0.41480000
H	1.19195000	-4.34118700	1.31602200
C	2.59855700	-4.69126100	-1.76218500
H	2.15897100	-3.44316700	-3.46750500
H	2.83048900	-5.75103200	0.10418600
H	3.32231500	-5.30343800	-2.29361600
P	-1.64721500	0.56666600	1.83791200
O	-2.30709800	2.07938000	1.68487000
O	-1.16887300	0.54819700	3.44322000
C	-3.13557400	-0.47760000	2.06828200
C	-3.20298600	2.60552500	2.67345400
C	-0.02778600	1.32915000	3.80741700
C	-4.20702300	-0.28320200	1.18270700
C	-3.19102400	-1.52117700	3.00024700
H	-3.37547400	3.65107900	2.40857700
H	-4.15518900	2.06374600	2.66696000
H	-2.76570900	2.54700200	3.67556200
H	0.80014500	1.18698300	3.10532000
H	-0.27779100	2.39659100	3.84096100
H	0.28094400	0.99981600	4.80276400
C	-5.32302200	-1.11857400	1.23452000
H	-4.15924800	0.51833700	0.44937400
C	-4.30623000	-2.36024500	3.04541000
H	-2.35693300	-1.68375800	3.67364800
C	-5.37198900	-2.16271800	2.16343500
H	-6.15038900	-0.95874900	0.54805700
H	-4.34224200	-3.17064700	3.76897300
H	-6.23801000	-2.81839500	2.19984300
P	-1.36547600	-0.04159700	-2.01527000
O	-2.12919300	-1.39653600	-2.61326400
O	-0.21097200	0.07921600	-3.18368000
C	-2.62172300	1.24787500	-2.43067300
C	-3.37504400	-1.81191900	-2.03383200
C	-0.50055200	0.12830700	-4.58761400

C	-2.79108500	2.35750400	-1.58807600	C	-1.83756700	-2.38934700	-0.32994200
C	-3.45928700	1.10554700	-3.55130200	C	0.85937400	-3.98571300	-0.85366300
H	-3.51678900	-2.85867900	-2.31347500	C	-1.26513900	-1.21570200	-3.32290700
H	-3.35737800	-1.73860000	-0.94510000	C	-2.43600700	-2.13851700	0.91182200
H	-4.20185700	-1.21193200	-2.43174900	C	-2.38473800	-3.39097800	-1.15076900
H	0.46401600	0.10445800	-5.09956200	H	1.80211500	-4.41112900	-0.50284100
H	-1.10145500	-0.73377500	-4.89443100	H	0.01923800	-4.55129700	-0.43528900
H	-1.02543400	1.05441200	-4.84577200	H	0.82012500	-4.02389400	-1.94583900
C	-3.77104200	3.31160300	-1.87178200	H	-1.11644300	-0.14060400	-3.44658400
H	-2.14726000	2.45832300	-0.72368900	H	-1.14371100	-1.72572900	-4.28214000
C	-4.43402300	2.06352800	-3.83405000	H	-2.27848500	-1.40081200	-2.94827800
H	-3.35687700	0.23680800	-4.19456600	C	-3.56449700	-2.85193600	1.31770600
C	-4.59108800	3.16979200	-2.99386100	H	-2.03645900	-1.37136700	1.56234800
H	-3.89349200	4.16684900	-1.21193100	C	-3.51381300	-4.10484000	-0.74705800
H	-5.07355200	1.94362700	-4.70469700	H	-1.92280200	-3.61375600	-2.10701700
H	-5.35379400	3.91322400	-3.21105500	C	-4.10873300	-3.83401100	0.48784700
C	3.02788200	6.01924800	1.46757300	H	-4.02339500	-2.62980900	2.27693500
H	3.16682100	6.91829400	0.85383600	H	-3.92773100	-4.87172200	-1.39636900
H	2.17844000	6.19587400	2.13810200	H	-4.99157900	-4.38524300	0.80032500
H	3.92747600	5.88979500	2.08331200	P	-1.31777000	1.31606300	0.96717300
C	2.78810500	4.77573800	0.58774300	O	-1.34747300	2.98716600	1.03691900
C	2.63984700	3.52407800	1.48823100	O	-1.51092400	0.97377200	2.60101800
C	1.52207700	4.97528900	-0.22923400	C	-3.04498300	0.92913200	0.46604700
C	1.97049900	2.36476700	0.74732700	C	-2.41761600	3.69657800	1.67168900
H	2.02500500	3.78560400	2.36252400	C	-0.45154700	1.40498900	3.46504100
H	3.62613000	3.23600600	1.87727800	C	-3.27523900	0.75401500	-0.90601100
C	0.52916500	4.08465800	-0.32583300	C	-4.11173900	0.78906900	1.36575000
H	1.45447000	5.92302800	-0.76689300	H	-2.11618900	4.74645500	1.70676200
H	1.95917100	1.44618800	1.34394100	H	-3.34670300	3.60045300	1.09928000
H	2.51960600	2.12922500	-0.17185700	H	-2.58752300	3.32994000	2.68976500
H	-0.35151000	4.29905500	-0.93027800	H	0.53185300	1.20585100	3.02407100
C	3.99034300	4.60907100	-0.37098600	H	-0.53499100	2.47929400	3.66857300
H	4.06494300	5.46244200	-1.05613900	H	-0.55411400	0.84951700	4.40064200
H	4.92991900	4.54752000	0.19397400	C	-4.55148300	0.43493100	-1.37252900
H	3.89509800	3.70277400	-0.97827800	H	-2.45531000	0.86653100	-1.60860100
O	-0.03374000	1.77613200	-0.50794300	C	-5.38478200	0.45899800	0.89880600
C	0.53411900	2.72776700	0.34983700	H	-3.93441900	0.91363000	2.42895600
H	-0.06288900	2.81466700	1.27562200	C	-5.60632300	0.27840200	-0.46993400
C	5.12950500	-0.74187900	-0.75702400	H	-4.71784700	0.30012100	-2.43796200
C	4.47416600	-0.99762000	0.65579100	H	-6.20418500	0.33800600	1.60279900
O	4.05914400	-0.07359900	-1.48843800	H	-6.59753600	0.01596400	-0.83025400
O	3.05058000	-1.00160200	0.34772800	P	2.01336700	-0.44048700	1.12276300
C	6.34914700	0.17548400	-0.74538600	O	1.82117400	-1.51405000	2.37133700
H	7.15290500	-0.25765300	-0.13963300	O	2.81588600	0.78943800	1.90599600
H	6.72152400	0.30242500	-1.76690500	C	3.39482300	-1.32257400	0.26852500
H	6.10438600	1.16399700	-0.35021900	C	0.52068300	-1.94190400	2.78222400
C	5.43841100	-2.03201500	-1.52512900	C	3.91835100	0.55937000	2.78996200
H	5.71068900	-1.77424200	-2.55339400	C	3.48780400	-1.22086600	-1.12636800
H	6.27159700	-2.57917100	-1.07224400	C	4.33081300	-2.11384200	0.95250400
H	4.56354000	-2.68710100	-1.55974200	H	-0.20957400	-1.13454200	2.69892400
C	4.83011000	-2.33755500	1.29497700	H	0.19143400	-2.78604400	2.16860800
H	5.91205300	-2.41897600	1.44689600	H	0.60199800	-2.25651400	3.82645500
H	4.34301900	-2.41921300	2.27229400	H	4.13031100	1.51600200	3.27356000
H	4.49138000	-3.17361300	0.67972000	H	3.66369300	-0.18563900	3.55122500
C	4.70741600	0.14484400	1.65026300	H	4.80556000	0.22854200	2.23832100
H	4.06439700	-0.00756100	2.52302900	C	4.51077500	-1.86471600	-1.82358300
H	5.74875300	0.17584900	1.98647700	H	2.72614700	-0.67078800	-1.66960400
H	4.45125300	1.11087600	1.20895400	C	5.35486500	-2.76057200	0.25665100
B	2.88116300	-0.37012400	-0.85650000	H	4.24217600	-2.24630900	2.02578700
H	1.82123600	-0.09490500	-1.30120800	C	5.45206800	-2.63106900	-1.13146300

TS III-IVb

$$E = -4181.589413$$

$$G_{\text{Corr}} = 0.656294$$

Co	0.37698700	0.43898700	-0.02501100
H	1.06002000	1.71555900	0.43536400
P	-0.28511900	-1.50584500	-0.81077300
O	0.84561300	-2.63095100	-0.39032000
O	-0.27497900	-1.78454100	-2.44420300

C	-1.83756700	-2.38934700	-0.32994200
C	0.85937400	-3.98571300	-0.85366300
C	-1.26513900	-1.21570200	-3.32290700
C	-2.43600700	-2.13851700	0.91182200
C	-2.38473800	-3.39097800	-1.15076900
H	1.80211500	-4.41112900	-0.50284100
H	0.01923800	-4.55129700	-0.43528900
H	0.82012500	-4.02389400	-1.94583900
H	-1.11644300	-0.14060400	-3.44658400
H	-1.14371100	-1.72572900	-4.28214000
H	-2.27848500	-1.40081200	-2.94827800
C	-3.56449700	-2.85193600	1.31770600
H	-2.03645900	-1.37136700	1.56234800
C	-3.51381300	-4.10484000	-0.74705800
H	-1.92280200	-3.61375600	-2.10701700
C	-4.10873300	-3.83401100	0.48784700
H	-4.02339500	-2.62980900	2.27693500
H	-3.92773100	-4.87172200	-1.39636900
H	-4.99157900	-4.38524300	0.80032500
P	-1.31777000	1.31606300	0.96717300
O	-1.34747300	2.98716600	1.03691900
O	-1.51092400	0.97377200	2.60101800
C	-3.04498300	0.92913200	0.46604700
C	-2.41761600	3.69657800	1.67168900
C	-0.45154700	1.40498900	3.46504100
C	-3.27523900	0.75401500	-0.90601100
C	-4.11173900	0.78906900	1.36575000
H	-2.11618900	4.74645500	1.70676200
H	-3.34670300	3.60045300	1.09928000
H	-2.58752300	3.32994000	2.68976500
H	0.53185300	1.20585100	3.02407100
H	-0.53499100	2.47929400	3.66857300
H	-0.55411400	0.84951700	4.40064200
C	-4.55148300	0.43493100	-1.37252900
H	-2.45531000	0.86653100	-1.60860100
C	-5.38478200	0.45899800	0.89880600
H	-3.93441900	0.91363000	2.42895600
C	-5.60632300	0.27840200	-0.46993400
H	-4.71784700	0.30012100	-2.43796200
H	-6.20418500	0.33800600	1.60279900
H	-6.59753600	0.01596400	-0.83025400
P	2.01336700	-0.44048700	1.12276300
O	1.82117400	-1.51405000	2.37133700
O	2.81588600	0.78943800	1.90599600
C	3.39482300	-1.32257400	0.26852500
C	0.52068300	-1.94190400	2.78222400
C	3.91835100	0.55937000	2.78996200
C	3.48780400	-1.22086600	-1.12636800
C	4.33081300	-2.11384200	0.95250400
H	-0.20957400	-1.13454200	2.69892400
H	0.19143400	-2.78604400	2.16860800
H	0.60199800	-2.25651400	3.82645500
H	4.13031100	1.51600200	3.27356000
H	3.66369300	-0.18563900	3.55122500
H	4.80556000	0.22854200	2.23832100
C	4.51077500	-1.86471600	-1.82358300
H	2.72614700	-0.67078800	-1.66960400
C	5.35486500	-2.76057200	0.25665100
H	4.24217600	-2.24630900	2.02578700
C	5.45206800	-2.63106900	-1.13146300
H	4.56392500	-1.77984100	-2.90575900
H	6.07251800	-3.37165600	0.79806000
H	6.24810400	-3.13660600	-1.67169100
C	3.50673000	3.64439000	-1.26950200
H	4.17746300	3.12586600	-0.57349600
H	3.70575400	3.26874500	-2.28056000
H	3.75609500	4.71226800	-1.25035900
C	2.02872600	3.43236300	-0.87234600
C	1.13499900	4.26738600	-1.82076100
C	1.74126100	1.92042500	-1.08319600
C	-0.30200800	3.73901900	-1.90414700
H	1.57131500	4.25039200	-2.82933900

H	1.14053500	5.31520800	-1.49528400
C	0.75488500	1.43679900	-1.97847500
H	2.65272500	1.33540800	-1.02047400
C	-0.31234700	2.32003200	-2.44971400
H	-0.92218200	4.35430600	-2.56377900
H	-0.76299800	3.73488700	-0.91169400
H	0.93825900	0.53994100	-2.56291500
C	1.85209400	3.89433400	0.58682600
H	2.43296900	3.25752300	1.26215600
H	2.20150100	4.92922100	0.69332500
H	0.80521300	3.84436900	0.89516500
O	-1.16064700	1.97401600	-3.28294800

Vb

E = -4593.690894

G_{Corr} = 0.836697

Co	-0.28231000	-0.42324800	0.36087900
H	0.74129400	-2.41495800	2.73261500
P	-1.14310800	0.45785400	-1.44626400
O	-0.46776800	-0.08910000	-2.84905600
O	-0.84462900	2.05920600	-1.63586500
C	-2.93946600	0.39948600	-1.84108300
C	-0.72222000	0.56332700	-4.10378600
C	-0.88667900	2.95886300	-0.51369000
C	-3.63937800	-0.81019600	-1.72179800
C	-3.63303300	1.55646000	-2.22826800
H	-0.21371800	-0.03169400	-4.86562000
H	-1.79640500	0.59394900	-4.31927200
H	-0.31963200	1.57974600	-4.09522300
H	-0.36187100	2.52346900	0.33658700
H	-0.36987700	3.86172800	-0.83759000
H	-1.92442700	3.18504200	-0.24705000
C	-5.01245000	-0.85613300	-1.96405300
H	-3.10426800	-1.70713800	-1.43672600
C	-5.00708600	1.50919600	-2.46987600
H	-3.09579500	2.49312300	-2.32969000
C	-5.70100300	0.30460200	-2.32967300
H	-5.54734000	-1.79664400	-1.86016900
H	-5.53583700	2.41302600	-2.76099200
H	-6.77257300	0.26931600	-2.50793800
P	-2.04230000	-0.30272900	1.62701300
O	-1.74317800	-0.67885300	3.21870800
O	-3.41453300	-1.20033700	1.33245000
C	-2.91343700	1.30803500	1.78794800
C	-2.80203800	-0.66757800	4.18625900
C	-3.28144400	-2.61980800	1.21654800
C	-2.29465100	2.31311900	2.55121500
C	-4.08042700	1.61425600	1.07459300
H	-2.38216600	-1.07686700	5.10820600
H	-3.15791200	0.35281900	4.36787000
H	-3.64446300	-1.28600900	3.85981300
H	-2.84387000	-3.05166700	2.12466700
H	-4.29115200	-3.01496000	1.07854200
H	-2.66201100	-2.89111700	0.35927900
C	-2.83034700	3.59913700	2.59821700
H	-1.39002100	2.08559700	3.10998400
C	-4.60876300	2.90740400	1.11272600
H	-4.56897200	0.84707200	0.48505800
C	-3.98671500	3.90198800	1.87044800
H	-2.34604600	4.36609000	3.19699500
H	-5.50669600	3.13473000	0.54411400
H	-4.39908100	4.90713800	1.89672800
P	0.07995000	-2.42125300	-0.46409500
O	-1.15785700	-2.84745900	-1.50296100
O	0.02073000	-3.66385900	0.64835700
C	1.57717900	-2.90476800	-1.44723700
C	-1.01685400	-3.51149300	-2.76118700
C	-0.46692400	-4.96696100	0.30911500
C	1.97185100	-2.06581000	-2.50442900

C	2.39792100	-3.99200100	-1.10878500
H	-0.57263500	-2.83711100	-3.49961600
H	-0.40420700	-4.41595800	-2.68534500
H	-2.02804300	-3.78177800	-3.07753600
H	-1.53347300	-4.93089700	0.06400100
H	0.07383800	-5.40581600	-0.53717600
H	-0.31843900	-5.59486100	1.19102900
C	3.14006500	-2.32777000	-3.22085500
H	1.36961500	-1.19736200	-2.74873600
C	3.57047100	-4.24937200	-1.82282100
H	2.14040100	-4.62581100	-0.26737500
C	3.94262600	-3.42147000	-2.88409700
H	3.43142600	-1.66689500	-4.03307600
H	4.19596500	-5.09339800	-1.54381300
H	4.85784600	-3.61911300	-3.43573900
C	3.05038500	-3.13101000	3.81634800
H	2.69296300	-3.07637000	4.85262700
H	2.53240100	-3.96453400	3.32520100
H	4.12200400	-3.36719400	3.84210700
C	2.79157000	-1.81038700	3.07416200
C	3.24858200	-1.95815900	1.60593900
C	1.27083100	-1.51627800	3.06834700
C	3.00246500	-0.71021300	0.74538800
H	2.70605100	-2.80529600	1.17570900
H	4.31466600	-2.22090300	1.56852500
C	0.91118800	-0.34481600	2.17541700
H	0.92465600	-1.31649200	4.08945600
C	1.70370200	-0.00281600	1.05778100
H	3.05514000	-0.94271700	-0.32104800
H	3.78040300	0.04400700	0.91598400
H	0.39725800	0.48888200	2.64120200
C	3.55853800	-0.67537900	3.77792800
H	3.27237700	-0.61321700	4.83546900
H	4.64142700	-0.84763500	3.73065400
H	3.35357900	0.29959400	3.32257200
O	1.29703700	0.97779000	0.31474400
C	3.01784900	4.20897900	-0.87334200
C	3.99605400	3.30975400	-0.02125700
O	2.14570100	3.23389800	-1.50436700
O	3.94486800	2.03853600	-0.72635400
C	2.16305700	5.17577900	-0.05692200
H	2.79488000	5.89004100	0.48300400
H	1.50599900	5.74088400	-0.72655000
H	1.53775400	4.64486600	0.66355800
C	3.71961300	4.96053100	-2.01205800
H	2.96001500	5.40673100	-2.66172100
H	4.36688100	5.75868800	-1.63405300
H	4.32243100	4.27637600	-2.61736200
C	5.44841000	3.78254100	0.00275500
H	5.52513500	4.77607300	0.45874600
H	6.04872600	3.08686200	0.59825200
H	5.87662300	3.82346400	-1.00129100
C	3.50355400	3.06594400	1.41130900
H	4.13773600	2.30591900	1.87969700
H	3.56444400	3.97921000	2.01259800
H	2.47643000	2.69703800	1.41159300
B	2.77655000	2.01355600	-1.45448200
H	2.47111600	1.09429500	-2.14146400

VIAdd

E = -4593.707909

G_{Corr} = 0.83986

Co	-0.30610800	0.24307800	-0.06235700
H	4.02585300	-0.82500600	-3.77187300
P	-1.97356300	0.88989800	1.09958400
O	-1.66254800	2.30568500	1.87370100
O	-2.38560900	-0.01244700	2.40939000
C	-3.60042900	1.16987800	0.30584100
C	-2.60687000	2.88785100	2.78775400

C	-2.43685800	-1.44986000	2.33147300
C	-3.62957800	1.75585600	-0.96869700
C	-4.80181800	0.77299400	0.91104500
H	-2.17817200	3.84092900	3.10339800
H	-3.57091500	3.06329900	2.29656100
H	-2.74995800	2.23835400	3.65572700
H	-1.52194100	-1.85057400	1.88845100
H	-2.53765700	-1.80390100	3.36011700
H	-3.30340900	-1.77219300	1.74621500
C	-4.84363000	1.94058700	-1.62967700
H	-2.70028100	2.05223200	-1.44293100
C	-6.01524100	0.95090400	0.24461200
H	-4.77991600	0.31595900	1.89504900
C	-6.03698200	1.53099400	-1.02697000
H	-4.85744500	2.39068100	-2.61850500
H	-6.94195300	0.63248900	0.71420100
H	-6.98162500	1.66262300	-1.54769600
P	-1.38131000	-0.99364900	-1.57377100
O	-0.32899200	-1.97990000	-2.38061600
O	-2.25224700	-0.30084300	-2.81332900
C	-2.68342600	-2.16828900	-1.04177700
C	-0.78888200	-2.84326200	-3.42974600
C	-1.61448300	0.73636800	-3.56640800
C	-2.26257200	-3.33825000	-0.38557200
C	-4.05236200	-1.88792800	-1.14640600
H	0.10506600	-3.24620100	-3.91174600
H	-1.38881000	-3.66547300	-3.02456000
H	-1.38528900	-2.29066300	-4.16329800
H	-0.96381200	1.34854900	-2.93221800
H	-1.01468900	0.30428200	-4.37648800
H	-2.40485100	1.35948100	-3.99354400
C	-3.20319400	-4.22044500	0.14454200
H	-1.20051900	-3.52619000	-0.25381700
C	-4.99025800	-2.76762800	-0.59903900
H	-4.38274400	-0.98257700	-1.64380200
C	-4.56952000	-3.93486100	0.04301500
H	-2.87106600	-5.12363400	0.64997700
H	-6.04973300	-2.53656000	-0.67369600
H	-5.30143500	-4.61716400	0.46751800
P	0.39778400	2.25703400	-0.52885100
O	-0.55318300	3.49968300	-1.12249100
O	1.39113600	2.12428200	-1.83718600
C	1.40050000	3.15217900	0.73715700
C	-1.34795700	4.38687300	-0.32919200
C	2.16707300	3.20863300	-2.36147700
C	1.78539600	2.42226700	1.87196300
C	1.79993500	4.49371900	0.61794300
H	-2.32089100	3.94224500	-0.10401100
H	-0.85449700	4.64765700	0.61125900
H	-1.49192200	5.29194000	-0.92653100
H	2.60891700	2.84789800	-3.29284300
H	1.53520800	4.07870200	-2.56736100
H	2.96645500	3.48772100	-1.66635000
C	2.57217600	3.01608200	2.86020800
H	1.47782000	1.38477400	1.96657800
C	2.58034800	5.08905700	1.61032900
H	1.49299900	5.07596400	-0.24601600
C	2.96971600	4.34931900	2.73140000
H	2.87211700	2.43715100	3.72961900
H	2.88372500	6.12794400	1.51042100
H	3.57867400	4.81355400	3.50273000
C	6.46315900	-0.33488800	-2.99160500
H	6.82787300	-1.21672100	-3.53378700
H	6.12826400	0.40131900	-3.73332200
H	7.31107100	0.09824100	-2.44604000
C	5.32441400	-0.71061500	-2.03046200
C	4.77365200	0.56413500	-1.35418000
C	4.17026000	-1.36935100	-2.82421900
C	3.62449300	0.27293100	-0.38040700
H	4.41202200	1.24320800	-2.13905100
H	5.58318100	1.08796600	-0.82826700
C	2.86239400	-1.40994400	-2.07425600

H	4.46346900	-2.38878000	-3.11582700
C	2.62268400	-0.66858100	-0.98801700
H	3.12235600	1.20196400	-0.10360100
H	3.99083200	-0.15571000	0.55874800
H	2.06598300	-2.04771100	-2.44330500
C	5.86450200	-1.69184700	-0.97162400
H	6.32783300	-2.56190900	-1.45308100
H	6.62413800	-1.20924600	-0.34384000
H	5.06819200	-2.05998900	-0.31723500
O	1.38681000	-0.77590000	-0.37028500
C	2.18886400	-2.18845500	2.83059000
C	1.58885300	-3.33811000	1.94088500
O	2.20933800	-1.08094400	1.92034500
O	0.65877800	-2.62601700	1.11281400
C	1.27693300	-1.81902000	4.01240900
H	1.27003700	-2.59455200	4.78606800
H	1.64186200	-0.88778400	4.45872600
H	0.25009700	-1.65209400	3.67310300
C	3.61291500	-2.43775500	3.32458200
H	3.94763600	-1.59144000	3.93464300
H	3.66107700	-3.34324900	3.94067000
H	4.30703900	-2.54494500	2.48730700
C	2.64004000	-3.98374700	1.02418900
H	3.35656600	-4.59770500	1.58131100
H	2.12610800	-4.62301400	0.29846600
H	3.18469300	-3.21674200	0.46584100
C	0.83019100	-4.41611700	2.71354700
H	0.45076000	-5.17277000	2.01753400
H	1.48433500	-4.91672300	3.43710500
H	-0.02397800	-3.99137400	3.24701400
B	1.12412600	-1.26342800	0.99862200
H	0.11135200	-0.46860800	1.36511700

VII

E = -4597.707535

G_{corr} = 0.644896

Co	0.04101200	-0.37931200	-0.82168000
H	-0.24076700	-0.87440300	-2.20830000
P	-1.13170600	-2.07832500	-0.27717000
O	-0.72487300	-3.02500800	1.04264200
O	-1.26439700	-3.21798100	-1.48708100
C	-2.89209500	-1.83913500	0.19239300
C	0.61455900	-3.53252800	1.06594800
C	-1.96973400	-4.44623200	-1.25810800
C	-3.83219000	-1.64368800	-0.83212000
C	-3.29805200	-1.70575200	1.52747500
H	1.33155900	-2.76511500	0.75519100
H	0.82887400	-3.83614000	2.09238900
H	0.70634300	-4.40133700	0.40305100
H	-1.79176600	-5.07460700	-2.13404600
H	-1.60016700	-4.95400200	-0.36083300
H	-3.04551000	-4.26923400	-1.14901300
C	-5.15604300	-1.32438600	-0.52572800
H	-3.51818200	-1.71936600	-1.86814900
C	-4.62064100	-1.37756500	1.83213700
H	-2.57475400	-1.84665900	2.32204700
C	-5.55242200	-1.18433600	0.80792900
H	-5.87502100	-1.17547500	-1.32711200
H	-4.92485000	-1.27258300	2.87064500
H	-6.58065000	-0.92587900	1.04716600
P	2.03435500	-0.62515000	-1.50748400
O	2.20262100	-0.47721100	-3.16671600
O	2.85952900	-2.06478400	-1.27025200
C	3.37047600	0.48404700	-0.90041000
C	3.49874500	-0.54209500	-3.77210900
C	2.28847000	-3.22933400	-1.87822000
C	3.05228500	1.84951000	-0.82685700
C	4.63881500	0.04983500	-0.49023800

H	3.33802400	-0.60897500	-4.85106400	C	-2.02102200	-4.51263600	-1.01258300
H	4.08382800	0.35715100	-3.54547100	C	-3.89461700	-1.72835100	-0.68117200
H	4.05575800	-1.42162800	-3.43081200	C	-3.33063100	-1.56367800	1.66649900
H	1.19650300	-3.23174500	-1.79365500	H	1.27154500	-2.65937900	0.98733800
H	2.56238200	-3.28049600	-2.93921100	H	0.77403700	-3.59401700	2.42496300
H	2.69856200	-4.09849100	-1.35737900	H	0.71341400	-4.34821500	0.80725600
C	3.98431600	2.76502500	-0.33576400	H	-1.85287400	-5.16433400	-1.87320500
H	2.05843000	2.17894800	-1.11497500	H	-1.63558500	-4.99296400	-0.10676900
C	5.56646500	0.96550200	0.01199200	H	-3.09558700	-4.33595000	-0.89285900
H	4.88566800	-1.00474500	-0.54825900	C	-5.21304500	-1.37333600	-0.39154800
C	5.24005200	2.32242800	0.09365000	H	-3.59483500	-1.90643900	-1.70941600
H	3.72822400	3.81978700	-0.27766500	C	-4.64775200	-1.19966000	1.95343500
H	6.54268800	0.62011500	0.34266500	H	-2.59656000	-1.62484400	2.46129800
H	5.96110500	3.03253700	0.49020700	C	-5.59190600	-1.10243900	0.92700100
P	-1.18496000	1.25142600	-1.48460000	H	-5.94152800	-1.229890500	-1.19472900
O	-2.41988600	0.71780000	-2.46419300	H	-4.93789900	-0.99055900	2.98014600
O	-0.55136000	2.50687100	-2.38552800	H	-6.61582600	-0.81606300	1.15241000
C	-2.08735400	2.33819700	-0.30077500	P	2.05720800	-0.80672100	-1.49265000
C	-3.37034800	1.63704200	-3.01793200	O	2.20697200	-0.82054300	-3.16326900
O	0.18708100	2.17090800	-3.56690400	O	2.91016100	-2.20459400	-1.11932600
C	-3.22353800	1.82342700	0.34017700	C	3.36719100	0.37607500	-0.97632500
C	-1.62359800	3.61227500	0.05313900	C	3.49174900	-0.97168000	-3.78000400
H	-3.87316300	1.11402800	-3.83547200	C	2.32576300	-3.43178800	-1.56658100
H	-4.10980000	1.93274200	-2.26542800	C	3.01606600	1.73570700	-0.98203300
H	-2.87593300	2.53364500	-3.40703800	C	4.65028000	-0.00049500	-0.55305200
H	0.78735600	3.04704200	-3.82778000	H	3.31674900	-1.07960200	-4.85329300
H	0.83921200	1.30987900	-3.39966200	H	4.11785600	-0.08969600	-3.59883100
H	-0.49958600	1.94679300	-4.39319500	H	4.01354500	-1.85829700	-3.40339400
C	-3.89454200	2.57484500	1.30523300	H	1.23288000	-3.41296200	-1.47708000
H	-3.58164300	0.83209200	0.08927800	H	2.59059600	-3.62491400	-2.61368300
C	-2.29051600	4.36165500	1.02606000	H	2.72854900	-4.23185200	-0.93989900
H	-0.74105100	4.01356200	-0.43240300	C	3.93075200	2.70253600	-0.56182900
C	-3.42878300	3.84599100	1.65327500	H	2.01012400	2.02263500	-1.27199800
H	-4.77566600	2.16042500	1.78827500	C	5.56071700	0.96728300	-0.12278900
H	-1.92445100	5.35106700	1.28948700	H	4.92207800	-1.05042900	-0.54430200
H	-3.94758200	4.43081000	2.40866000	C	5.20243600	2.31879200	-0.12402000
P	0.34296400	0.41979700	1.16933200	H	3.64724000	3.75180200	-0.56378100
O	-1.07025200	0.32734400	2.01025900	H	6.54866200	0.66693500	0.21684200
O	0.78711000	2.00420300	1.12763700	H	5.91064700	3.06959800	0.21681100
C	1.52223400	-0.26549200	2.40719200	P	-1.16914200	1.15754800	-1.64041200
C	-1.35284100	1.00585900	3.23547700	O	-2.37963100	0.52701700	-2.59788400
C	1.09503100	2.86493200	2.22828200	O	-0.54895100	2.36998000	-2.61501700
C	2.86184800	0.15208600	2.43594500	C	-2.08980800	2.29858400	-0.52789000
C	1.10433600	-1.27844200	3.28412300	C	-3.32078300	1.38423400	-3.25916500
H	-2.27133700	0.56119900	3.62668400	C	0.26914600	1.97362800	-3.72106200
H	-0.54786300	0.87650700	3.96859900	C	-3.21962000	1.80606900	0.14099000
H	-1.52767900	2.06875000	3.04679000	C	-1.63805300	3.59426900	-0.24178300
H	0.26899500	3.57030700	2.36128700	H	-3.87488400	0.75922100	-3.96383300
H	1.26644500	2.31346300	3.15738200	H	-4.01705200	1.82623000	-2.53750500
H	2.00808800	3.40929200	1.96813500	H	-2.81075600	2.18691800	-3.80271800
C	3.76739700	-0.44131100	3.31681500	H	0.88129200	2.83719800	-3.99611100
H	3.19832000	0.94396100	1.77691200	H	0.91699500	1.13062200	-3.46003100
C	2.00929500	-1.86555700	4.16950900	H	-0.35697500	1.69022000	-4.57683200
H	0.07283200	-1.61548200	3.25598000	C	-3.89736800	2.60017400	1.06628100
C	3.34421400	-1.45131000	4.18465400	H	-3.56628900	0.79880900	-0.05587300
H	4.80258600	-0.11084100	3.32290300	C	-2.31169000	4.38628400	0.69136700
H	1.67313700	-2.64792700	4.84499200	H	-0.75929800	3.97827500	-0.74755400
H	4.04992000	-1.91202500	4.87076000	C	-3.44401400	3.89225300	1.34645300
				H	-4.77268300	2.20156400	1.57238600
				H	-1.95512000	5.39147600	0.90290300
				H	-3.96744300	4.51017600	2.07174300
				P	0.34954400	0.54062200	1.19927200
				O	-1.06054400	0.49995400	2.06098300
				O	0.77340800	2.12713000	1.02666600
				C	1.54841600	-0.02043300	2.48467400
				C	-1.34325500	1.27754200	3.22557800
				C	1.07951900	3.07477400	2.05290300
				C	2.89295500	0.38093200	2.43280100
				C	1.15591100	-0.95934900	3.45139500
				H	-2.24552200	0.85064600	3.67164300
				H	-0.52556100	1.23405200	3.95506300
				H	-1.54581000	2.31545100	2.94586800

VIII

E = -4597.101945

G_{Corr} = 0.631905

Co	0.04776800	-0.44000700	-0.78295900
P	-1.18412400	-2.10186600	-0.11431600
O	-0.78149200	-2.96666400	1.25671500
O	-1.31989900	-3.28845400	-1.28014700
C	-2.94225000	-1.83067400	0.34609100
C	0.57518900	-3.41512900	1.36652500

H	0.23919600	3.76898700	2.15434200
H	1.28491100	2.59723100	3.01581300
H	1.97234700	3.62265400	1.73512700
C	3.82397000	-0.14899300	3.32734200
H	3.21367300	1.10963800	1.69650100
C	2.08652900	-1.48400900	4.34974700
H	0.12101500	-1.28683500	3.48691000
C	3.42398700	-1.08235600	4.28764100
H	4.86163900	0.16920300	3.27113900
H	1.76851800	-2.20766800	5.09596200
H	4.14979500	-1.49456500	4.98362100

IX

E = -5009.173919

G_{Corr} = 0.812113

Co	0.06380800	-0.12957100	0.14753900
P	0.20305200	1.01468000	1.99705200
O	1.38253300	0.61855300	3.11394900
O	-1.18942400	0.99109700	2.91857000
C	0.56364000	2.81784700	1.96560800
C	1.45573100	-0.76049800	3.50095600
C	-1.23237100	1.60016300	4.21623100
C	-0.49917100	3.69912500	1.70851600
C	1.86455500	3.32952800	2.06289300
H	1.30037200	-1.41823100	2.63893800
H	2.45172000	-0.92889400	3.91427300
H	0.69885800	-0.98260700	4.26326000
H	-2.17920300	1.29897500	4.67130100
H	-0.39976400	1.25658700	4.83947100
H	-1.19406600	2.69259400	4.14204100
C	-0.26519700	5.06712000	1.55968500
H	-1.50574000	3.30631100	1.60464000
C	2.09941600	4.69643900	1.90187300
H	2.69107400	2.65560500	2.25498700
C	1.03689600	5.56893800	1.64952900
H	-1.09675200	5.73946500	1.36458800
H	3.11343600	5.08170700	1.97585900
H	1.22168300	6.63274400	1.52483600
P	-0.43559000	-2.23665000	0.21268300
O	-1.89557900	-2.67533800	-0.50239800
O	-0.59265000	-3.05635300	1.66790300
C	0.71066000	-3.44177000	-0.57594900
C	-2.34446800	-4.03452600	-0.43959000
C	-1.51686000	-2.48845300	2.60563800
C	1.04989500	-3.20077600	-1.91731400
C	1.25562300	-4.55552800	0.07797000
H	-3.18902500	-4.12256400	-1.12602100
H	-1.55644200	-4.73149400	-0.74739900
H	-2.67211000	-4.29373900	0.57290400
H	-1.31209700	-1.42589300	2.77098700
H	-2.54915000	-2.58739400	2.24916800
H	-1.39649000	-3.03911300	3.54252100
C	1.92047500	-4.05736600	-2.59196300
H	0.65726900	-2.32054200	-2.41669000
C	2.13430200	-5.40813000	-0.59567400
H	0.99314700	-4.74734500	1.11267900
C	2.46857000	-5.16154400	-1.92982900
H	2.17832900	-3.85949500	-3.62917300
H	2.55863300	-6.26447900	-0.07783900
H	3.15433100	-5.82421600	-2.45131800
P	-0.52924600	1.20530200	-1.48811200
O	-1.67801100	2.26589800	-0.92667500
O	-1.16235200	0.69719900	-2.94734900
C	0.69138900	2.35050800	-2.25984000
C	-2.44309800	3.07594800	-1.82331900
C	-2.05161900	-0.42581500	-2.96860800
C	0.98388800	3.56971800	-1.63360700
C	1.41982800	1.97665000	-3.39800800

H	-2.94220700	3.83255800	-1.21148600
H	-1.80445000	3.57357600	-2.56280400
H	-3.19677000	2.46945500	-2.33451500
H	-2.06422600	-0.79981500	-3.99694400
H	-1.71232800	-1.21272200	-2.28939400
H	-3.06004400	-0.12215500	-2.67100700
C	1.97686800	4.40745600	-2.14316100
H	0.44036500	3.86061900	-0.74243800
C	2.41545200	2.81403800	-3.90709900
H	1.20575600	1.03042500	-3.88262400
C	2.69580100	4.03298700	-3.28149300
H	2.19001300	5.34940200	-1.64416100
H	2.96772200	2.51780100	-4.79581800
H	3.47123300	4.68392600	-3.67764700
P	2.26179100	-0.11174000	-0.32153300
O	2.83087800	1.42236500	-0.10581000
O	2.55299900	-0.52852300	-1.89537600
C	3.56949200	-1.07209000	0.56311300
C	4.10278000	1.92323700	-0.51988300
C	3.81754800	-0.57632500	-2.56231200
C	3.89914000	-2.37801700	0.16979100
C	4.16443800	-0.54225300	1.71965500
H	4.25578200	2.86063400	0.02161800
H	4.91606700	1.22893500	-0.27724100
H	4.09146400	2.13328100	-1.59281700
H	3.92953000	0.32081600	-3.17986000
H	4.65602600	-0.65042100	-1.86287300
H	3.81462700	-1.46448400	-3.20196600
C	4.80156100	-3.13741000	0.91646000
H	3.45395500	-2.80290700	-0.72218200
C	5.07119200	-1.29950000	2.46258600
H	3.89950300	0.45837500	2.04594300
C	5.39054200	-2.60101100	2.06412500
H	5.04000000	-4.14894800	0.59861500
H	5.52629200	-0.87478000	3.35379400
H	6.09305500	-3.19252700	2.64534300
C	-5.60750100	0.22585000	-0.49226600
C	-5.63458500	-1.09568800	0.36049800
O	-4.18183300	0.51643500	-0.56584600
O	-4.42185200	-0.96990000	1.16311600
C	-6.15078200	0.09359200	-1.91176000
H	-7.20725400	-0.19640700	-1.89556600
H	-6.06833300	1.05620400	-2.42686000
H	-5.59295500	-0.64721400	-2.48865300
C	-6.25703900	1.41960300	0.21771400
H	-6.01669900	2.33303900	-0.33502700
H	-7.34589600	1.31645300	0.26485200
H	-5.86988500	1.52711200	1.23583700
C	-6.82808300	-1.23771900	1.29902600
H	-7.76473800	-1.25426800	0.73060600
H	-6.74919800	-2.17771900	1.85470000
H	-6.87083400	-0.41952900	2.02138500
C	-5.46461600	-2.35788300	-0.49065800
H	-5.28451900	-3.21027500	0.17098300
H	-6.35798100	-2.56258900	-1.08930000
H	-4.60229800	-2.25956800	-1.15549100
B	-3.58216900	-0.11901200	0.49123600
H	-2.46429800	0.07519400	0.82001100

TS IX-X^{BS}

E = -5396.62933

G_{Corr} = 0.98479

Co	-0.75868500	-0.25524000	0.09777500
H	1.55080500	-0.94600900	0.43493900
P	-0.07393600	1.20496300	-1.44606700
O	-1.08238300	1.40824900	-2.75903000
O	1.39000500	0.93088500	-2.17393200
C	0.08377500	2.97439000	-0.99893500

C	-1.36267400	0.21773500	-3.51065300	H	-4.31735800	2.94260000	1.44988200
C	1.87901800	1.82819900	-3.18546600	H	-5.08824600	0.89497400	2.42490600
C	1.26313300	3.36817000	-0.34653500	H	-5.75035000	0.36095600	0.84812500
C	-0.93570400	3.91251700	-1.20609400	H	-5.52896200	-0.81683000	2.16511800
H	-1.63942300	-0.60793700	-2.84583800	C	-5.83580600	-1.17714100	-2.54036700
H	-2.19924800	0.44625500	-4.17245500	H	-4.93212200	-1.71473700	-0.66633600
H	-0.48812500	-0.07644100	-4.10300200	C	-5.13423700	0.93183100	-3.49043500
H	2.65063300	2.47318200	-2.75603100	H	-3.66476000	2.02867700	-2.36431500
H	2.31027800	1.21399100	-3.98065200	C	-5.91271000	-0.22765700	-3.56166800
H	1.07540200	2.44002500	-3.60518600	H	-6.42879700	-2.08606900	-2.58935200
C	1.42446300	4.68695400	0.07897100	H	-5.18799300	1.67445100	-4.28230600
H	2.04121400	2.63632600	-0.15886200	H	-6.57206100	-0.39015600	-4.41012900
C	-0.77542400	5.22949900	-0.77057000	C	7.72917800	1.56565000	-2.53530800
H	-1.84983600	3.61013100	-1.70322500	H	7.98421300	2.59773300	-2.80607800
C	0.40379600	5.62033200	-0.12960000	H	8.17675400	1.34984900	-1.55840700
H	2.34307500	4.98377000	0.57834700	H	8.18841000	0.89925800	-3.27632400
H	-1.57071300	5.95228600	-0.93419700	C	6.19853700	1.36241800	-2.50162700
H	0.52639500	6.64642000	0.20705900	C	5.88557700	-0.11513500	-2.16068500
P	-0.78122600	-2.42251000	-0.52411800	C	5.60896500	2.26664600	-1.44229100
O	-0.04505800	-3.44658400	0.55657600	C	4.44972300	-0.34751300	-1.66010700
O	-0.12904100	-2.90114100	-1.97049100	H	6.57649500	-0.44585100	-1.37403400
C	-2.40466600	-3.25987900	-0.73775200	H	6.08259600	-0.74377000	-3.03824300
C	0.13632800	-4.83423100	0.23708400	C	4.71517800	1.85509800	-0.49306800
C	1.20931900	-2.45487700	-2.27559200	H	5.96216100	3.29689900	-1.43011800
C	-3.17270200	-3.48575900	0.41663800	C	4.15954300	0.53986400	-0.47683900
C	-2.90303400	-3.66917800	-1.98152900	H	4.28532700	-1.38827000	-1.38613600
H	0.58274800	-5.29992100	1.11835100	H	3.72081000	-0.10581100	-2.44543100
H	-0.82108900	-5.31949500	0.01354400	H	4.40499300	2.52910800	0.30266900
H	0.80975800	-4.95129000	-0.61761500	C	5.62708100	1.73721100	-3.88959500
H	1.24388200	-1.36675700	-2.37305300	H	5.78105500	2.80180200	-4.10233400
H	1.91348700	-2.76373500	-1.49718900	H	6.12650800	1.15765400	-4.67660600
H	1.47334500	-2.92165100	-3.22834200	H	4.55489900	1.53590800	-3.94767500
C	-4.41173600	-4.12120000	0.32884100	O	3.44629100	0.19560000	0.53993400
H	-2.79796000	-3.16512900	1.38427000	C	4.21965100	-2.83993700	1.29469800
C	-4.14692600	-4.29973200	-2.06908900	C	3.50675200	-2.45771100	2.65019000
H	-2.31059500	-3.50432400	-2.87526900	O	3.32389300	-2.30960000	0.31320700
C	-4.90150800	-4.52990400	-0.91655600	O	2.76810700	-1.27760300	2.32072400
H	-4.99459200	-4.29730600	1.22907000	C	5.60151300	-2.17437300	1.14205400
H	-4.52539800	-4.61237900	-3.03864100	H	6.33483800	-2.60191100	1.83480200
H	-5.86720300	-5.02345900	-0.98653000	H	5.96473700	-2.33526300	0.12143500
P	-0.38138300	0.74344400	2.11501600	H	5.54536100	-1.09738300	1.31677000
O	1.10538900	1.42858300	2.10452300	C	4.36424700	-4.34189400	1.03826600
O	-0.43292000	-0.22448000	3.45547500	H	4.86309900	-4.50187100	0.07549500
C	-1.41593400	2.09232900	2.81780200	H	4.96651500	-4.82375400	1.81742800
C	1.83164200	1.70280000	3.31007500	H	3.38805700	-4.83078100	0.99512700
C	-0.39001300	-1.64870400	3.25537000	C	2.51806400	-3.54058500	3.11078400
C	-1.14628400	3.42618700	2.48388000	H	3.02797000	-4.46807700	3.39476900
C	-2.53617600	1.79721000	3.60805400	H	1.96881000	-3.17470700	3.98337700
H	2.27172300	0.77388600	3.67891500	H	1.79583500	-3.75254400	2.31935400
H	2.62499500	2.40285600	3.03622900	C	4.46301800	-2.13023000	3.80177900
H	1.18874000	2.15977100	4.07199200	H	3.88248400	-1.87151000	4.69452900
H	-1.36330400	-2.00519900	2.89912900	H	5.10089200	-2.98803000	4.04808000
H	0.38277000	-1.92497000	2.54164900	H	5.10067100	-1.27672400	3.55918600
H	-0.17266600	-2.08911700	4.23176100	B	2.67847400	-1.14073900	0.88079300
C	-1.97523400	4.45037100	2.94424200				
H	-0.29041000	3.66294700	1.86250800				
C	-3.36439000	2.82282700	4.07059400				
H	-2.75048600	0.76592600	3.86816600				
C	-3.08456400	4.15281800	3.74051600				
H	-1.75227300	5.48032500	2.67778200				
H	-4.22269100	2.58475900	4.69423300				
H	-3.72894700	4.95089200	4.10034500				
P	-2.97897000	0.40801300	-0.00902900				
O	-2.98378900	2.04524600	0.14361400				
O	-3.77873700	-0.23819200	1.28474500				
C	-4.20588600	0.19161200	-1.36880000				
C	-4.11524700	2.89070200	0.37759900				
C	-5.11637600	0.07991800	1.69508100				
C	-4.98767200	-0.96950200	-1.45141900				
C	-4.28432500	1.13896900	-2.40366100				
H	-3.83788600	3.88540500	0.01945500				
H	-5.00410600	2.54626300	-0.16224100				

X

$$E = -5396.678373$$

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Co	-1.15302000	-0.23998500	0.02522000
H	0.01324000	-1.09252000	0.37915100
P	0.35194600	0.80459500	-1.06874600
O	0.05584100	1.43618200	-2.59086300
O	1.69571300	-0.13279600	-1.32789100
C	1.08648600	2.33140600	-0.36086500
C	-0.49947100	0.53251900	-3.55282800
C	2.79353800	0.32427600	-2.12675600
C	2.07621600	2.20217400	0.62580300
C	0.58171100	3.60460800	-0.66178200
H	-1.25906100	-0.11117800	-3.09591300

H	-0.95923500	1.13440300	-4.33915100
H	0.28784400	-0.09419300	-3.98902100
H	3.21976200	1.25290700	-1.73608500
H	3.54511100	-0.46433300	-2.07017900
H	2.48583900	0.47690800	-3.16737900
C	2.54946400	3.32853800	1.30176700
H	2.47089900	1.22298200	0.87222800
C	1.05829700	4.72975200	0.01380100
H	-0.19182900	3.70797300	-1.41381600
C	2.04061000	4.59535800	0.99961500
H	3.31154800	3.21321500	2.06829900
H	0.66022800	5.71241000	-0.22687900
H	2.40539800	5.47093000	1.53026200
P	-1.84188200	-2.11843100	-0.66215900
O	-1.14216700	-3.40828100	0.14836200
O	-1.60023300	-2.62184700	-2.24327900
C	-3.63133100	-2.54472200	-0.58748100
C	-1.53405200	-4.75263300	-0.14110300
C	-0.24003100	-2.74512600	-2.67506100
C	-4.31711100	-2.13137300	0.56568000
C	-4.33555900	-3.20008700	-1.60763700
H	-0.80441100	-5.40340500	0.34809100
H	-2.53515400	-4.96433500	0.25336300
H	-1.53113500	-4.94840200	-1.21901000
H	0.39066800	-1.95425900	-2.25633400
H	0.16904100	-3.71745400	-2.37495800
H	-0.24002900	-2.67516500	-3.76603900
C	-5.68829200	-2.35932600	0.69187700
H	-3.77830600	-1.58728600	1.33466400
C	-5.71025500	-3.41614000	-1.48607300
H	-3.80768200	-3.51721600	-2.50052500
C	-6.38896700	-2.99455200	-0.33874700
H	-6.21155100	-2.03060300	1.58612400
H	-6.25286700	-3.91056500	-2.28781800
H	-7.45969900	-3.15851500	-0.24889400
P	-1.05948400	0.24760500	2.11127500
O	0.52362200	0.29091300	2.60624800
O	-1.78748700	-0.69946600	3.27738600
C	-1.71206500	1.83642700	2.77911800
C	0.89087400	0.50666500	3.97250000
C	-1.64819100	-2.12262800	3.20585600
C	-0.95690700	3.00292300	2.59402900
C	-2.98416500	1.93368100	3.36019400
H	0.28175100	-0.10535900	4.64676000
H	1.93968400	0.21172600	4.05774100
H	0.77911900	1.56216300	4.24567300
H	-2.61014200	-2.56732600	3.48104100
H	-1.36889300	-2.45135200	2.20213000
H	-0.88370100	-2.45115800	3.91885800
C	-1.45737800	4.24273800	2.99330700
H	0.02168400	2.94385700	2.13344100
C	-3.48711300	3.17538300	3.75694000
H	-3.57820200	1.03735900	3.49835700
C	-2.72472100	4.33354700	3.57513500
H	-0.85568900	5.13524400	2.84246800
H	-4.47236200	3.23758700	4.21286300
H	-3.11726100	5.29918500	3.88380700
P	-2.82186400	1.06595300	-0.39373800
O	-2.32871500	2.63396500	-0.28253500
O	-4.04799000	0.86311400	0.68898000
C	-3.73977000	1.10367800	-1.99021600
C	-3.19455700	3.76509900	-0.16796200
C	-5.32767900	1.50233900	0.70538300
C	-4.79334600	0.20825300	-2.23364100
C	-3.33050200	1.97047000	-3.01499600
H	-2.56859100	4.64753100	-0.32182000
H	-3.98840400	3.74925200	-0.92446200
H	-3.62669000	3.80858100	0.83566700
H	-5.34582800	2.22811700	1.52442700
H	-5.55843400	2.00352300	-0.23923500
H	-6.07692500	0.72472000	0.88357000
C	-5.41652900	0.17453000	-3.48191600

H	-5.13247700	-0.45805200	-1.44864300
C	-3.95984300	1.94061100	-4.26048900
H	-2.50622000	2.65437800	-2.83769000
C	-5.00128700	1.03936400	-4.49815400
H	-6.22756900	-0.52735400	-3.65667600
H	-3.63491600	2.61821500	-5.04576400
H	-5.48781800	1.01275000	-5.46954600
C	8.46514600	2.07240500	-2.53270200
H	8.22279400	2.97291300	-3.11063800
H	9.04278000	2.38082400	-1.65338700
H	9.10518300	1.43509600	-3.15573200
C	7.18289100	1.32499700	-2.11883200
C	7.56849600	0.06403000	-1.30555200
C	6.31882500	2.21920100	-1.25691500
C	6.36717100	-0.63319400	-0.64162500
H	8.27093900	0.36665900	-0.51806400
H	8.09797100	-0.64636700	-1.95288400
C	5.55130400	1.71822400	-0.21569900
H	6.27221300	3.27778700	-1.50112000
C	5.51963600	0.36478900	0.09322100
H	6.72225400	-1.40190800	0.05808700
H	5.76502200	-1.17194300	-1.38644900
H	4.92147300	2.38567600	0.36427000
C	6.40427100	0.92711100	-3.39693900
H	6.11690100	1.81766000	-3.96794300
H	7.02202600	0.29103400	-4.04503400
H	5.48843900	0.38004500	-3.15345600
O	4.74114900	-0.05010900	1.14946300
C	3.47358300	-3.38050200	0.65406300
C	3.11937400	-3.07934600	2.16830500
O	3.83548900	-2.06627000	0.13958000
C	3.85801200	-1.84880700	2.43534500
C	4.71645200	-4.26102400	0.47840400
H	4.53268200	-5.28897200	0.80598700
H	4.99129700	-4.27752500	-0.58090500
H	5.56583600	-3.86115200	1.04197300
C	2.31272500	-3.92398300	-0.17310400
H	2.63004800	-4.03221100	-1.21584100
H	2.01367800	-4.91181200	0.19624500
H	1.44219800	-3.26807500	-0.14257300
C	1.64119300	-2.77158500	2.39760000
H	1.01834500	-3.65787400	2.24511300
H	1.51145000	-2.42550300	3.42733900
H	1.28248100	-1.98184700	1.73612200
C	3.59830700	-4.14048500	3.15618800
H	3.32863000	-3.83939700	4.17351600
H	3.11873100	-5.10302100	2.94685300
H	4.68206800	-4.27222100	3.11806600
B	4.15480700	-1.28862200	1.22204900

TS X-XI

E = -5396.650143

G_{Corr} = 0.987578

Co	-0.75222200	0.23842500	0.03741500
H	0.68572300	1.01260200	-0.13782700
P	0.22973100	-0.88367500	1.60779100
O	-0.65989900	-1.31340600	2.96847200
O	1.52243700	-0.15234200	2.35266800
C	0.84026400	-2.59413000	1.27020000
C	-1.17411800	-0.24438900	3.76356800
C	2.40728300	-0.88782900	3.20356300
C	1.70957200	-2.77094600	0.18445100
C	0.43526300	-3.71572600	2.00984300
H	-1.74262800	0.46524500	3.15353700
H	-1.83827900	-0.68964000	4.50752100
H	-0.36021900	0.28498700	4.27288100
H	3.09298200	-1.49502300	2.60371300
H	2.97816000	-0.14843000	3.77353600

H	2.32195300	2.51641800	3.07215200
C	0.86122800	5.39457500	1.98612100
H	-0.92752700	5.49096200	0.77976700
H	2.60720600	4.97769300	3.18288200
H	0.98756100	6.47307000	2.03155800
P	0.74530300	-2.21659200	-0.49027000
O	0.01355600	-2.66863000	-1.92715300
O	-0.17261400	-3.07573700	0.60956700
C	2.14056500	-3.43379500	-0.49117000
C	-0.30393600	-4.03653900	-2.20570800
C	-1.45950800	-2.56532800	0.97616000
C	3.07769000	-3.35244600	-1.53499700
C	2.29008800	-4.43978200	0.47288300
H	-0.96345900	-4.03259000	-3.07747400
H	0.60173100	-4.61058500	-2.43344400
H	-0.81936600	-4.50225300	-1.35908000
H	-1.46396000	-1.47512200	1.01892600
H	-2.21669100	-2.89902000	0.25728400
H	-1.69854900	-2.97346200	1.96257900
C	4.13438000	-4.26012100	-1.61644800
H	2.99004000	-2.56855100	-2.27798900
C	3.35336200	-5.34363900	0.39708100
H	1.56882800	-4.51680600	1.27869600
C	4.27650300	-5.25904300	-0.64697600
H	4.84830400	-4.18638900	-2.43288800
H	3.45950700	-6.11447900	1.15604600
H	5.10151100	-5.96408800	-0.70626200
P	1.41341800	1.36048600	-1.79836500
O	0.14348900	2.40658100	-2.02551800
O	1.69812700	0.91691000	-3.38596600
C	2.78682100	2.60632000	-1.70654700
C	0.11636500	3.35478500	-3.09765900
C	2.00238000	-0.42952000	-3.73498600
C	2.65603200	3.72591800	-0.87299300
C	3.96807800	2.44528300	-2.44146900
H	0.21851100	2.85389000	-4.06536600
H	-0.85571300	3.85204200	-3.04419000
H	0.91309500	4.09921700	-2.98899100
H	3.08894900	-0.58569100	-3.73034800
H	1.53637700	-1.13172900	-3.04121200
H	1.61427200	-0.60379200	-4.74313400
C	3.67927000	4.66967800	-0.78418100
H	1.75173500	3.86004200	-0.29261000
C	4.99856200	3.38648400	-2.34930500
H	4.07773200	1.58912000	-3.09834300
C	4.85519600	4.50382500	-1.52244600
H	3.55572700	5.53194200	-0.13392500
H	5.90712900	3.25144100	-2.93142100
H	5.65339800	5.23858600	-1.45347900
P	3.17122400	-0.08361700	0.40006600
O	3.51348000	1.42895300	0.95343300
O	4.13812000	-0.37663100	-0.90974500
C	4.01872800	-1.07223000	1.71621100
C	4.81016400	1.98051700	1.19067400
C	5.56954000	-0.32756600	-0.95754900
C	4.63503000	-2.29996900	1.43702600
C	4.02151900	-0.60275600	3.04106500
H	4.65710000	2.86380800	1.81555600
H	5.46632700	1.27580600	1.71399800
H	5.26167500	2.29040500	0.24521200
H	5.87881100	0.62741300	-1.39331400
H	6.02461500	-0.44738300	0.02984300
H	5.89975100	-1.14959600	-1.59957100
C	5.23063300	-3.04618500	2.45578100
H	4.65851800	-2.67527200	0.42207400
C	4.61819100	-1.34722200	4.05862100
H	3.53781700	0.33887500	3.27413300
C	5.22287100	-2.57420600	3.76943500
H	5.69530000	-3.99849300	2.21584900
H	4.61104400	-0.96874700	5.07757600
H	5.68551200	-3.15555500	4.56267000
C	-1.39833400	-0.23245300	-3.61900400

H	-0.97397800	0.75495300	-3.81786000
H	-0.62022800	-0.85751100	-3.18471900
H	-1.71163500	-0.67146300	-4.57617100
C	-2.59033300	-0.13787600	-2.66044300
C	-3.13609700	-1.55809400	-2.38153500
C	-2.21126100	0.51847000	-1.33816300
C	-4.31266800	-1.57984000	-1.39144900
H	-2.31095200	-2.14781500	-1.97477300
H	-3.43876400	-2.03019500	-3.32556200
C	-3.11626800	0.32824500	-0.25014700
H	-1.71869600	1.48016600	-1.41437000
C	-4.07959100	-0.62883700	-0.25791200
H	-4.46005200	-2.59333300	-0.99119900
H	-5.25686800	-1.31359800	-1.88883700
H	-3.03393800	0.95970000	0.62379700
C	-3.68615700	0.74002100	-3.32066900
H	-3.29264000	1.73962300	-3.54242600
H	-4.01691900	0.29017400	-4.26664000
H	-4.55934900	0.85945300	-2.67087100
O	-4.90718200	-0.77210800	0.85277700
C	-8.27346200	-0.00181200	-0.10642500
C	-8.35510200	-0.09994000	1.46477900
O	-6.83801600	0.09153200	-0.33192400
O	-7.09749000	-0.75421100	1.79988700
C	-8.74940400	-1.27605600	-0.81384500
H	-9.83578700	-1.39160900	-0.74661500
H	-8.46996200	-1.21950000	-1.87039400
H	-8.27595300	-2.16422000	-0.38312800
C	-8.94250000	1.22708400	-0.71285600
H	-8.82468400	1.21111900	-1.80111300
H	-10.01403200	1.23340200	-0.48469700
H	-8.49780100	2.15133900	-0.33764000
C	-8.33947100	1.27063500	2.15190200
H	-9.28275500	1.80558800	2.00277500
H	-8.18674400	1.12662100	3.22578200
H	-7.52173500	1.89117700	1.77142000
C	-9.50372200	-0.95043500	1.99717300
H	-9.47660000	-0.96372100	3.09145200
H	-10.46730100	-0.53365000	1.68390900
H	-9.43566300	-1.98168800	1.64394700
B	-6.23611800	-0.48594200	0.76408500

XI

$$E = -799.5872832$$

$$G_{\text{corr}} = 0.335457$$

C	-5.13623400	1.35905800	-0.00519600
H	-5.50839900	1.73172400	0.95712700
H	-4.67679700	2.19898700	-0.53929300
H	-5.99859500	1.01410100	-0.58936500
C	-4.12683500	0.21037100	0.19629000
C	-3.66026800	-0.31325300	-1.18444800
C	-2.93436600	0.72600400	0.97991500
C	-2.36297300	-1.12577400	-1.10112500
H	-3.49658400	0.54535000	-1.85114500
H	-4.45867600	-0.91320400	-1.63849700
C	-1.65632800	0.52953200	0.64446800
H	-3.16881100	1.29488400	1.88070900
H	-2.09068500	-1.53625800	-2.07998600
H	-2.48072900	-1.97435500	-0.41709000
H	-0.85192500	0.95088200	1.24422100
C	-4.81110200	-0.91394900	1.00803600
H	-5.09457200	-0.55712100	2.00553500
H	-5.72206600	-1.25494600	0.50024600
H	-4.14770500	-1.77505300	1.13966400
O	-0.12080600	-1.12094000	-0.24418900
C	2.88956800	0.81700700	-0.32296400
C	3.32115700	-0.49679200	0.43218100
O	1.43686900	0.73292700	-0.27510800

O	2.21950100	-1.40024600	0.13635600	H	-4.83386300	-4.52888100	-2.78085000
C	3.32554400	2.11769000	0.34354800	H	-6.20664600	-4.62811900	-0.70994900
H	4.41808600	2.16963900	0.40659800	P	-0.45377800	0.67427900	2.08233700
H	2.97666600	2.97069400	-0.24743900	O	1.04393000	1.30953300	2.27815100
H	2.91109300	2.21038700	1.34984600	O	-0.62014800	-0.27247600	3.44551500
C	3.28483400	0.81495700	-1.80429800	C	-1.45962600	2.10407400	2.69868400
H	2.77594800	1.64245700	-2.30810800	C	1.59273100	1.59714200	3.56561900
H	4.36459500	0.94074900	-1.93237700	C	-1.26558600	-1.54434100	3.35992300
H	2.98194200	-0.11852200	-2.28939100	C	-1.11553900	3.40847100	2.31574600
C	4.61795300	-1.12770800	-0.06481900	C	-2.56778100	1.91251100	3.53348300
H	5.45640800	-0.43384300	0.06193600	H	1.86983100	0.66628000	4.06503800
H	4.83282100	-2.03241300	0.51286200	H	2.48944500	2.19723200	3.38932500
H	4.54940000	-1.40709000	-1.11849700	H	0.89008900	2.16813600	4.18523300
C	3.35931600	-0.32565800	1.95575100	H	-2.35578400	-1.41949200	3.33484300
H	3.45500600	-1.31171200	2.42024000	H	-0.94651900	-2.09388900	2.47296400
H	4.20679300	0.29161900	2.27042400	H	-0.98619500	-2.10300200	4.25711000
H	2.43624100	0.13519700	2.32211500	C	-1.86057700	4.49888900	2.76509200
B	1.12846300	-0.60578500	-0.13450800	H	-0.26505200	3.56971200	1.66428200
C	-1.22731900	-0.25357300	-0.57247000	C	-3.31951400	3.00393200	3.98035100
H	-0.89396300	0.44536800	-1.35346800	H	-2.83524600	0.90957100	3.84954300

TS IX-X

E = -5396.617177

G_{Corr} = 0.990557

Co	-0.58209500	-0.23108500	0.04413600	C	-3.88038800	0.37695700	-1.56602800
H	1.07388900	-0.89591400	0.50915400	C	-3.68354900	3.07792300	0.14748500
P	0.19885500	1.13423700	-1.49109700	C	-4.90844500	0.34490600	1.43143000
O	-0.82428400	1.39293900	-2.79695800	C	-4.78524900	-0.69277300	-1.62532600
O	1.60881800	0.80586600	-2.32029700	C	-3.88236500	1.32097300	-2.60795800
C	0.44610900	2.90248200	-1.05334600	H	-3.32627800	4.07317800	-0.12597700
C	-1.06367100	0.24275200	-3.61674400	H	-4.55623400	2.82291400	-0.46395900
C	2.09298300	1.73630100	-3.29852200	H	-3.94720200	3.07381200	1.20767700
C	1.54571900	3.20703500	-0.23412500	H	-4.90400800	1.08108700	2.24045800
C	-0.43704000	3.92392000	-1.42686000	H	-5.45646700	0.74252900	0.57274300
H	-1.32561600	-0.62922100	-3.00638700	H	-5.39815600	-0.57340500	1.76831400
H	-1.89775800	0.48607400	-4.27682900	C	-5.66175300	-0.82476600	-2.70375700
H	-0.17573400	0.00464000	-4.21452300	H	-4.81767600	-1.41984900	-0.82463400
H	2.70340400	2.50843500	-2.81773900	C	-4.76082100	1.19036400	-3.68334900
H	2.70734300	1.16975300	-4.00365300	H	-3.18110700	2.14659200	-2.57991700
H	1.27017900	2.21207600	-3.84183600	C	-5.65130800	0.11363900	-3.73724700
C	1.76411900	4.51900000	0.18919900	H	-6.34912400	-1.66565900	-2.73045400
H	2.20077300	2.40827600	0.09596600	H	-4.74996600	1.93018400	-4.47959800
C	-0.22609700	5.23229100	-0.98545800	H	-6.33317100	0.01035500	-4.57718500
H	-1.28856800	3.69221600	-2.05605900	C	8.08442600	0.72160100	-2.00454400
C	0.87589900	5.53431000	-0.18009800	H	8.55221100	1.71187500	-2.06767000
H	2.62003300	4.74594400	0.81990400	H	8.44101000	0.23533400	-1.08911300
H	-0.92026300	6.01781900	-1.27422200	H	8.42973500	0.13009600	-2.86135600
H	1.03973600	6.55367800	0.15996500	C	6.54694900	0.83393100	-2.01015700
P	-0.95029400	-2.33379300	-0.46695900	C	5.92702600	-0.58140100	-1.93104200
O	-0.29278400	-3.41655000	0.61869900	C	6.09073200	1.64367000	-0.81879100
O	-0.39502600	-2.93818200	-1.91777300	C	4.42243200	-0.58156700	-1.63096000
C	-2.63772500	-3.06634100	-0.62041100	H	6.44092000	-1.13324600	-1.13399200
C	-0.26830700	-4.81920100	0.33456700	H	6.12244300	-1.12050000	-2.86658400
C	0.93552600	-2.58810600	-2.33392400	C	4.95248100	1.36517900	-0.11230000
C	-3.41984700	-3.12587800	0.54500200	H	6.69147700	2.51013400	-0.54674500
C	-3.15816700	-3.57961300	-1.81544200	C	4.07402900	0.30345500	-0.46638300
H	0.08613900	-5.31399300	1.24227700	H	4.04788600	-1.58716000	-1.42881900
H	-1.26682200	-5.19653900	0.08425100	H	3.84379900	-0.21928100	-2.49046100
H	0.41619600	-5.03663300	-0.49158200	H	4.65620800	1.98323900	0.73202200
H	1.06891900	-1.50336500	-2.35074400	C	6.10421000	1.55950000	-3.30497900
H	1.67950500	-3.01615700	-1.65738000	H	6.53282200	2.56737600	-3.35304800
H	1.05828200	-2.99257100	-3.34272700	H	6.44269300	1.00321700	-4.18867100
C	-4.69651100	-3.68779400	0.51535800	H	5.01599100	1.65744900	-3.35522900
H	-3.03207700	-2.71809300	1.47173100	O	2.93696700	0.20510600	0.14874500
C	-4.43913600	-4.13794200	-1.84666000	C	3.61435500	-2.97202800	1.27850700
H	-2.55619500	-3.54548900	-2.71680200	C	3.07337900	-2.34674800	2.61673200
C	-5.21078500	-4.19366100	-0.68405600	O	2.79907300	-2.33158200	0.28007800
H	-5.29088300	-3.72945900	1.42449600	O	2.62249600	-1.05505400	2.19874700
				C	5.08801600	-2.61819300	1.01798300

H	5.75281500	-3.11016600	1.73594800
H	5.36720000	-2.95180300	0.01367000
H	5.25495200	-1.53841400	1.07768300
C	3.43459900	-4.48443200	1.15343700
H	3.82155800	-4.82342600	0.18565200
H	3.98339800	-5.01134100	1.94293400
H	2.38201000	-4.76253700	1.21199900
C	1.87462700	-3.11409200	3.19230300
H	2.16972400	-4.09056600	3.59418300
H	1.44215600	-2.52153100	4.00443300
H	1.10940200	-3.25336700	2.42713700
C	4.12818600	-2.15655700	3.70952300
H	3.65812700	-1.71601900	4.59575600
H	4.57246400	-3.11547400	4.00199400
H	4.92547300	-1.48385600	3.38397000
B	2.31437200	-1.08603400	0.80428300

XBS

E = -5396.636734

G_{Corr} = 0.987256

Co	-0.84362500	-0.17146800	0.01355500
H	1.68010100	-0.83548300	0.49814100
P	0.03786300	1.46585100	-1.11288900
O	-0.76572200	1.94579700	-2.50385900
O	1.59377000	1.28155700	-1.70329000
C	0.18866900	3.13361200	-0.35829400
C	-0.87938800	0.93365700	-3.51340700
C	2.17388400	2.30932700	-2.52092400
C	1.28985500	3.36816800	0.48334000
C	-0.79489200	4.12174000	-0.49622700
H	-1.19046000	-0.02266800	-3.07727000
H	-1.63292000	1.27064800	-4.22681800
H	0.07996800	0.79744500	-4.02829700
H	2.98150100	2.80395400	-1.97295500
H	2.57968900	1.83063500	-3.41820700
H	1.43365900	3.05392700	-2.82626700
C	1.40363600	4.57828400	1.16906800
H	2.04821700	2.60064000	0.61245600
C	-0.67906000	5.32992900	0.19470900
H	-1.65205000	3.93580600	-1.13278400
C	0.41820400	5.56151800	1.02891400
H	2.25883700	4.75181200	1.81747100
H	-1.44775600	6.09081700	0.08380900
H	0.50466900	6.50130500	1.56826100
P	-0.76860500	-2.18579500	-0.77697400
O	0.13465100	-3.29142600	0.11674800
O	-0.15420800	-2.50406700	-2.30492800
C	-2.33869800	-3.12289200	-0.99599600
C	0.37687500	-4.60545600	-0.39570600
C	1.16073500	-1.99827600	-2.57416000
C	-3.17726700	-3.21645900	0.12712400
C	-2.73952200	-3.71942400	-2.19954700
H	0.81764800	-5.18778100	0.41720000
H	-0.55339800	-5.08849100	-0.71782500
H	1.07499100	-4.57792800	-1.23844700
H	1.22089700	-0.92400200	-2.37598000
H	1.91202700	-2.50717900	-1.95801000
H	1.36192300	-2.19174500	-3.63158900
C	-4.39436400	-3.89402100	0.04723400
H	-2.88983900	-2.72474700	1.05094300
C	-3.96348600	-4.38910100	-2.28159300
H	-2.09421800	-3.65131200	-3.06857600
C	-4.79252400	-4.47810800	-1.16044800
H	-5.03631600	-3.95760900	0.92208300
H	-4.26971200	-4.84052700	-3.22184100
H	-5.74531000	-4.99692600	-1.22677900
P	-0.84516000	0.28109400	2.16822800
O	0.65047200	0.85360100	2.59062900

O	-1.18861900	-0.83989600	3.35618500
C	-1.95589100	1.56692400	2.88577300
C	1.04658300	0.99174300	3.95799200
C	-0.65294200	-2.16081700	3.22967200
C	-1.59110200	2.91655700	2.78996800
C	-3.19841000	1.23435400	3.44480400
H	1.22830000	0.00928900	4.40490600
H	1.97796900	1.56350300	3.95385000
H	0.29145800	1.52941500	4.54397000
H	-1.28753700	-2.82431100	3.82550900
H	-0.64311600	-2.49011400	2.18664300
H	0.37237500	-2.18711200	3.60539300
C	-2.44817700	3.91614800	3.25303000
H	-0.63797800	3.18688800	2.35062600
C	-4.05517900	2.23471100	3.91031400
H	-3.48919200	0.19239300	3.51711200
C	-3.68208800	3.57921100	3.81544000
H	-2.14838600	4.95748400	3.16866400
H	-5.01170000	1.96416000	4.35148200
H	-4.35003200	4.35763000	4.17587000
P	-2.98325700	0.46595100	-0.29468700
O	-3.09835800	2.08751600	-0.00258400
O	-3.97485000	-0.29728800	0.78922600
C	-3.97908800	0.34300000	-1.84738200
C	-4.30456600	2.82618100	0.19904100
C	-5.38801500	-0.13522300	0.94119700
C	-4.65984700	-0.84031000	-2.17309100
C	-3.97511600	1.39905200	-2.77298900
H	-4.04439300	3.88187900	0.08448600
H	-5.07501800	2.56365900	-0.53556100
H	-4.67754600	2.66287300	1.21345700
H	-5.58378100	0.50419500	1.80817200
H	-5.85711100	0.29646900	0.05172800
H	-5.81263600	-1.12893300	1.11479700
C	-5.31877800	-0.96599000	-3.39714400
H	-4.68239700	-1.66322100	-1.46856400
C	-4.64015800	1.27545000	-3.99393600
H	-3.43075100	2.30864400	-2.54039600
C	-5.31186000	0.09105600	-4.31075300
H	-5.83613500	-1.89223000	-3.63283600
H	-4.63157700	2.10274800	-4.69916700
H	-5.82564100	-0.00668800	-5.26352000
C	8.11840500	1.53496000	-2.63100700
H	8.45051400	2.50486800	-3.02048600
H	8.63543600	1.35306400	-1.68186900
H	8.42967200	0.76035700	-3.34209400
C	6.58699100	1.50170600	-2.44668900
C	6.15660200	0.10206400	-1.94643900
C	6.18966200	2.55958500	-1.43950200
C	4.74596100	0.08086700	-1.34177600
H	6.86868700	-0.22798000	-1.17753400
H	6.22805600	-0.61899400	-2.76978800
C	5.32059300	2.37707200	-0.42981600
H	6.65949400	3.53577200	-1.56639000
C	4.62240300	1.09208400	-0.21908400
H	4.46747500	-0.90411800	-0.96669800
H	3.99368800	0.34958300	-2.09343700
H	5.09912500	3.16708200	0.28379600
C	5.91535400	1.83930100	-3.79948400
H	6.18097300	2.85094900	-4.12766600
H	6.24797500	1.13434200	-4.57068700
H	4.82536500	1.78491500	-3.73175400
O	3.97223700	0.88643400	0.80276700
C	4.13869000	-3.08074500	1.27873600
C	3.36127100	-2.90315500	2.64260200
O	3.25130400	-2.43685800	0.32151600
O	2.51424900	-1.75111300	2.38119000
C	5.47111300	-2.32143300	1.24124500
H	6.19700900	-2.75403300	1.93705200
H	5.88991900	-2.38067700	0.23149200
H	5.32219400	-1.26647600	1.48615000
C	4.34408300	-4.52627700	0.83296200

H	4.86001800	-4.53944100	-0.13275500
H	4.95833100	-5.07430300	1.55608700
H	3.39159300	-5.04719300	0.71345500
C	2.43170700	-4.07871200	2.96806100
H	2.99448700	-5.00073400	3.14440900
H	1.86283700	-3.84951400	3.87372300
H	1.71869000	-4.23965600	2.15612500
C	4.24018700	-2.58078000	3.84901300
H	3.60761200	-2.44187100	4.73175500
H	4.93780800	-3.40067900	4.05371800
H	4.81027100	-1.66215600	3.69524100
B	2.41500400	-1.59795100	1.02276200

C	2.53790300	0.69022700	-3.93708400
H	-1.99843100	1.48585700	-3.56201600
H	-1.69883200	3.21090600	-3.22020000
H	-0.50612000	2.27994100	-4.17137400
H	-0.71216000	-2.28290800	-3.46630200
H	-1.22318400	-1.54953500	-1.90924300
H	-1.95884800	-0.99698700	-3.41728500
C	3.36830000	3.26178200	-3.23281900
H	1.80447600	3.19950700	-1.76158500
C	3.60633000	1.29032900	-4.61122500
H	2.20642100	-0.30415800	-4.21443700
C	4.02390700	2.57723000	-4.26081400
H	3.68664500	4.26127500	-2.94810100
H	4.10600500	0.75478000	-5.41471000
H	4.85431900	3.04299000	-4.78516000
P	2.71603700	-0.50121300	-0.16900800
O	3.51621600	0.91638900	-0.32275400
O	2.87315300	-1.32436700	-1.57414000
C	3.86048900	-1.42323900	0.94412100
C	4.81443500	1.08046500	-0.90732000
C	4.07635400	-1.83611900	-2.16722200
C	3.95581100	-2.82226800	0.88577300
C	4.66282100	-0.72582800	1.86205200
H	5.11976000	2.10255300	-0.67557000
H	5.53922600	0.37559100	-0.48535100
H	4.75199800	0.96317600	-1.99156700
H	4.31087800	-1.22900400	-3.04519200
H	4.91934000	-1.82714200	-1.47180800
H	3.87230700	-2.86751900	-2.46687400
C	4.81094800	-3.51049500	1.74746900
H	3.38144700	-3.37799900	0.15708300
C	5.52378700	-1.41525000	2.71630400
H	4.59580000	0.35411600	1.91829700
C	5.59387400	-2.81018500	2.66748300
H	4.86415100	-4.59405400	1.69117900
H	6.13864700	-0.86186400	3.42098400
H	6.26062200	-3.34648200	3.33719800
C	-3.71105000	2.83022300	3.75452800
H	-4.49471100	2.40404700	4.39333300
H	-2.74022000	2.55977900	4.18390700
H	-3.80621000	3.92248600	3.78744300
C	-3.83783000	2.32094700	2.30717600
C	-2.74608400	2.96422400	1.42789300
C	-3.67284800	0.81904400	2.27385600
C	-2.61785900	2.30693500	0.05416000
H	-1.79552500	2.88010300	1.95351700
H	-2.95986700	4.03425200	1.29985300
C	-3.08526200	0.12925500	1.28454600
H	-4.15155400	0.26332800	3.08213200
C	-2.53238700	0.78140600	0.07815000
H	-1.78390400	2.70487800	-0.51982500
H	-3.52107300	2.48619800	-0.54232000
H	-3.08304000	-0.94971800	1.26472100
C	-5.25043700	2.65413300	1.76980600
H	-6.02327300	2.19425900	2.39816400
H	-5.41226500	3.74001200	1.77722600
H	-5.38152900	2.27622000	0.75241000
O	-2.76087600	0.22308500	-1.09148900
C	-6.36467800	-0.29019700	-1.14603100
C	-5.81565900	-1.69494200	-0.64979700
O	-5.19663300	0.52374800	-1.16027700
O	-4.43952900	-1.67198200	-1.02478300
C	-6.94424400	-0.34379000	-2.57570900
H	-7.88237000	-0.90857000	-2.62115900
H	-7.14133600	0.68174300	-2.90704000
H	-6.23339400	-0.78952200	-3.27616700
C	-7.41209100	0.34092700	-0.22435200
H	-7.71214200	1.31637900	-0.62418200
H	-8.30697100	-0.28966600	-0.15771800
H	-7.02162200	0.49890400	0.78243200
C	-5.90983500	-1.86643800	0.87628300
H	-6.94533800	-2.00481400	1.20979200

TS VII-XII

E = -5397.210579

G_{corr} = 1.005622

Co	0.57853100	-0.00677500	0.16425600
H	-1.04765100	0.50703100	0.29403600
P	1.12354600	1.46209900	1.68494400
O	2.36958300	1.09150800	2.73262500
O	-0.06530300	1.86511600	2.76707300
C	1.75608400	3.10657200	1.16485100
C	2.14716400	-0.03548700	3.59360400
C	0.19411600	2.84971000	3.78441500
C	0.84233300	4.00037200	0.58568400
C	3.11176300	3.45655600	1.22111800
H	1.81433300	-0.90855700	3.02314400
H	3.09969800	-0.25955400	4.07524100
H	1.39652500	0.20670800	4.35393400
H	0.01138500	3.85539800	3.39235400
H	-0.49653700	2.64416500	4.60464800
H	1.22424300	2.78177200	4.14618300
C	1.27590000	5.22246500	0.06976900
H	-0.20769700	3.73613500	0.52286600
C	3.54668000	4.67403500	0.69368400
H	3.82299300	2.77296000	1.66948200
C	2.63217200	5.55834400	0.11437500
H	0.55741100	5.90599500	-0.37434800
H	4.60139900	4.93366100	0.73675500
H	2.97344000	6.50451500	-0.29684400
P	-0.08805800	-2.02018700	0.75883100
O	-1.60775100	-2.32299800	0.21548500
O	-0.17918500	-2.41328600	2.37667900
C	0.78669000	-3.55515500	0.24499200
C	-2.30912200	-3.54881800	0.47454000
C	-0.91374300	-1.54161300	3.24459900
C	1.11243700	-3.67588100	-1.11505300
C	1.10823900	-4.60081100	1.12220000
H	-3.27627100	-3.41835300	-0.00961500
H	-1.77069300	-4.40340900	0.04914600
H	-2.43294400	-3.70404300	1.55271500
H	-0.81699900	-0.49507700	2.93991800
H	-1.97411600	-1.81633400	3.24485800
H	-0.50648800	-1.67130000	4.25090500
C	1.76704300	-4.81487300	-1.58657900
H	0.89200100	-2.86062100	-1.79350400
C	1.77081500	-5.73641000	0.65057000
H	0.85051700	-4.51583400	2.17176900
C	2.10519300	-5.84433400	-0.70210700
H	2.01690200	-4.89651300	-2.64111300
H	2.02658100	-6.53685100	1.33981600
H	2.62389000	-6.72702500	-1.06648400
P	0.45171800	0.65825600	-1.97131600
O	-0.58644200	1.92944900	-2.10379200
O	0.00904200	-0.39173000	-3.15940000
C	1.87636800	1.37252900	-2.90859200
C	-1.22900400	2.23285400	-3.34863100
C	-1.03543700	-1.36438200	-2.96649900
C	2.30218100	2.66322800	-2.56166600

H	-5.33576100	-2.75262800	1.17004400
H	-5.48806100	-1.00384300	1.39236300
C	-6.48853900	-2.90436800	-1.31483400
H	-6.05632300	-3.82951700	-0.91499400
H	-7.56788700	-2.92327900	-1.11844100
H	-6.32958300	-2.90247400	-2.39591200
B	-4.09931400	-0.35625500	-1.57850600
H	-3.91725500	-0.39349000	-2.79539000

H	-1.06313900	-3.32843700	3.24134400
H	-0.32436300	1.54236100	3.49310900
H	-1.08595700	1.09851100	1.91830100
H	-1.92850500	0.72526100	3.41425300
C	3.05306800	-4.13506100	2.76997700
H	1.46436500	-3.89962400	1.33816900
C	3.36686900	-2.29960900	4.31427100
H	2.02201300	-0.63111700	4.07478800
C	3.73867100	-3.56399400	3.84539700
H	3.33710200	-5.11550400	2.39710900
H	3.89102300	-1.85465200	5.15637300
H	4.55874400	-4.09966800	4.31635300
P	3.04501000	0.41806500	0.46088400
O	3.68146400	-1.09034300	0.47357300
O	3.12029900	1.05406600	1.97317500
C	4.32401500	1.36526400	-0.45371700
C	4.95819900	-1.47061200	1.00983800
C	4.31403500	1.25987500	2.74733100
C	4.46229000	2.74669700	-0.24881600
C	5.07869600	0.74172700	-1.46074100
H	5.22270900	-2.41743900	0.53404200
H	5.72924900	-0.72426100	0.79125000
H	4.86797000	-1.62395300	2.08716700
H	4.47610200	0.39199500	3.39308600
H	5.18938300	1.42256200	2.11107300
H	4.14636400	2.14882900	3.36004300
C	5.34650500	3.48936600	-1.03222000
H	3.88138900	3.24290500	0.52060500
C	5.96623700	1.48610500	-2.23872800
H	4.95548400	-0.32082500	-1.64519700
C	6.10091600	2.86141400	-2.02656300
H	5.43978900	4.55863100	-0.86506400
H	6.54999300	0.99362300	-3.01171700
H	6.78874500	3.44085300	-2.63621100
C	-3.96500500	-1.20523200	-4.48817400
H	-4.64195600	-0.53112700	-5.02877200
H	-2.93924100	-0.85177800	-4.65269700
H	-4.05856800	-2.20443700	-4.93367700
C	-4.29666400	-1.24165000	-2.98308800
C	-3.35679800	-2.24448400	-2.27127400
C	-4.11099600	0.14231200	-2.39150700
C	-3.30710600	-2.04428900	-0.75250300
H	-2.34358300	-2.11221200	-2.66899100
H	-3.66501300	-3.26991400	-2.52069100
C	-3.47059400	0.40309500	-1.24700100
H	-4.58932000	0.95861400	-2.93828000
C	-2.78833800	-0.64138900	-0.39515100
H	-2.65473400	-2.79100300	-0.28756600
H	-4.29900800	-2.14414700	-0.30344700
H	-3.41603800	1.41162500	-0.85960000
C	-5.77442300	-1.65899500	-2.80456800
H	-6.44565300	-0.92498000	-3.26850300
H	-5.96468500	-2.63362500	-3.27390500
H	-6.03656700	-1.72404300	-1.74443400
O	-2.84176500	-0.38881200	0.98722900
C	-6.36478300	0.26568900	1.53388500
C	-5.73639700	1.72813300	1.42997200
O	-5.28736400	-0.58455300	1.19442900
O	-4.33946500	1.51757300	1.56253300
C	-6.84310300	-0.08415600	2.96065900
H	-7.71363300	0.50712200	3.26875100
H	-7.12146900	-1.14411900	2.98067800
H	-6.04217100	0.06246900	3.68956800
C	-7.52125400	0.00211100	0.56095300
H	-7.87504500	-1.02796600	0.68815800
H	-8.36653900	0.67672500	0.74574700
H	-7.20090100	0.11724500	-0.47717300
C	-6.00797700	2.39891500	0.06942100
H	-7.06333600	2.67230900	-0.05395600
H	-5.41108900	3.31673500	0.00235700
H	-5.71586600	1.74623100	-0.75405900
C	-6.20597700	2.69053000	2.53465300

XII³

E = -5397.255153

G_{Corr} = 0.999779

Co	0.78179300	0.16675000	-0.07435100
H	-1.70964500	-0.60900300	-0.65886100
P	1.15635200	-1.24372900	-1.86456400
O	2.47158100	-0.87252000	-2.80539300
O	-0.07561800	-1.34720300	-2.95461000
C	1.55604900	-2.98964300	-1.51946500
C	2.46768200	0.43889300	-3.39729900
C	0.04216600	-2.15449700	-4.14382400
C	0.48862700	-3.86034500	-1.24662900
C	2.87449600	-3.45552100	-1.42820400
H	2.20334000	1.20350300	-2.65903500
H	3.47778300	0.62697500	-3.76156100
H	1.75811300	0.47981500	-4.23098900
H	0.04095400	-3.21815400	-3.88866100
H	-0.82925500	-1.92306200	-4.75753400
H	0.95997000	-1.90981600	-4.68712200
C	0.74063100	-5.18992400	-0.90609600
H	-0.53389100	-3.49752300	-1.29210100
C	3.12163700	-4.78395000	-1.07829500
H	3.69822300	-2.77974500	-1.62714500
C	2.05733600	-5.65267900	-0.81986300
H	-0.08922500	-5.86033300	-0.70140000
H	4.14530600	-5.14192100	-1.00880600
H	2.25297900	-6.68639500	-0.54822500
P	0.07346000	2.28901600	-0.75603500
O	-1.35748800	2.42316500	-0.00066500
O	-0.12529200	2.81874700	-2.29774100
C	1.05666900	3.68905800	-0.11619300
C	-2.14432200	3.62388100	0.14031200
C	-0.88646500	1.99346000	-3.20736500
C	1.28639300	3.70390100	1.26972500
C	1.61370500	4.68966700	-0.92231500
H	-3.02146700	3.30736500	0.70761200
H	-1.57624100	4.39034500	0.67845100
H	-2.43612400	4.00376200	-0.84437900
H	-0.56726600	0.94859800	-3.15729800
H	-1.95181300	2.04366700	-2.96888300
H	-0.70483600	2.39259300	-4.20733300
C	2.05427800	4.71698100	1.84344300
H	0.87544600	2.91630800	1.89489800
C	2.38963100	5.69817600	-0.34559100
H	1.43760300	4.67790300	-1.99270300
C	2.60911500	5.71482200	1.03439400
H	2.22385900	4.72545300	2.91650100
H	2.82139900	6.47196000	-0.97435500
H	3.21252300	6.50127800	1.47925000
P	0.29095500	-1.26067400	1.76870300
O	-0.74243400	-2.45191600	1.35877800
O	-0.28553300	-0.47230600	3.07413100
C	1.61508500	-2.18608100	2.63842100
C	-1.62119100	-3.02883100	2.34664700
C	-0.94196500	0.81119000	2.95972800
C	1.99561000	-3.45036500	2.16928100
C	2.31377200	-1.60975000	3.70918100
H	-2.39993300	-2.30345400	2.59078900
H	-2.06344500	-3.91043400	1.87864700

H	-5.72542300	3.66688700	2.39511300
H	-7.29275600	2.84324900	2.50990000
H	-5.92814500	3.22284400	3.52574100
B	-4.04965400	0.04776600	1.69510800
H	-3.82007600	-0.23208100	2.89089800

XIII³

E = -4985.141958

G_{Corr} = 0.814076

Co	-0.09186400	-0.23221700	-0.29148800
H	-2.42402000	-0.47490900	-0.81258300
P	-0.61171200	0.52390200	1.82807500
O	0.47611900	0.15803600	3.03122500
O	-2.04125900	-0.00776200	2.44920400
C	-0.69752100	2.32868700	2.09910500
C	0.75107200	-1.24020800	3.21778000
C	-2.49763600	0.35525400	3.76373900
C	-1.86405600	2.99317300	1.68877000
C	0.37392000	3.06696200	2.61906000
H	0.99281700	-1.72500400	2.26614700
H	1.61283100	-1.30896200	3.88248900
H	-0.10975000	-1.74510800	3.67036200
H	-3.43580400	-0.18159100	3.91617500
H	-1.76720900	0.05743400	4.52276200
H	-2.67460200	1.43297200	3.83101900
C	-1.96117300	4.37989000	1.81355900
H	-2.68953700	2.42845500	1.26654100
C	0.27702000	4.45467200	2.73249600
H	1.27649400	2.55519400	2.93213100
C	-0.88970200	5.11282000	2.33248900
H	-2.86857600	4.88685900	1.49772800
H	1.11112700	5.02250300	3.13618500
H	-0.96287600	6.19326100	2.42232700
P	-0.14130700	-2.57308100	-0.39971800
O	-1.00789500	-3.01909700	-1.71710700
O	-0.67192800	-3.52198900	0.83404200
C	1.45111400	-3.44404400	-0.67556700
C	-1.20964000	-4.40276200	-2.05445000
C	-1.94635200	-3.22060400	1.44535600
C	2.10026900	-3.23105300	-1.90340600
C	2.04012200	-4.28783000	0.27523500
H	-1.91496000	-4.41362300	-2.88687900
H	-0.26652000	-4.86971800	-2.35857100
H	-1.63211700	-4.95016600	-1.20623600
H	-1.96190300	-2.20191800	1.83983800
H	-2.75724900	-3.32988100	0.72080100
H	-2.06737000	-3.93929700	2.25900500
C	3.31065000	-3.86685400	-2.18087600
H	1.65442700	-2.57702900	-2.64756100
C	3.25464000	-4.91944300	-0.00305300
H	1.54118600	-4.45929400	1.22310400
C	3.88965100	-4.71405000	-1.22984200
H	3.79987600	-3.70385100	-3.13724600
H	3.70365600	-5.57332500	0.73948100
H	4.83244400	-5.20953400	-1.44510500
P	-0.41763500	1.64798700	-1.72821700
O	-1.84712800	2.37607300	-1.45122200
O	-0.30554500	1.18885200	-3.29286500
C	0.70462800	3.09826200	-1.85247900
C	-2.64391100	2.91072200	-2.53213700
C	-0.50906700	-0.21772100	-3.60233100
C	0.51381300	4.19134800	-0.99624600
C	1.78986300	3.10296900	-2.74034400
H	-3.35906100	3.59494400	-2.06855900
H	-2.02214700	3.46207600	-3.24703400
H	-3.15263000	2.05820100	-2.99373300
H	-0.38539900	-0.30120900	-4.68555500
H	0.26973000	-0.81337000	-3.10941200

H	-1.52734500	-0.50607800	-3.29079500
C	1.38806300	5.27834600	-1.03497100
H	-0.31944200	4.19280600	-0.30290400
C	2.65947300	4.19606800	-2.78462500
H	1.93947800	2.25919600	-3.40529300
C	2.46038500	5.28625100	-1.93161000
H	1.22796200	6.11946200	-0.36544300
H	3.48709100	4.19955900	-3.48967900
H	3.13779000	6.13557100	-1.96560500
P	2.22155400	0.24312000	-0.04450600
O	2.24215200	1.78908200	0.49827400
O	2.91691700	0.18030900	-1.53423800
C	3.49765000	-0.53009100	1.03129000
C	3.37689200	2.66402600	0.57479500
C	4.24357700	0.62727400	-1.86274700
C	4.23646200	-1.63374800	0.58157200
C	3.66255500	-0.09061900	2.35563500
H	3.13552500	3.41583100	1.32941700
H	4.28526900	2.12852200	0.87011500
H	3.51970800	3.15735800	-0.38854300
H	4.20719400	1.67918600	-2.15981600
H	4.93585900	0.49892800	-1.02493400
H	4.58367800	0.02014500	-2.70501800
C	5.13317200	-2.27837700	1.43481500
H	4.10855400	-1.99370200	-0.43327600
C	4.56017300	-0.73569600	3.20666400
H	3.07444800	0.74443600	2.72180800
C	5.29869200	-1.83060400	2.74735500
H	5.69413900	-3.13479600	1.07209300
H	4.68277000	-0.38440100	4.22771300
H	5.99607900	-2.33391800	3.41146600
C	-5.66490200	-2.22825300	1.88321900
H	-6.21974100	-3.17182200	1.79709500
H	-4.65136100	-2.46304100	2.23114700
H	-6.15401600	-1.62059300	2.65661800
C	-5.62642900	-1.47237000	0.53865300
C	-4.83664500	-0.15498900	0.71803500
C	-4.94213000	-2.33413100	-0.50760200
C	-4.37559900	0.45719200	-0.60780200
H	-3.94877200	-0.36457300	1.32222400
H	-5.44731800	0.55785100	1.29376400
C	-3.96105600	-1.91015500	-1.31539100
H	-5.31652900	-3.35870000	-0.59024500
C	-3.43351200	-0.47792400	-1.41674100
H	-3.86776900	1.41248600	-0.44287200
H	-5.23422200	0.66003400	-1.26236200
H	-3.52334000	-2.59030100	-2.04337900
C	-7.07950300	-1.19062900	0.09355600
H	-7.62479300	-2.12687500	-0.08230500
H	-7.62134800	-0.62470700	0.86349100
H	-7.10193700	-0.61301200	-0.83626600
O	-3.27315600	-0.10832600	-2.69555200

XIII³ Sep

E = -800.2350086

G_{Corr} = 0.342194

H	1.18798400	0.53726500	-1.86087000
C	5.15021200	-1.09612800	-0.43049200
H	5.37733100	-2.00139000	0.14784800
H	4.90905000	-1.40273100	-1.45530600
H	6.05957300	-0.48088700	-0.46340300
C	3.98100300	-0.31191600	0.19962900
C	3.71878500	0.97286500	-0.62531100
C	2.73460300	-1.18063800	0.20525100
C	2.33573600	1.57654900	-0.35852700
H	3.78898800	0.72190600	-1.69410700
H	4.51489600	1.70398100	-0.42455900
C	1.52985000	-0.78808500	-0.22269900
H	2.86806000	-2.18936200	0.60427800

C	1.21786100	0.60182700	-0.75255000	H	-0.70220900	-5.09418900	0.06218400
H	2.20708400	2.52028200	-0.90288800	H	-1.48734800	-2.37137000	2.39267100
H	2.21094100	1.80600100	0.70774700	H	-1.52818600	-4.12550400	2.12743300
H	0.67258300	-1.45612200	-0.19384200	H	-0.44612500	-3.44961800	3.37950500
C	4.35933800	0.04439300	1.65582200	C	2.77330300	-3.10598700	-2.86411800
H	4.49078500	-0.86405300	2.25747700	H	1.16149600	-1.72791700	-2.50100600
H	5.30055800	0.61006500	1.68882500	C	3.26533700	-4.64813900	-1.06917200
H	3.57904100	0.64712900	2.13177900	H	1.98935400	-4.50577200	0.66468000
O	-0.00573100	1.07776400	-0.26758000	C	3.54658000	-4.14852800	-2.34288600
C	-3.03991500	0.53351500	0.47864900	H	2.98603100	-2.71092000	-3.85440800
C	-2.82952800	-0.87745400	-0.18610700	H	3.85891200	-5.46149000	-0.65929000
O	-2.39434000	1.40120700	-0.43714900	H	4.36177700	-4.56866800	-2.92641500
O	-1.54872500	-0.76869300	-0.77411000	P	-0.36367000	0.79470800	-1.88287500
C	-4.50536800	0.96054400	0.62190400	O	-1.60373000	1.88727400	-2.04326300
H	-5.07052000	0.24886300	1.23794700	O	-0.46163400	-0.07830400	-3.30670500
H	-4.56018300	1.94449300	1.10374200	C	1.03612600	1.84411400	-2.49116500
H	-4.99090300	1.04044000	-0.35462200	C	-1.96574500	2.42421400	-3.31603200
C	-2.34784700	0.63757300	1.85486600	C	-1.37027900	-1.17788700	-3.43999200
H	-2.35913700	1.68770500	2.16952800	C	1.07180700	3.20180300	-2.14111500
H	-2.85131100	0.03963900	2.62583700	C	2.09950800	1.30712400	-3.22919200
H	-1.30390400	0.32686000	1.77160300	H	-2.66199200	3.24498900	-3.12145800
C	-2.83851800	-2.05364100	0.79836500	H	-1.09654700	2.81199300	-3.86005700
H	-3.79085800	-2.11784400	1.34151200	H	-2.46298200	1.66530900	-3.93027000
H	-2.69409200	-2.99495300	0.25351700	H	-1.04266800	-1.74334300	-4.31775100
H	-2.02666800	-1.96038300	1.52474800	H	-1.35722700	-1.81965300	-2.55718000
C	-3.85921200	-1.14431100	-1.30429700	H	-2.39197400	-0.81654500	-3.58992000
H	-3.53276500	-2.02024400	-1.87676500	C	2.13851400	4.01041500	-2.53641100
H	-4.86856700	-1.33853500	-0.91839000	H	0.26246400	3.62548500	-1.55606200
H	-3.89992300	-0.28855100	-1.98508300	C	3.17209000	2.11332800	-3.61851800
B	-1.23647900	0.68288600	-1.00034300	H	2.08949400	0.25737700	-3.49973500
H	-1.08729500	0.93319800	-2.21113800	C	3.19297000	3.46898800	-3.27697800

XIV

$$E = -5008.574472$$

$$G_{\text{Corr}} = 0.810602$$

Co	-0.29144500	-0.19017500	0.05774500	C	3.36121000	2.54332100	0.41362200
P	-0.94879800	1.16206000	1.60203800	C	4.22885700	-0.31528100	-0.83744400
O	-0.22394000	1.08935300	3.10713000	C	3.18583400	-1.59066800	2.04134600
O	-2.56110800	1.17042500	2.02153200	C	2.88567600	0.59009700	3.03718700
C	-0.70501300	2.97505600	1.36220900	H	3.21487400	3.56769900	0.76552600
C	-0.14939000	-0.20410800	3.71599500	H	4.10979300	2.04755700	1.04238900
C	-3.05127000	2.01090700	3.07130500	H	3.69633300	2.56668000	-0.62623800
C	-1.56544200	3.62905200	0.46754900	H	4.56495000	0.49823700	-1.48801500
C	0.30397200	3.71100100	1.99637100	H	4.69656200	-0.22233600	0.14760200
H	0.26257900	-0.93452200	3.01427200	H	4.50597600	-1.27643200	-1.27963900
H	0.51383300	-0.11250000	4.57839500	C	3.77526200	-2.04858100	3.22015800
H	-1.14213600	-0.53411800	4.04601800	H	3.08525700	-2.26308400	1.19736100
H	-4.08768800	1.71080900	3.24722800	C	3.47996500	0.13402000	4.21509500
H	-2.46935400	1.87444100	3.98867600	H	2.52411800	1.60982000	2.97478100
H	-3.02178900	3.06732300	2.78141900	C	3.92171800	-1.18798600	4.31167500
C	-1.40427100	4.98920700	0.19579800	H	4.12242500	-3.07652800	3.28419900
H	-2.34422400	3.06621400	-0.03480100	H	3.59357800	0.81036900	5.05830100
C	0.47043600	5.06921000	1.71897200	H	4.37953600	-1.54460300	5.23051000
H	0.95763300	3.21874500	2.70643600	B	-2.23222000	-0.67903000	-0.06148300
C	-0.37905500	5.71119600	0.81329800	O	-2.92705500	-1.37984300	0.91973800
H	-2.07623400	5.48304800	-0.50162400	O	-3.09379700	-0.35596700	-1.10214500
H	1.26098000	5.62795000	2.21409400	C	-4.28315800	-1.62675800	0.48588500
H	-0.24792800	6.76827000	0.59661700	C	-4.45944000	-0.60085000	-0.69688800
P	-0.00586400	-2.31255700	0.05210700	C	-5.21108800	-1.39789800	1.67835500
O	-1.21745900	-3.20544600	-0.68400400	C	-4.35809000	-3.09044800	0.03445400
O	0.20655000	-3.18672600	1.46336400	C	-5.23129800	-1.12996300	-1.90509900
C	1.44759500	-3.05211400	-0.82820100	C	-5.04009000	0.75156800	-0.26048400
C	-1.10195200	-4.62192900	-0.84122200	H	-6.26278300	-1.49296000	1.38417500
C	-0.88149300	-3.27888100	2.39072800	H	-5.00475800	-2.14669700	2.45104200
C	1.73542700	-2.55969400	-2.10934300	H	-5.05197400	-0.40976500	2.11493800
C	2.21427500	-4.11057000	-0.32020900	H	-4.04058200	-3.73255800	0.86264800
H	-2.10981400	-5.00026700	-1.03111600	H	-5.37646500	-3.37250800	-0.25445900
H	-0.45110200	-4.86870500	-1.68775600	H	-3.68083300	-3.26663500	-0.80242300
				H	-6.26095100	-1.38667300	-1.63060300

H	-5.26827500	-0.35702100	-2.68033900
H	-4.75266600	-2.01366800	-2.33325900
H	-4.97348400	1.44899000	-1.10235900
H	-6.09105200	0.66619500	0.03687100
H	-4.46072700	1.16364600	0.56820600

XV

E = -798.9498486

G_{Corr} = 0.320432

C	5.46665600	0.11381300	-0.51961700
H	6.16327300	0.04691300	0.32531300
H	5.58879800	-0.78854700	-1.13024800
H	5.75772100	0.97954900	-1.12754500
C	4.01508400	0.25514500	-0.02401000
C	3.06508300	0.33969500	-1.24529600
C	3.63254000	-0.94571500	0.81374400
C	1.57371600	0.26763600	-0.87038300
H	3.29519000	-0.49815500	-1.91632700
H	3.26269800	1.26303600	-1.80410200
C	2.33704900	-1.44321400	0.82729000
H	4.38933800	-1.38553800	1.45877600
C	1.32340300	-0.87904000	0.06465600
H	0.96218900	0.14441500	-1.77392000
H	1.23660900	1.20872400	-0.41392600
H	2.08048700	-2.28947200	1.46090100
C	3.90182300	1.53774500	0.83698800
H	4.57643100	1.48531300	1.69956500
H	4.17069400	2.42483500	0.24796800
H	2.88465300	1.67313200	1.21909400
O	0.07117100	-1.44818300	0.13116800
C	-2.63673200	0.90669500	0.25455300
C	-3.32549600	-0.42834700	-0.22159700
O	-1.22330500	0.61349600	0.04588500
O	-2.30313600	-1.42500600	0.06857900
C	-2.99994800	2.14617400	-0.55609300
H	-4.07554400	2.34431400	-0.49278900
H	-2.46837100	3.01624800	-0.15760300
H	-2.72512000	2.03280000	-1.60703300
C	-2.81313800	1.17438700	1.75341100
H	-2.14216700	1.98639300	2.04967800
H	-3.84063600	1.46803200	1.99004900
H	-2.55797200	0.28847100	2.34359600
C	-4.59772600	-0.80008500	0.53273200
H	-5.36016900	-0.02376500	0.40517200
H	-4.99793300	-1.73996200	0.13945200
H	-4.40679800	-0.93313100	1.59980500
C	-3.56720400	-0.47171400	-1.73506000
H	-3.84721500	-1.49032000	-2.01990700
H	-4.37247000	0.20722300	-2.03276400
H	-2.66048500	-0.20102400	-2.28575600
B	-1.10434000	-0.75619400	0.07791800

XVI

E = -4204.979099

G_{Corr} = 0.635653

Co	0.37972100	-0.08108600	-0.28760600
P	0.54587200	1.04188700	1.47371100
O	0.40360700	2.70182500	1.50879900
O	1.89694800	0.80175500	2.41524100
C	-0.79610600	0.63911100	2.65625700
C	1.12382200	3.40796300	0.48753700
C	2.02523700	1.44244700	3.69065700
C	-0.82371000	-0.66436200	3.17821600
C	-1.82766800	1.53069200	2.97697100
H	1.07252800	2.87111600	-0.46584500
H	0.65267200	4.38702300	0.37996100

H	2.17620800	3.52582000	0.77129500
H	3.03515600	1.22553500	4.04738400
H	1.89097700	2.52578700	3.60151300
H	1.29312000	1.04571400	4.40361500
C	-1.87071400	-1.06727800	4.00833400
H	-0.03882700	-1.36697100	2.90906000
C	-2.87872000	1.12233300	3.80143200
H	-1.80067600	2.54153500	2.58424700
C	-2.90400000	-0.17652800	4.31633000
H	-1.88462900	-2.07788800	4.40837000
H	-3.67641600	1.81982500	4.04460400
H	-3.72328000	-0.49313300	4.95646800
P	0.08117400	-2.12858400	-0.55752400
O	0.65109700	-2.95102400	0.76714200
O	0.62235300	-3.05343300	-1.83460900
C	-1.66717700	-2.71204300	-0.60711100
C	0.54786100	-4.37869700	0.84417700
C	1.77044600	-2.60110400	-2.55623900
C	-2.42408000	-2.66867700	0.57268800
C	-2.30599400	-3.02965400	-1.81357200
H	1.05426400	-4.67799600	1.76492100
H	-0.49979100	-4.70036000	0.88316100
H	1.03676800	-4.85174800	-0.01389800
H	1.80948900	-3.17523100	-3.48590800
H	1.68721700	-1.53173600	-2.78765100
H	2.68505500	-2.76681600	-1.97772200
C	-3.79211200	-2.94202400	0.55009600
H	-1.94479800	-2.40206000	1.50850000
C	-3.67585400	-3.30036100	-1.83834200
H	-1.72862500	-3.05716300	-2.73138100
C	-4.42318200	-3.25501000	-0.65707800
H	-4.36469800	-2.90153700	1.47326200
H	-4.15992300	-3.54951200	-2.77950200
H	-5.48990600	-3.46347500	-0.67810900
P	-1.52636300	0.65364800	-1.04874000
O	-2.79715900	0.44401400	-0.03203600
O	-1.89591500	-0.02515300	-2.51098000
C	-1.63496300	2.44458400	-1.45605600
C	-4.17471500	0.71511600	-0.31278500
C	-3.04825700	0.26745400	-3.31051800
C	-1.06239200	2.92204700	-2.64561200
C	-2.12675900	3.36316100	-0.51735100
H	-4.65583200	0.91103100	0.64899500
H	-4.29872300	1.59030200	-0.96006100
H	-4.63515100	-0.16394800	-0.77357700
H	-3.86913700	-0.40015600	-3.03019200
H	-3.36353400	1.31191100	-3.21120000
H	-2.77214100	0.07866400	-4.35131500
C	-0.98960200	4.29354400	-2.89413300
H	-0.67690700	2.21722000	-3.37780400
C	-2.06039700	4.73424900	-0.76947700
H	-2.55323400	3.00180500	0.41264700
C	-1.48907200	5.20212700	-1.95627000
H	-0.54598900	4.65304200	-3.81874300
H	-2.44916600	5.43735800	-0.03766800
H	-1.43197300	6.26994900	-2.14914200
B	2.29758400	-0.32524100	-0.19156600
O	2.94089300	0.76253500	-0.79568100
O	3.22024500	-1.28601500	0.18866300
C	4.34779800	0.44621200	-0.96286700
C	4.55399400	-0.72285500	0.07303000
C	5.15408000	1.71146500	-0.67348500
C	4.55379100	0.02176000	-2.42173800
C	5.50603900	-1.82565200	-0.38467500
C	4.95166500	-0.23073600	1.47067800
H	6.23040800	1.50576200	-0.70142300
H	4.93207100	2.46981800	-1.43194200
H	4.90156500	2.12745900	0.30444800
H	4.20814600	0.82814500	-3.07683300
H	5.60860100	-0.17525300	-2.64114900
H	3.97608700	-0.87496300	-2.65723000
H	6.51423500	-1.42686600	-0.54575100

H	5.56491500	-2.60160600	0.38561400
H	5.16514600	-2.29529500	-1.31053400
H	4.90493700	-1.07532600	2.16583000
H	5.96958000	0.17362700	1.48293700
H	4.25147400	0.53012200	1.82235400

CoP₄^T

E = -4596.968604

G_{Corr} = 0.629992

Co	0.13542200	-0.67986700	-0.65087300
P	-0.98284100	-1.98299600	0.90927000
O	-0.42669600	-1.93181600	2.46278900
O	-0.98672400	-3.58187700	0.51039200
C	-2.73372500	-1.61092700	1.26464100
C	0.96972900	-2.19885100	2.68226900
C	-1.57020500	-4.57021900	1.38910800
C	-3.71574500	-2.11874700	0.39904600
C	-3.10729200	-0.75273600	2.30890900
H	1.59142300	-1.69705100	1.93426300
H	1.21625200	-1.81131000	3.67080400
H	1.15749000	-3.27713700	2.65132200
H	-1.32179600	-5.54326000	0.96293300
H	-1.14959300	-4.48546600	2.39557300
H	-2.65649000	-4.45163800	1.43683800
C	-5.05738600	-1.78164100	0.58537300
H	-3.43069100	-2.76761500	-0.42308800
C	-4.44906400	-0.41259500	2.48727500
H	-2.35059400	-0.35250700	2.97312200
C	-5.42524100	-0.92557500	1.62793300
H	-5.81285000	-2.18329000	-0.08380800
H	-4.73348400	0.25084400	3.29927600
H	-6.46884900	-0.65922200	1.76959900
P	2.31139700	-1.45350300	-1.03027800
O	2.37044800	-2.09556000	-2.54420600
O	3.10051800	-2.53543400	-0.08044600
C	3.54388700	-0.11445600	-1.04034100
C	3.63580100	-2.43949300	-3.15253000
C	2.52942200	-3.85486400	0.04925500
C	3.16436800	1.06555000	-1.70128400
C	4.79732700	-0.19456600	-0.41865500
H	3.39872700	-2.93919300	-4.09256400
H	4.22317700	-1.53641800	-3.34637600
H	4.20483200	-3.11490200	-2.50632100
H	1.44116500	-3.81083200	0.16339200
H	2.77866100	-4.45770600	-0.82976300
H	2.97802500	-4.30043000	0.93840500
C	4.03522400	2.15401900	-1.74690200
H	2.17783200	1.14397600	-2.15149600
C	5.66080700	0.90195600	-0.45572700
H	5.08635100	-1.10442700	0.09638200
C	5.28298500	2.07306900	-1.11967400
H	3.73763400	3.06474600	-2.25841400
H	6.62917800	0.84238000	0.03261300
H	5.95820400	2.92357700	-1.14492900
P	-1.59219900	0.21970900	-1.98364000
O	-2.72794700	-0.90156800	-2.35140300
O	-1.04371000	0.80620500	-3.42079900
C	-2.52585500	1.68620600	-1.44331700
C	-3.83948900	-0.59245200	-3.22296700
C	-0.12817500	-0.00421500	-4.18291100
C	-3.60711700	1.50955500	-0.56706400
C	-2.11207800	2.98165100	-1.78528900
H	-4.30311900	-1.54697000	-3.47576300
H	-4.56105200	0.04748900	-2.70768100
H	-3.48994900	-0.09627400	-4.13316900
H	0.39635900	0.66842900	-4.86394400
H	0.59780200	-0.51010900	-3.53506900
H	-0.67842500	-0.75515300	-4.75931700
C	-4.28541200	2.61769100	-0.06075700

H	-3.92019900	0.51213800	-0.27983000
C	-2.79262400	4.08838700	-1.27264400
H	-1.26901500	3.12213100	-2.45267300
C	-3.88124700	3.90838400	-0.41363400
H	-5.12573900	2.46957700	0.61137000
H	-2.47786800	5.09045700	-1.55080100
H	-4.40972000	4.77149500	-0.01855600
P	0.38357400	1.19387300	0.72382800
O	-1.06165600	1.43399600	1.45091300
O	0.71689300	2.46599400	-0.25393400
C	1.56640500	1.38417600	2.10806700
C	-1.45453500	2.62918600	2.14842200
C	0.89228200	3.83523600	0.15531200
C	2.89397500	1.76636800	1.85737400
C	1.19114800	1.01068200	3.40884300
H	-2.31421700	2.35650000	2.76354300
H	-0.65027300	3.00526400	2.78897000
H	-1.75729100	3.39071600	1.42628300
H	-0.03866500	4.37907500	-0.02713700
H	1.17359700	3.91310400	1.20935000
H	1.69232200	4.25277000	-0.46061900
C	3.82765200	1.78104500	2.89397100
H	3.19888000	2.05551500	0.85763300
C	2.12662100	1.03208100	4.44397000
H	0.17199500	0.69212100	3.60607500
C	3.44634500	1.41527800	4.18771900
H	4.85201600	2.07774100	2.68779900
H	1.82621100	0.74882800	5.44887100
H	4.17464300	1.42759600	4.99358600

XVII

E = -411.3780814

G_{Corr} = 0.148196

C	0.00000000	0.78759600	-0.15405800
C	0.00000000	-0.78759600	-0.15405800
O	0.32897600	1.10229400	1.25287800
O	-0.32897600	-1.10229400	1.25287800
C	1.05439600	1.43429300	-1.04441700
H	0.88793000	1.16245100	-2.09285900
H	0.98934900	2.52351000	-0.95977800
H	2.06410400	1.13115900	-0.75991600
C	-1.37811800	1.39972500	-0.41950900
H	-1.33783000	2.47198800	-0.20616800
H	-1.67889400	1.26392800	-1.46338900
H	-2.14017800	0.95265800	0.22602800
C	-1.05439600	-1.43429300	-1.04441700
H	-0.88793000	-1.16245100	-2.09285900
H	-0.98934900	-2.52351000	-0.95977800
H	-2.06410400	-1.13115900	-0.75991600
C	1.37811800	-1.39972500	-0.41950900
H	1.33783000	-2.47198800	-0.20616800
H	1.67889400	-1.26392800	-1.46338900
H	2.14017800	-0.95265800	0.22602800
B	0.00000000	0.00000000	1.97638400

XVIII

E = -4597.536952

G_{Corr} = 0.640895

Co	0.21532300	0.10948000	-0.55174000
H	0.68290000	0.46905900	-1.93701700
P	0.80577100	2.26194700	-0.48382300
O	0.36369400	3.32200400	0.69495800
O	0.23248300	3.07682900	-1.76853800
C	2.62417800	2.44369100	-0.56409000
C	0.70949500	3.13852300	2.08151300

C	0.52173900	4.47752200	-1.96199500
C	3.36928600	1.49474300	-1.28474400
C	3.28643700	3.52408300	0.04119300
H	-0.21187600	3.17841400	2.66465300
H	1.20924900	2.18320700	2.26297200
H	1.37515500	3.95165600	2.38369700
H	0.08107900	4.74145100	-2.92398300
H	0.07199000	5.07460200	-1.16477300
H	1.60266300	4.64966400	-1.99212300
C	4.75636800	1.61455600	-1.37854000
H	2.86498400	0.66691800	-1.77487400
C	4.67407600	3.63958300	-0.05495100
H	2.71971000	4.27899600	0.57526700
C	5.41041900	2.68304200	-0.75917600
H	5.32390600	0.87412500	-1.93494000
H	5.17913700	4.47793100	0.41605200
H	6.49050700	2.77398200	-0.83003800
P	-1.82258900	0.14079700	-1.70247800
O	-1.53132000	-0.73909000	-3.04940300
O	-2.30172800	1.55154000	-2.41234600
C	-3.44009400	-0.48084400	-1.07755100
C	-2.49234500	-0.88632900	-4.11398900
C	-2.78194600	2.65081700	-1.62655700
C	-3.47040700	-1.33792600	0.03157600
C	-4.65246500	-0.11119700	-1.68634500
H	-1.98882300	-1.45736800	-4.89519900
H	-3.37444500	-1.43400000	-3.76638200
H	-2.78862700	0.09225500	-4.50022300
H	-2.05646200	2.95085500	-0.86633100
H	-2.92638300	3.48237800	-2.31833000
H	-3.73878800	2.40276900	-1.15210700
C	-4.68300400	-1.82517000	0.52090400
H	-2.54377000	-1.62773200	0.51063700
C	-5.86517200	-0.59665700	-1.19611500
H	-4.64399100	0.56114400	-2.53871000
C	-5.88215000	-1.45423300	-0.09209700
H	-4.69189200	-2.48911500	1.38083400
H	-6.79622800	-0.30497200	-1.67363400
H	-6.82753700	-1.82853400	0.29017600
P	1.10866200	-1.89240600	-1.18594800
O	2.02198700	-1.65265700	-2.51929700
O	0.29512100	-3.25427000	-1.57927300
C	2.31570500	-2.54823300	0.02769600
C	2.82979500	-2.71855400	-3.06613900
C	-1.07039600	-3.50789400	-1.21025800
C	3.38185700	-1.72658700	0.42713200
C	2.19289800	-3.83412500	0.57171100
H	3.34425600	-2.29260900	-3.92834100
H	3.56244400	-3.06625800	-2.33048500
H	2.19609800	-3.55099800	-3.38309300
H	-1.73630300	-2.78379700	-1.68018100
H	-1.29916100	-4.50843000	-1.58204800
H	-1.19014000	-3.48151200	-0.12450300
C	4.32685500	-2.19673300	1.33867000
H	3.47993900	-0.72254100	0.02705100
C	3.13215900	-4.29592800	1.49725000
H	1.37483600	-4.47473600	0.25965800
C	4.20262400	-3.48158100	1.87602800
H	5.15614800	-1.55924300	1.63222400
C	3.03384900	-5.29488700	1.91274400
H	4.93664600	-3.84591800	2.58914400
P	-0.18686200	-0.41097300	1.58842800
O	1.21170400	-0.27157200	2.43974300
O	-0.65423800	-1.97753300	1.77373900
C	-1.35680300	0.58482900	2.57069400
C	1.72777700	-1.25287200	3.35679200
C	-1.35317200	-2.51879200	2.91385600
C	-2.29741100	1.36150600	1.88205300
C	-1.29219400	0.66535900	3.97186000
H	2.77741100	-1.00377800	3.50873800
H	1.20073400	-1.20888900	4.31614200
H	1.65774400	-2.25616200	2.93139100

H	-1.63255200	-3.53622600	2.63576900
H	-0.70857100	-2.54686700	3.79642300
H	-2.25086800	-1.93350300	3.13216800
C	-3.17319900	2.19649200	2.57532900
H	-2.32693800	1.32595700	0.80133500
C	-2.16630900	1.50082400	4.66561400
H	-0.55152700	0.09547100	4.52235700
C	-3.10791700	2.26635200	3.96869200
H	-3.89453100	2.79650200	2.02853600
H	-2.10939300	1.56179300	5.74841100
H	-3.78274600	2.92094500	4.51245800

XIX

$$E = -387.5145578$$

$$G_{\text{Corr}} = 0.146287$$

C	-2.51843100	0.22669400	-0.79679800
H	-3.11489200	1.05141200	-0.38217400
H	-2.31055600	0.46256100	-1.84790800
H	-3.13857900	-0.68144000	-0.76456500
C	-1.20695500	0.05029400	-0.00609700
C	-0.38013800	-1.09439600	-0.64573600
C	-0.38325800	1.31800700	-0.05155600
C	1.03333400	-1.22742900	-0.05511600
H	-0.28781200	-0.87923900	-1.72031000
H	-0.93077500	-2.04543000	-0.56023200
C	1.02027100	1.27540400	-0.01779200
H	-0.91280600	2.26744600	0.03615600
C	1.80963600	0.10040200	-0.01794100
H	1.62174600	-1.94896600	-0.64049900
H	0.97692600	-1.65217000	0.96231200
H	1.57576100	2.21633300	0.00972800
C	-1.57224700	-0.32125100	1.45550300
H	-2.18069100	0.47144700	1.91079200
H	-2.14357400	-1.26251200	1.51155000
H	-0.66846900	-0.43202200	2.06310200
O	3.08755600	0.05827800	0.02940600

XX

$$E = -5008.438823$$

$$G_{\text{Corr}} = 0.806435$$

Co	-0.37620000	-0.13423100	0.17487500
P	-1.12419700	1.79475400	1.12989200
O	-0.95711700	1.77184400	2.76675400
O	-2.71641600	2.10123900	0.88095600
C	-0.37382400	3.43107100	0.82161400
C	-1.39752000	0.59060800	3.46842400
C	-3.41210800	3.10087400	1.65480900
C	-0.85983200	4.20516000	-0.24428900
C	0.68642400	3.91566600	1.59990200
H	-0.69754800	-0.22864700	3.29301700
H	-1.39801600	0.84547800	4.52942700
H	-2.39971000	0.29365200	3.14793000
H	-4.43645500	3.11422300	1.27944900
H	-3.40892300	2.83240100	2.71477500
H	-2.95868600	4.08756800	1.52356300
C	-0.26680400	5.43123300	-0.54842700
H	-1.69081000	3.84162000	-0.83662500
C	1.27687500	5.14166300	1.29233100
H	1.04799900	3.33607100	2.43987900
C	0.81038400	5.89532400	0.21127500
H	-0.64655900	6.02237800	-1.37671300
H	2.09775100	5.51168400	1.90033300
H	1.27595500	6.84683200	-0.02938000
P	-0.24548200	-2.38499500	-0.11220400
O	-1.48844200	-2.98580700	-1.00447900
O	-0.24328000	-3.25898400	1.26934400
C	1.20975100	-3.18315200	-0.89134100

C	-1.57849600	-4.39441900	-1.30315400
C	-0.97336700	-2.86170100	2.44707900
C	1.54676600	-2.82357600	-2.20409200
C	1.98515200	-4.14027900	-0.22089300
H	-2.55812200	-4.54449900	-1.75983700
H	-0.79168600	-4.68824100	-2.00391500
H	-1.50151300	-4.98866900	-0.38787000
H	-1.68626300	-2.06677500	2.22579500
H	-1.51227100	-3.74239700	2.80546500
H	-0.25158800	-2.54093200	3.20315900
C	2.65613600	-3.39404900	-2.82769300
H	0.95727700	-2.08895500	-2.73895800
C	3.09847500	-4.70626400	-0.84695700
H	1.71347000	-4.44760600	0.78237800
C	3.43987700	-4.33104000	-2.14842700
H	2.90928900	-3.10514300	-3.84409100
H	3.69364500	-5.44558700	-0.31826500
H	4.30663500	-4.77135200	-2.63316200
P	0.03764100	0.70204900	-1.99426200
O	-0.96066200	1.97616200	-2.27002000
O	-0.09361400	-0.21310500	-3.36412200
C	1.70768600	1.36649000	-2.35307400
C	-0.86997500	2.75564800	-3.47960900
C	-1.33099700	-0.88690900	-3.68070000
C	2.06143900	2.61413600	-1.81758700
C	2.67399600	0.61330300	-3.03517000
H	-1.82317700	3.27765600	-3.58223600
H	-0.05513100	3.48135900	-3.40268600
H	-0.70703000	2.11053900	-4.34768700
H	-1.14261200	-1.42851300	-4.61008300
H	-1.61846400	-1.57495600	-2.88563500
H	-2.13307600	-0.15924300	-3.82780200
C	3.35651000	3.10823700	-1.97719300
H	1.33167300	3.19962400	-1.27134600
C	3.97168500	1.10532900	-3.18499900
H	2.41558100	-0.35449200	-3.44799200
C	4.31604100	2.35355200	-2.65741000
H	3.61258900	4.08097700	-1.56644300
H	4.71240800	0.51600700	-3.71865000
H	5.32573500	2.73626100	-2.77856300
P	1.78885100	0.04466000	0.89193400
O	2.29437800	1.58788000	1.03260800
O	2.77472600	-0.75546200	-0.11880400
C	2.16819800	-0.65582200	2.53963300
C	3.62670300	1.99716200	1.38479600
C	4.19808800	-0.93637900	-0.00557000
C	2.53469500	-2.00316500	2.67467000
C	1.94545000	0.11845500	3.68984500
H	3.54752700	3.03313500	1.72025400
H	4.03665600	1.38031600	2.19089300
H	4.26875200	1.95226100	0.50180400
H	4.69504200	-0.19282700	-0.63360100
H	4.53967300	-0.85063400	1.03024600
H	4.41057200	-1.94014700	-0.37889700
C	2.67678100	-2.56803800	3.94288100
H	2.70858700	-2.60674000	1.79115200
C	2.08920000	-0.44888500	4.95626800
H	1.64698600	1.15815100	3.59278500
C	2.45171800	-1.79313500	5.08429600
H	2.96408500	-3.61115900	4.03958200
H	1.91762900	0.15636000	5.84178900
H	2.56020400	-2.23462300	6.07074700
B	-2.33129000	-0.45042400	-0.07536500
O	-3.10748500	-0.86804500	0.98630000
O	-3.04417000	-0.32150200	-1.23273700
C	-4.45170000	-1.17234400	0.50571700
C	-4.45363800	-0.57608700	-0.96792100
C	-5.44133500	-0.51358200	1.46481600
C	-4.59255200	-2.69634200	0.56870600
C	-4.95244200	-1.54035800	-2.04402200
C	-5.16852400	0.77161300	-1.10249600
H	-6.47374500	-0.67728300	1.13828500

H	-5.32646900	-0.95202000	2.46154000
H	-5.26306000	0.56066000	1.54477100
H	-4.46544200	-3.02155900	1.60643800
H	-5.57732900	-3.02642000	0.22384600
H	-3.82066600	-3.17963100	-0.03277700
H	-6.00449500	-1.79895200	-1.88374200
H	-4.86475600	-1.06265500	-3.02505500
H	-4.36136500	-2.45849700	-2.06223100
H	-5.02562300	1.14629400	-2.12108300
H	-6.24328400	0.67961100	-0.91715800
H	-4.74303400	1.50360200	-0.41464100

VIIoEt

E = -4911.79625

G_{corr} = 0.847746

Co	0.06726800	-0.55453400	-0.29585000
P	-1.07860600	-1.47851700	1.31163900
O	-0.78850300	-1.19424500	2.93365900
O	-0.99925800	-3.14066700	1.21169700
C	-2.89366500	-1.20654100	1.44014300
C	0.54016400	-1.40928700	3.43291800
C	-1.67808500	-3.99356400	2.15767900
C	-3.74207200	-1.89184000	0.55589900
C	-3.43725200	-0.23267400	2.28929800
H	1.25317500	-0.79893000	2.86629000
H	0.81136300	-2.46318200	3.29859400
H	-1.79006800	-3.46972600	3.11343700
H	-2.68048600	-4.21941100	1.77524100
C	-5.10722000	-1.60551100	0.51914200
H	-3.32450400	-2.62826700	-0.12188600
C	-4.80274600	0.05793000	2.24772200
H	-2.78743900	0.30179300	2.97162500
C	-5.64078200	-0.62373000	1.36040100
H	-5.75289100	-2.14167800	-0.17186400
H	-5.21248100	0.81811900	2.90838800
H	-6.70221300	-0.39279700	1.32498500
P	2.09831700	-1.20312700	-0.74565000
O	2.09431700	-2.32885100	-1.98284200
O	3.11951100	-1.93026900	0.36559700
C	3.32434600	0.05595300	-1.30569900
C	3.25145700	-2.71663700	-2.74702600
C	2.62184300	3.07302100	1.07647100
C	2.84464900	1.10803200	-2.10092500
C	4.67670700	0.04877300	-0.92665500
H	2.85154300	-3.07741100	-3.70078800
H	3.87140900	-1.83615100	-2.95563000
H	1.54739800	-2.95817500	1.25733800
H	2.75692600	-3.96777000	0.45558300
C	3.69602300	2.13920200	-2.50178100
H	1.79107600	1.14612900	-2.35253000
C	5.52527100	1.08478700	-1.32120200
H	5.05050500	-0.75529600	-0.30261200
C	5.03664900	2.13324200	-2.10740600
H	3.30739400	2.95515100	-3.10552200
H	6.56732000	1.07691400	-1.01181400
H	5.69715600	2.94296800	-2.40660100
P	-1.26494800	-0.03690300	-1.95450400
O	-2.41093800	-1.23013700	-2.14041200
O	-0.78438200	0.23364800	-3.53637600
C	-2.29214900	1.48608900	-1.83706700
C	-3.48557900	-1.11832900	-3.09249500
C	0.24430800	-0.58848600	-4.11444700
C	-3.36678900	1.49968900	-0.93538500
C	-1.95946000	2.66512200	-2.51726400
H	-4.26330400	-0.46728900	-2.67520200
H	-3.11462100	-0.66076100	-4.01636600
H	0.61071700	-0.02412400	-4.97881000
H	1.06416700	-0.70947100	-3.40337600
C	-4.10085000	2.66662400	-0.72460800

H	-3.62596900	0.59983800	-0.39134400	C	0.08678900	3.04422900	-1.39766300
C	-2.68975800	3.83647600	-2.30064700	C	-1.66237700	0.16785700	-3.54831700
H	-1.12619800	2.66394900	-3.21149300	C	2.16802200	1.74671300	-3.27661400
C	-3.76175000	3.84110200	-1.40358500	C	1.23647400	3.54897000	-0.76762000
H	-4.93256500	2.65599300	-0.02486100	C	-0.98151000	3.90944500	-1.67069500
H	-2.42137700	4.74544500	-2.83347300	H	-1.98716300	-0.40259900	-2.67177200
H	-4.32884100	4.75324900	-1.23554400	H	-2.55288600	0.56712200	-4.04045300
P	0.27252600	1.51791000	0.52179600	H	1.57950800	2.64598200	-3.48304100
O	-1.12424700	2.02945700	1.23995100	H	3.12855300	2.06335400	-2.85800800
O	0.64155300	2.58224800	-0.68707400	C	1.32216900	4.90110900	-0.43397400
C	1.52047900	1.91701700	1.82540200	H	2.05869200	2.88063000	-0.53448200
C	-1.43338700	3.35366300	1.71065500	C	-0.89664100	5.26082500	-1.32808700
C	0.61060200	4.01872300	-0.77336300	H	-1.87633600	3.51898600	-2.14061900
C	2.87691700	2.04033200	1.48118100	C	0.25449800	5.76091300	-0.71227500
C	1.16536100	1.93163200	3.18197100	H	2.21895200	5.28105800	0.04850600
H	-0.52400200	3.86432600	2.05091900	H	-1.72936100	5.92512300	-1.54503300
H	-1.86666600	3.91619700	0.87769000	H	0.31836300	6.81310600	-0.44767100
H	-0.38133500	4.38198300	-0.49479400	P	-0.58653100	-2.30553500	-0.53432800
H	0.73117900	4.21854200	-1.84327100	O	0.04778200	-3.13762000	0.74569700
C	3.84983200	2.18410200	2.46973300	O	0.32936500	-2.82642900	-1.81822700
H	3.17278500	2.03167400	0.43919300	C	-2.04652500	-3.34966600	-0.93789400
C	2.13838200	2.08592400	4.17238800	C	0.57852000	-4.47430700	0.60285400
H	0.12493100	1.80545000	3.46262700	C	1.69820500	-2.35711300	-1.91513800
C	3.48385000	2.20985600	3.81934600	C	-2.80475500	-3.87926600	0.11838500
H	4.89421600	2.27773300	2.18358600	C	-2.43691000	-3.61286500	-2.25824700
H	1.84497700	2.10068100	5.21876500	H	1.66939900	-4.37868700	0.61631900
H	4.24229300	2.32311800	4.58938600	H	0.28230900	-4.90161800	-0.36099800
C	-2.44918500	3.23865400	2.83429300	H	1.70414000	-1.26556000	-1.94235300
H	-3.34156700	2.71718500	2.47617100	H	2.25477600	-2.67737400	-1.03024500
H	-2.03972500	2.67989300	3.68258000	C	-3.91837500	-4.67966100	-0.14086300
H	-2.74027100	4.23624700	3.18277700	H	-2.51154300	-3.67368300	1.14386200
C	1.70427900	4.73338900	0.00887800	C	-3.55786200	-4.40449600	-2.51660300
H	2.69112300	4.36188400	-0.28262100	H	-1.84679200	-3.22044900	-3.07978300
H	1.65603700	5.80680300	-0.21149800	C	-4.29582400	-4.94485900	-1.46063100
H	1.59483800	4.59859800	1.08786900	H	-4.48924300	-5.09660700	0.68482200
C	3.40184400	-3.20121500	2.37365500	H	-3.85140400	-4.60519200	-3.54358800
H	3.05127600	-4.06857900	2.94527200	H	-5.16287700	-5.56750400	-1.66464100
H	4.47036300	-3.33044400	2.16922400	P	-0.47401700	1.04493500	1.90679400
H	3.27812900	-2.30343200	2.98811000	O	1.03825500	1.66901000	1.97121500
C	0.54724000	-1.05793100	4.90974400	O	-0.64606400	0.12674800	3.26827300
H	-0.14361800	-1.70463400	5.46126000	C	-1.47049800	2.47319300	2.51421400
H	1.55404700	-1.18694900	5.32264000	C	1.63965800	2.07732300	3.21977100
H	0.24406000	-0.01838100	5.06156200	C	-0.61603000	-1.31049700	3.11526600
C	-0.85245300	-5.25859000	2.32236200	C	-1.20790800	3.75156200	2.00276200
H	0.14001900	-5.01956500	2.72020900	C	-2.50392200	2.31167600	3.44878800
H	-1.34748200	-5.95135700	3.01269600	H	0.90977800	2.64134600	3.81509700
H	-0.72328900	-5.76114000	1.35785000	H	1.93021100	1.17267900	3.75802000
C	4.07608200	-3.80307100	-2.06840800	H	-1.34206100	-1.59486900	2.34639100
H	4.52248900	-3.42901700	-1.14346000	H	0.37341600	-1.61122600	2.77350700
H	3.44732800	-4.66762500	-1.82956400	C	-1.96358700	4.84949600	2.41729200
H	4.87887000	-4.13504100	-2.73790900	H	-0.40955000	3.89065700	1.28434600
C	-4.02520100	-2.51444400	-3.35144900	C	-3.25979100	3.41059300	3.86399400
H	-4.37805100	-2.96772300	-2.41881000	H	-2.70424000	1.32601700	3.85289600
H	-4.86364900	-2.47473000	-4.05641700	C	-2.99282500	4.68258500	3.34724300
H	-3.24378700	-3.15602800	-3.77178800	H	-1.74608300	5.83270800	2.00823400
C	-0.26793100	-1.95931800	-4.53920700	H	-4.05396200	3.27460200	4.59404100
H	-1.12368800	-1.86453800	-5.21682900	H	-3.58253100	5.53689200	3.66964000
H	0.52770500	-2.50828100	-5.05714600	P	-3.02250400	0.46744800	-0.12403900
H	-0.57654600	-2.54221600	-3.66689000	O	-3.14699800	2.08610200	-0.42929700

TS IX-X^{BS}_{OEt}

E = -5711.328231

G_{Corr} = 1.206303

Co	-0.78057800	-0.06953000	-0.09690300	H	-4.03144800	2.88047100	1.26930700
H	1.72712900	-0.82747300	0.62800600	H	-5.00849600	1.29628200	2.40421000
P	-0.01358100	1.23663600	-1.71414500	H	-5.66582100	0.27132900	1.10664400
O	-0.90706900	1.31873300	-3.11752900	C	-5.98189200	-1.94241900	-1.71679200
O	1.52936900	0.94806200	-2.25229200	H	-4.70737100	-1.95840500	0.01100400
				C	-5.74690000	-0.04307300	-3.19257400

H	-4.30799900	1.44058800	-2.58903100
C	-6.35643500	-1.26080600	-2.87683400
H	-6.44128900	-2.89401200	-1.46761500
H	-6.03292600	0.49324000	-4.09367600
H	-7.11614000	-1.67689600	-3.53313000
C	7.98106300	1.34748100	-2.26343800
H	8.25749000	2.32811200	-2.66990400
H	8.34042800	1.29346300	-1.22951400
H	8.50410800	0.58016700	-2.84788700
C	6.45350900	1.12769900	-2.33303100
C	6.11386600	-0.28673200	-1.80223600
C	5.77442800	2.17626500	-1.48108000
C	4.64899900	-0.44798200	-1.35849900
H	6.75449800	-0.50118800	-0.93700200
H	6.35702400	-1.03440200	-2.56744300
C	4.83691600	1.90674200	-0.52574300
H	6.10468300	3.20412000	-1.62604300
C	4.30816500	0.59168900	-0.32278200
H	4.46304400	-1.44233800	-0.95558100
H	3.96949500	-0.30440500	-2.20995200
H	4.46787000	2.69474600	0.12603400
C	6.00506100	1.27997300	-3.80507600
H	6.15942700	2.30604400	-4.15936000
H	6.58326400	0.60663700	-4.45052000
H	4.94744200	1.03847300	-3.92628400
O	3.59569300	0.37159500	0.72036000
C	4.36157300	-2.46656400	1.99505500
C	3.52582600	-1.91370600	3.21299300
O	3.51880900	-2.15472600	0.87957300
O	2.77053900	-0.84185300	2.64279200
C	5.71714800	-1.75200600	1.83033900
H	6.41987100	-2.03250200	2.62279100
H	6.15513600	-2.04007800	0.86855000
H	5.59936700	-0.66634900	1.83938900
C	4.60149300	-3.97789400	2.00580300
H	5.17276200	-4.26431700	1.11540600
H	5.17439800	-4.28177400	2.88983500
H	3.66003300	-4.53194700	1.99289500
C	2.53802800	-2.95542000	3.75929600
H	3.04634800	-3.79157800	4.25274100
H	1.88173400	-2.47374900	4.49022700
H	1.91667600	-3.34325100	2.94926300
C	4.36848600	-1.36226100	4.36711700
H	3.70656300	-1.00342400	5.16340000
H	5.02145300	-2.13539000	4.79029300
H	4.98501900	-0.52097800	4.04117600
B	2.79352100	-0.94004700	1.20161700
C	-5.15270600	-0.80186100	2.92020000
H	-6.13861800	-0.70645600	3.38909000
H	-5.09114600	-1.77843600	2.42843000
H	-4.38747800	-0.76410700	3.70299200
C	-5.41979800	3.10176300	-0.38866200
H	-5.98875300	3.89313300	0.11425100
H	-5.39673100	3.32294600	-1.46033200
H	-5.95161800	2.15647200	-0.25013200
C	-0.88331700	-0.73292400	-4.49186900
H	-1.52727500	-1.55780500	-4.82019100
H	-0.55286000	-0.18565100	-5.38021500
H	-0.01284800	-1.15948100	-3.98786000
C	2.35491900	0.92832900	-4.54381100
H	2.86098300	-0.01883400	-4.32803700
H	1.39065800	0.70256400	-5.00131500
H	2.96059900	1.48781800	-5.26627300
C	2.85236800	2.92576100	2.88495500
H	3.55164200	2.33309100	2.29052600
H	2.55729500	3.81051600	2.30916700
H	3.35070000	3.25560400	3.80422800
C	-0.96902100	-1.92499100	4.45516100
H	-0.93891600	-3.01835800	4.38194800
H	-0.25892500	-1.61132700	5.22802200
H	-1.97551200	-1.62434400	4.76914500
C	0.08335700	-5.33721000	1.75238600

H	0.31436100	-4.87042700	2.71504600
H	-0.99919400	-5.48368300	1.68928400
H	0.56930200	-6.31960200	1.72067100
C	2.29906900	-2.94704900	-3.17830000
H	3.34566900	-2.63469400	-3.27015400
H	2.26701500	-4.04179000	-3.15025200
H	1.75987400	-2.60992700	-4.07019900

HOEt

E = -4417.627179

G_{Corr} = 0.80798

Co	-0.26057000	0.33158500	-0.08203600
H	-1.36573000	0.84353200	0.79428200
P	1.30153500	-0.36596500	-1.44908200
O	1.85349500	0.73895400	-2.55310200
O	0.81150600	-1.64502900	-2.37347800
C	2.95441300	-0.92095600	-0.87617800
C	0.96338800	1.76364700	-3.04707000
C	1.58507200	-2.10002500	-3.50268700
C	3.12593300	-2.24511700	-0.44510500
C	4.03056900	-0.02672900	-0.78817900
H	1.60332700	2.62383700	-3.26506000
H	0.26277900	2.04664500	-2.25675200
H	1.42664800	-1.40967900	-4.33853300
H	2.65324300	-2.09284800	-3.25433500
C	4.35207800	-2.66488300	0.07281000
H	2.30609900	-2.94924700	-0.52275900
C	5.25838600	-0.45028300	-0.27611100
H	3.90647700	0.99362400	-1.13186800
C	5.42078100	-1.76877100	0.15962600
H	4.46757000	-3.69280900	0.40574500
H	6.08833500	0.24927700	-0.21736800
H	6.37570700	-2.09561800	0.56289900
P	-0.95534800	-1.40317300	0.88783800
O	-2.49802200	-1.86647600	0.42566100
O	-1.09942000	-1.37456900	2.54699400
C	-0.08435800	-3.02899400	0.85592200
C	-3.21845200	-2.87538300	1.16081700
C	-1.65882800	-0.23681900	3.22328800
C	-0.23021900	-3.84964500	-0.27361900
C	0.80189400	-3.41922900	1.87108200
H	-3.76856800	-2.38849500	1.97608300
H	-2.51978400	-3.59099600	1.60875700
H	-2.72079800	-0.14144900	2.95622200
H	-1.14882400	0.67588900	2.90495700
C	0.48880400	-5.04097700	-0.38046000
H	-0.89900100	-3.54630000	-1.07283500
H	1.53221000	-4.60460500	1.75682500
H	0.91075000	-2.79669200	2.75278400
C	1.37803700	-5.41833600	0.63164200
H	0.35872400	-5.67399300	-1.25430000
H	2.21936000	-4.89348900	2.54796700
H	1.94471000	-6.34143800	0.54313000
P	0.84540300	1.82669000	0.90410300
O	2.21292000	1.35185600	1.73295800
O	-0.01975400	2.61118900	2.09529000
C	1.63461300	3.26503200	0.05874000
C	2.16128200	0.09836300	2.43865900
C	0.61514200	3.56966500	2.96262400
C	0.77927000	4.18830000	-0.56424600
C	3.02018300	3.42862200	-0.07525500
H	1.94576900	-0.70669100	1.73017800
H	1.34684300	0.12227600	3.17419000
H	1.63642900	3.24495600	3.19039800
H	0.67219200	4.53661600	2.44646700
C	1.29472100	5.25020300	-1.30643400
H	-0.29841400	4.06683000	-0.47322300
C	3.53811900	4.48422300	-0.83124000
H	3.68771600	2.73136800	0.41871100

C	2.67892400	5.39560100	-1.44942100	H	-0.24865400	-1.81314700	1.78138800
H	0.62019800	5.95978500	-1.77880900	C	-2.32336800	-4.73135300	0.30632000
H	4.61469800	4.59709700	-0.93236400	H	-1.90159400	-3.85279300	-1.61622300
H	3.08331500	6.21529900	-2.03736500	C	-2.13122500	-4.64178800	1.68818800
C	-6.91312100	1.92982600	-0.70542400	H	-1.22249000	-3.51398300	3.29136800
H	-7.13766300	2.39227800	0.26339300	H	-2.91728600	-5.54097800	-0.10946900
H	-6.88322800	2.72310100	-1.46173800	H	-2.57701000	-5.38109700	2.34833700
H	-7.73871400	1.25320900	-0.95573400	P	-1.62023900	0.85739400	0.97580600
C	-5.58215800	1.15830000	-0.65369500	O	-2.01874900	2.45615600	1.22904100
C	-5.29658200	0.52377700	-2.03567400	O	-1.57016000	0.29829600	2.54926600
C	-4.44775200	2.09981400	-0.30853400	C	-3.27102900	0.15182700	0.56464700
C	-3.89844900	-0.09750700	-2.13237100	C	-3.12552700	2.84377500	2.06784600
H	-5.39456900	1.30878800	-2.79720600	C	-0.54096700	0.83905700	3.40143500
H	-6.05991100	-0.23228400	-2.25803600	C	-4.00813400	0.77225000	-0.45784400
C	-3.17800600	1.90881800	-0.71529900	C	-3.77213900	-1.01875400	1.15002200
H	-4.67918800	2.93578000	0.35146100	H	-4.05050100	2.79197100	1.48156300
C	-2.80449000	0.76889400	-1.54825000	H	-3.21623400	2.14329400	2.90543800
H	-3.63350200	-0.34467300	-3.16687100	H	0.27969600	1.23821000	2.79686800
H	-3.83680600	-1.03661700	-1.56700500	H	-0.97900600	1.66882900	3.97232800
H	-2.35976800	2.54403900	-0.38938200	C	-5.21612300	0.22765600	-0.89235900
C	-5.65739900	0.07515800	0.45208600	H	-3.62605200	1.66913200	-0.93675500
H	-5.87086200	0.53131900	1.42598200	C	-4.97646000	-1.57027700	0.70569500
H	-6.45980400	-0.63990300	0.22996600	H	-3.21965700	-1.50003900	1.94741300
H	-4.71252400	-0.46941100	0.53729700	C	-5.69967600	-0.95164900	-0.31672600
O	-1.61735500	0.45401000	-1.73489200	H	-5.77355700	0.71771900	-1.68616000
C	-0.21829800	3.66928800	4.22947700	H	-5.34621300	-2.48603000	1.15980300
H	-0.25481100	2.70044600	4.73949400	H	-6.63491600	-1.38368400	-0.66302500
H	0.21281800	4.40880600	4.91408500	P	1.97983200	0.02023100	0.70694200
H	-1.24424400	3.97146300	3.99264600	O	2.14303300	-1.24225100	1.78567500
C	3.50298200	-0.11152900	3.11575500	O	2.37549200	1.24433100	1.74434000
H	3.50268800	-1.06386200	3.65879600	C	3.51213300	-0.19921300	-0.31967200
H	4.30134500	-0.13989100	2.36890700	C	2.49540200	-2.59422200	1.43615700
H	3.71189000	0.69485800	3.82753500	C	3.37257500	1.21358800	2.78391900
C	-1.49267000	-0.46609300	4.71607600	C	3.38790700	-0.11132500	-1.71265400
H	-1.91652600	0.37542100	5.27615600	C	4.78307200	-0.45064500	0.22606800
H	-1.99728400	-1.38570900	5.03164500	H	1.77226900	-2.99577700	0.72283500
H	-0.43040300	-0.55191500	4.97199200	H	3.48064400	-2.60582500	0.95693800
C	-4.16638300	-3.58011000	0.20470800	H	2.84870300	1.47613900	3.71045400
H	-4.86561700	-2.86780100	-0.24586100	H	3.76535100	0.20152000	2.91205300
H	-3.60255700	-4.06593800	-0.59876200	C	4.50400100	-0.23924700	-2.54249600
H	-4.74666800	-4.34374700	0.73571800	H	2.40209400	0.02380300	-2.14261300
C	0.21389500	1.29307000	-4.28423200	C	5.89982500	-0.58437600	-0.59983400
H	-0.40408500	2.10847800	-4.67986500	H	4.90610400	-0.56157600	1.29832000
H	0.91226500	0.97772100	-5.06736700	C	5.76347300	-0.47200500	-1.98710200
H	-0.44247600	0.45594100	-4.02952400	H	4.38636700	-0.16655800	-3.62039400
C	1.12067800	-3.50381600	-3.84799500	H	6.87489200	-0.78108700	-0.16202500
H	1.65558700	-3.87483500	-4.72971000	H	6.63374300	-0.57513000	-2.62963200
H	1.30745100	-4.18266200	-3.01060500	C	2.19104500	4.47674300	-1.60669600
H	0.04671400	-3.50999800	-4.06390200	H	3.06167000	4.10504200	-1.05221200

TS III-IV_{OEt}

E = -4417.620013

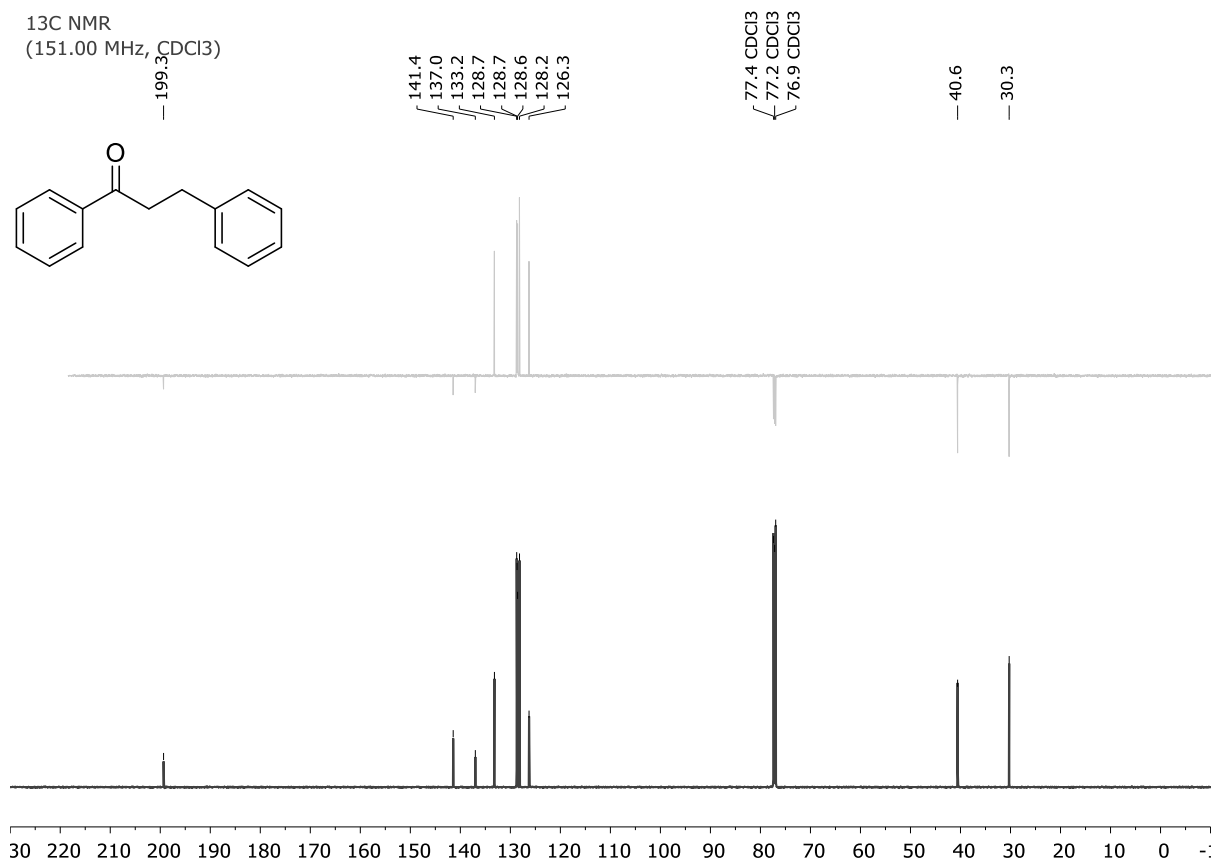
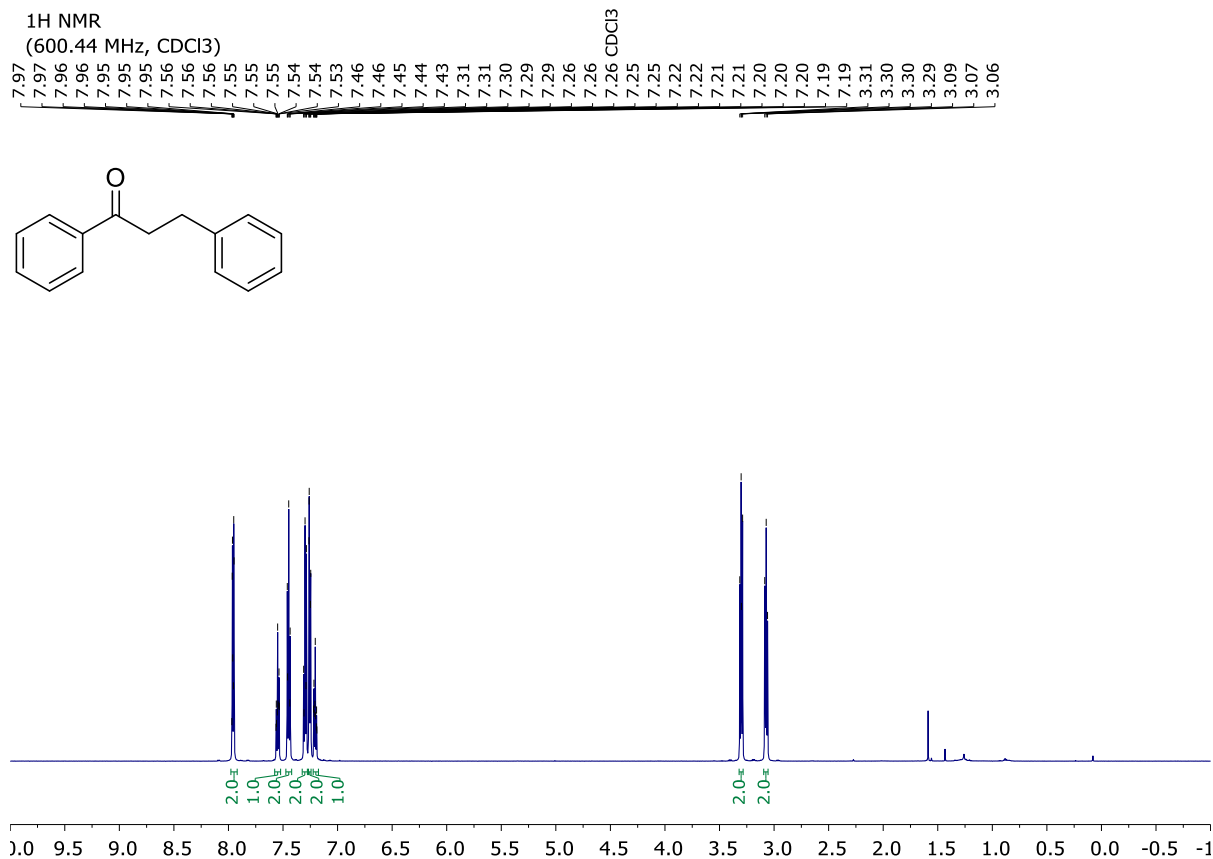
G_{Corr} = 0.817469

Co	0.11620800	0.53776200	-0.27186100	H	2.17569200	5.57013800	-1.52141600
H	0.52096300	1.91838500	0.20903500	C	0.88193400	3.87681300	-1.04729100
P	-0.22022800	-1.44461500	-1.09934600	C	-0.31594000	4.51664100	-1.78989900
O	1.19387500	-2.16647600	-1.54810100	C	0.94006500	2.35436600	-1.35559000
O	-1.04674800	-1.68555900	-2.50650600	C	-1.57308900	3.63852500	-1.75059000
C	-0.99511500	-2.72294800	-0.01818500	H	-0.03949600	4.68276300	-2.84051400
C	1.27151100	-3.47501800	-2.15052600	H	-0.52336500	5.50508200	-1.36087600
C	-2.39630400	-1.16749800	-2.60437700	C	-0.00792200	1.69481400	-2.17870300
C	-0.81076300	-2.64047800	1.36876500	H	1.96528100	2.01008100	-1.44349200
C	-1.75388700	-3.78076300	-0.54309600	C	-1.30263600	2.31801900	-2.45899000
H	0.81066300	-4.21371200	-1.48265100	H	-2.41863400	4.12046000	-2.25197000
H	0.71387200	-3.46936700	-3.09270500	H	-1.85736500	3.43955400	-0.71287100
H	-2.40499200	-0.13753800	-2.25702600	H	0.30156100	0.90947500	-2.86350000
H	-3.05687500	-1.76276700	-1.96206300	C	0.81116100	4.19227600	0.45927300
C	-1.36909600	-3.59687500	2.21758300	H	1.61829900	3.68503300	0.99872400
				H	0.91046300	5.27366400	0.61842300
				H	-0.13711700	3.86053700	0.88903600
				O	-2.11760500	1.85293800	-3.26384500
				C	-0.03620000	-0.25265700	4.33027900
				H	0.51339100	-1.01135900	3.76669000
				H	0.64295000	0.17556100	5.07738400
				H	-0.87172400	-0.72866800	4.85540400

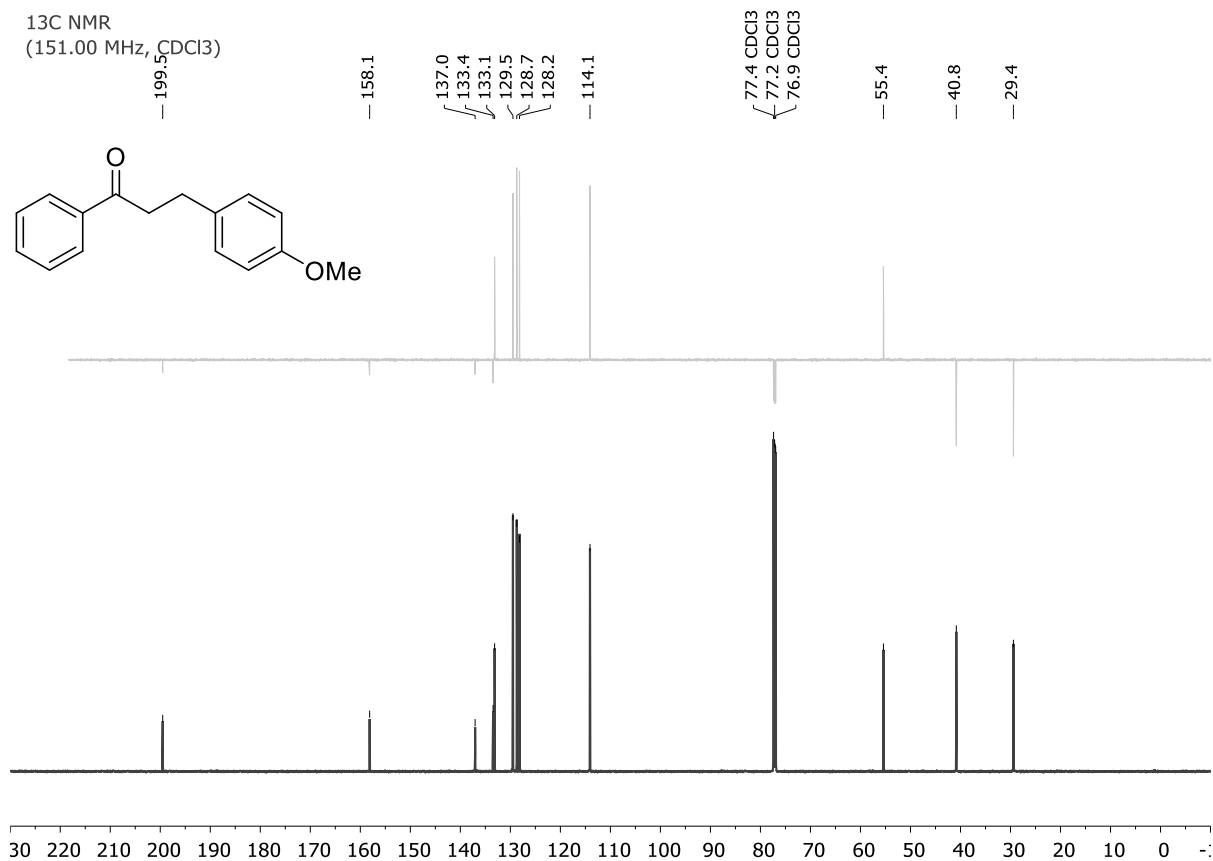
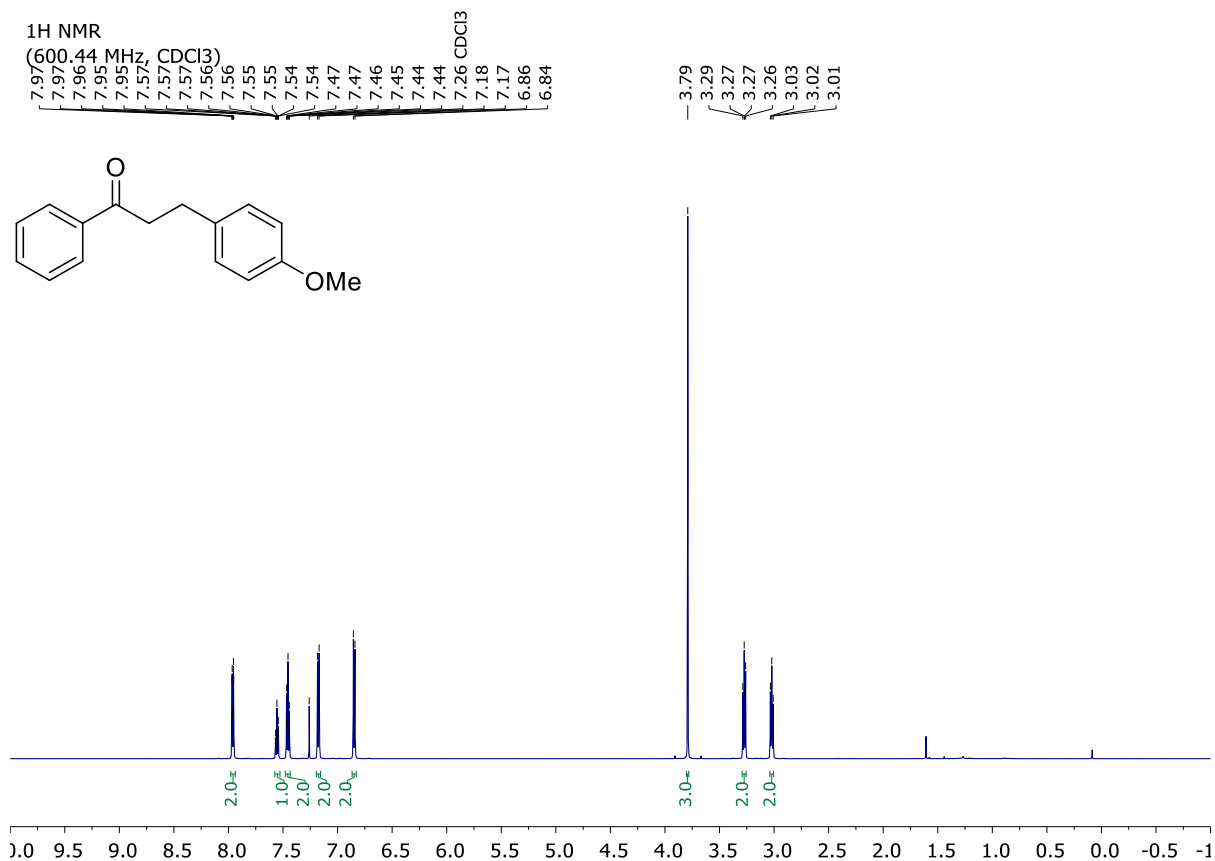
C	-2.86022200	4.25739600	2.55653000	H	3.19994900	-3.02339300	-3.01617300
H	-2.74729800	4.94125200	1.70846700	H	3.28157200	-3.78038600	-1.41767300
H	-3.69142100	4.60843900	3.17859600	C	-2.81897000	-1.23524100	-4.05652100
H	-1.94002900	4.29161000	3.14958200	H	-3.85579500	-0.89403700	-4.15127800
C	4.46750200	2.22400900	2.47897400	H	-2.18596000	-0.57673200	-4.65745400
H	5.19392500	2.25694300	3.29968100	H	-2.75036800	-2.25932200	-4.44092700
H	4.99338400	1.96132700	1.55626900				
H	4.03617000	3.22323500	2.35717600				
C	2.49957700	-3.40594400	2.71865000				
H	2.79691400	-4.43914200	2.50674500				
H	3.20267400	-2.98067100	3.44270700				
H	1.50114300	-3.41870700	3.16692000				
C	2.74315200	-3.78014700	-2.37111200				
H	2.85942300	-4.76351900	-2.84025700				

8. NMR Spectra

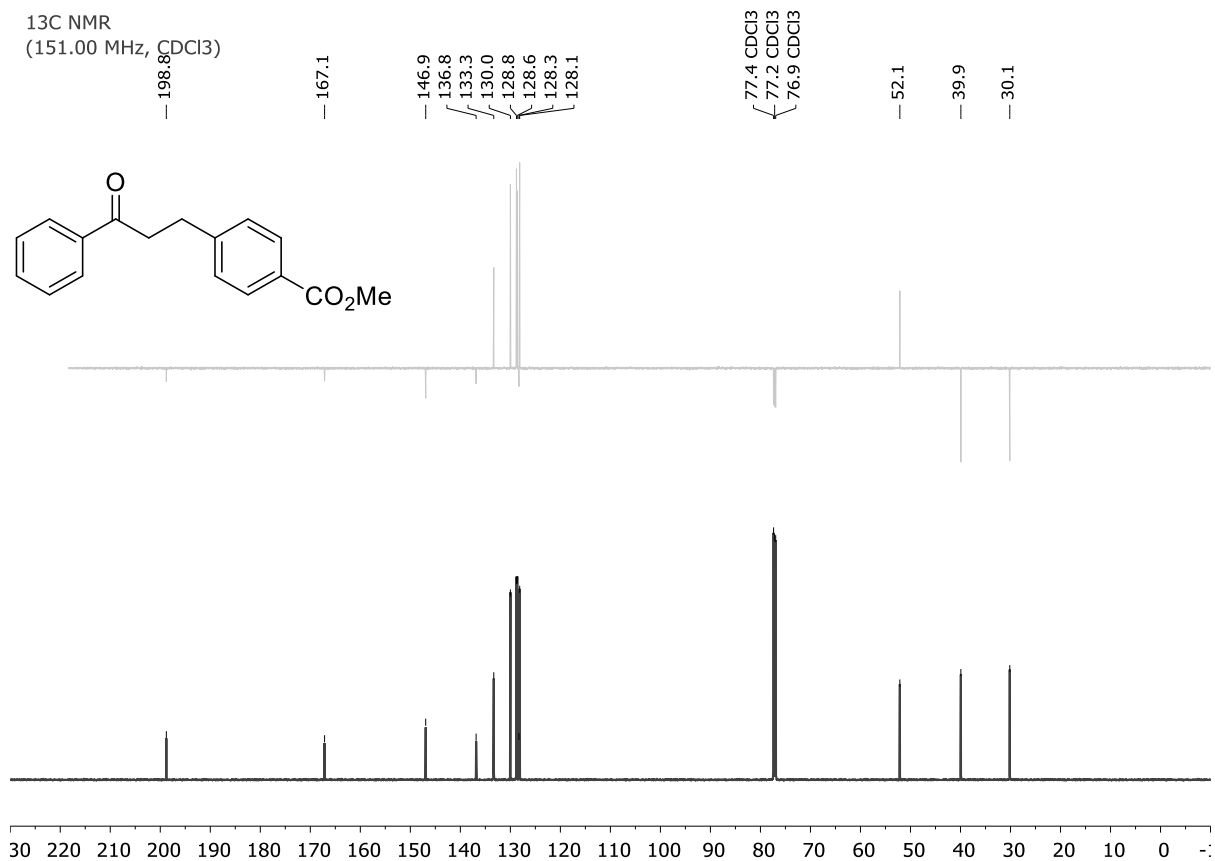
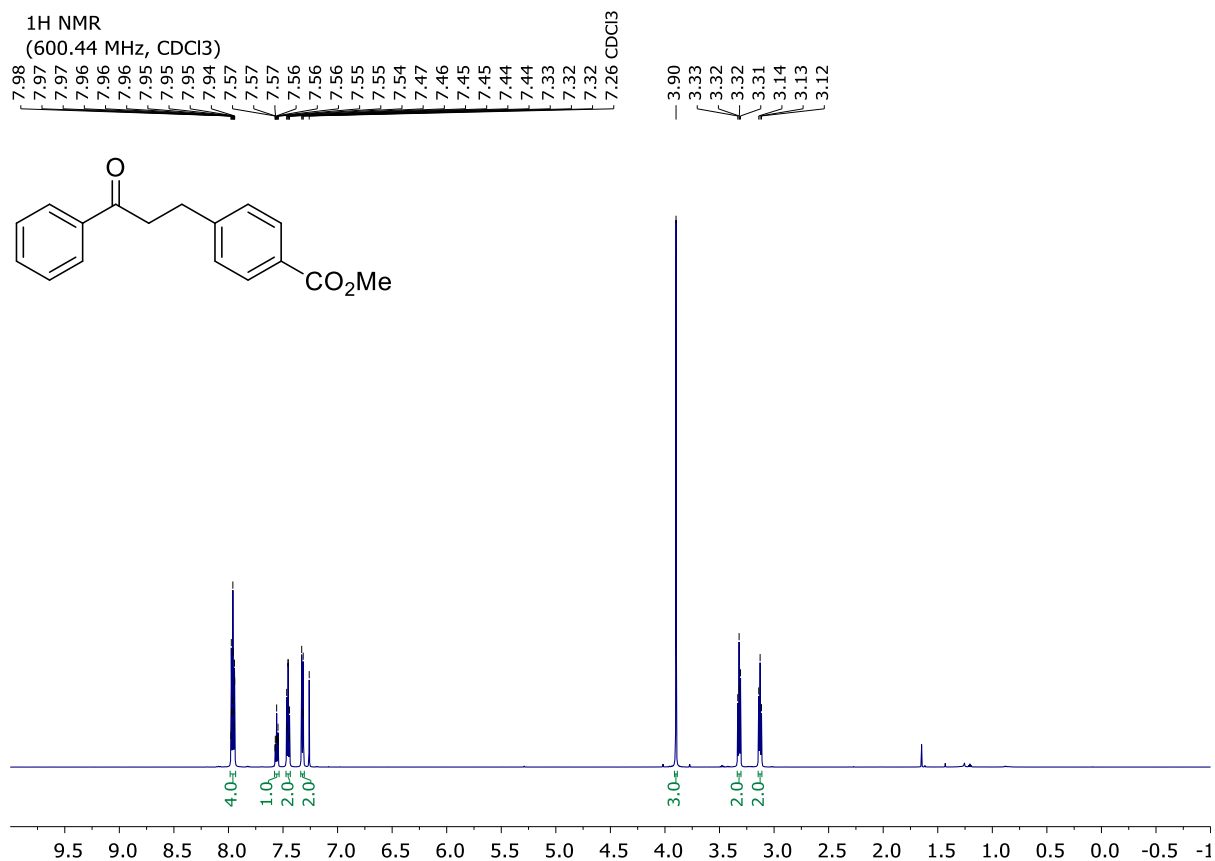
1,3-diphenylpropan-1-one (2a)



3-(4-methoxyphenyl)-1-phenylpropan-1-one (2b)

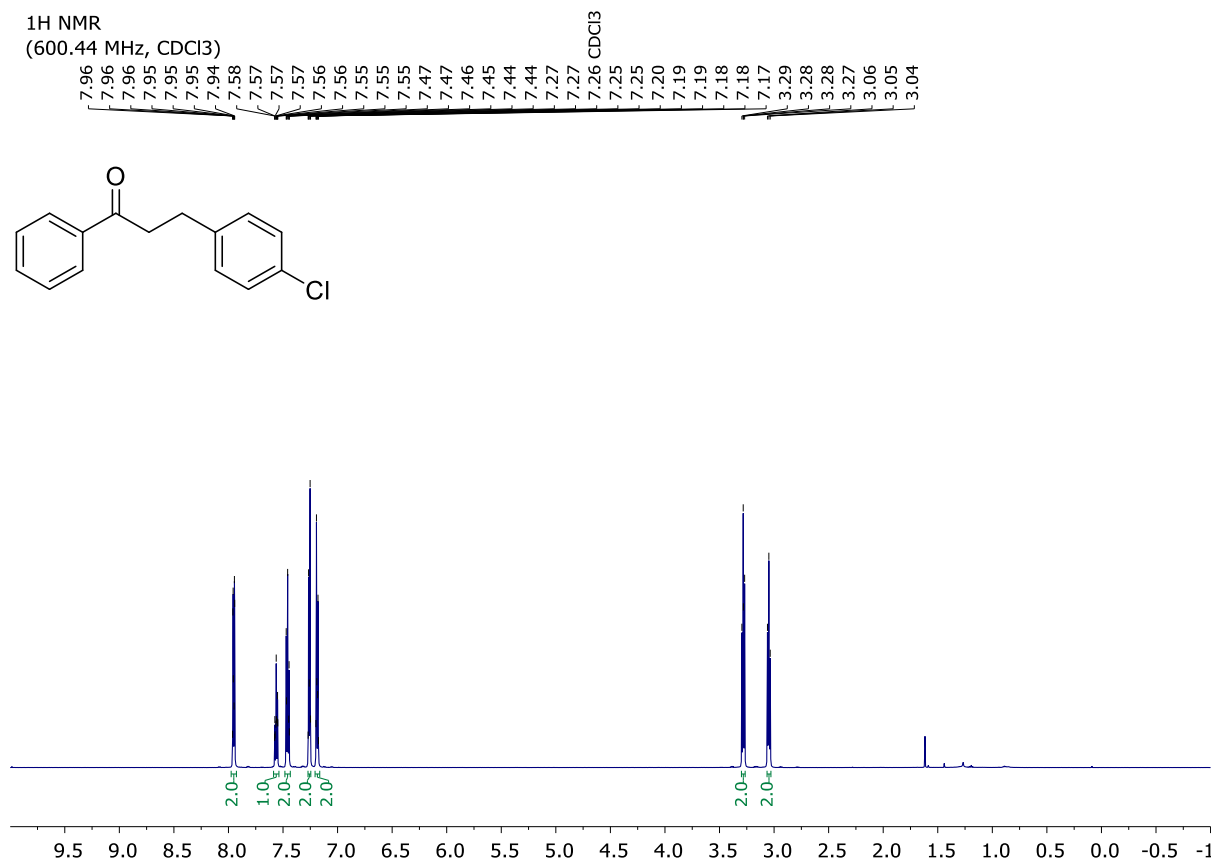


methyl 4-(3-oxo-3-phenylpropyl)benzoate (2c)

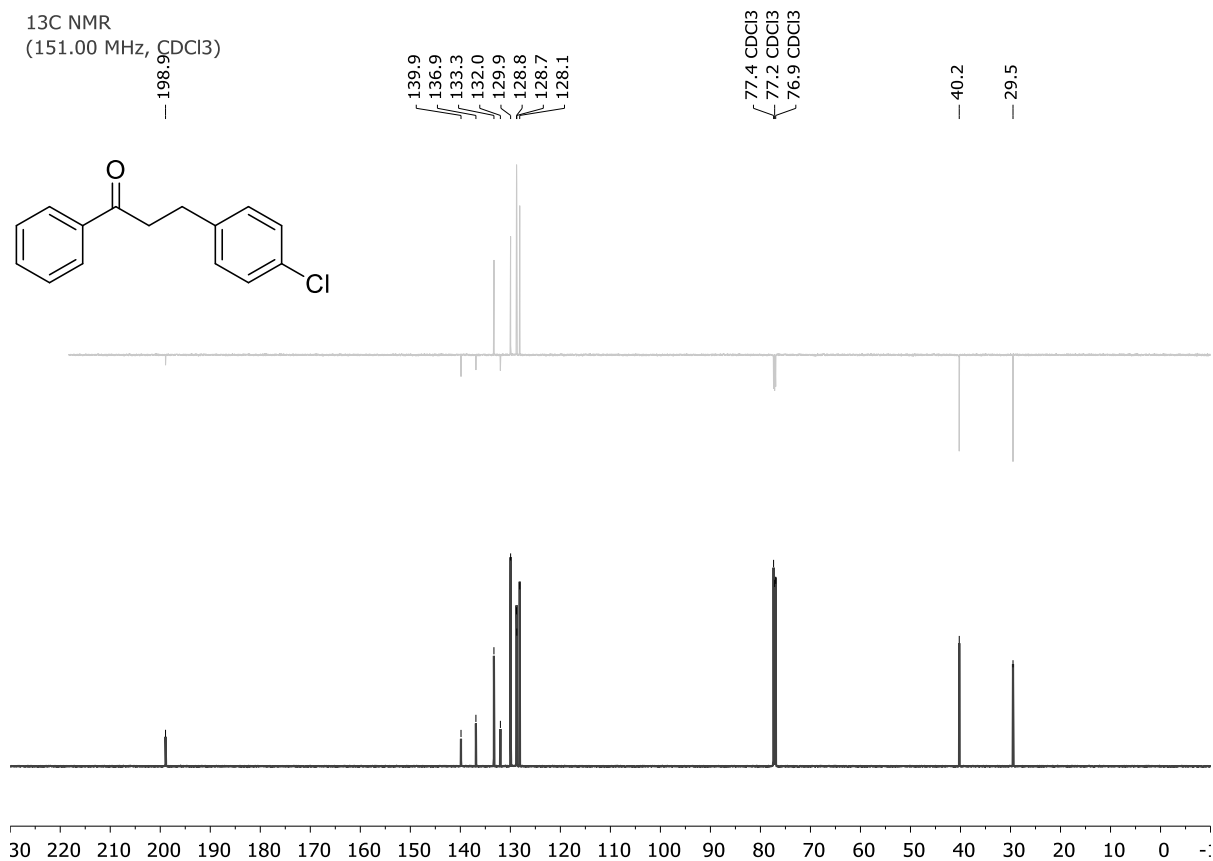


3-(4-chlorophenyl)-1-phenylpropan-1-one (2d)

¹H NMR
(600.44 MHz, CDCl₃)

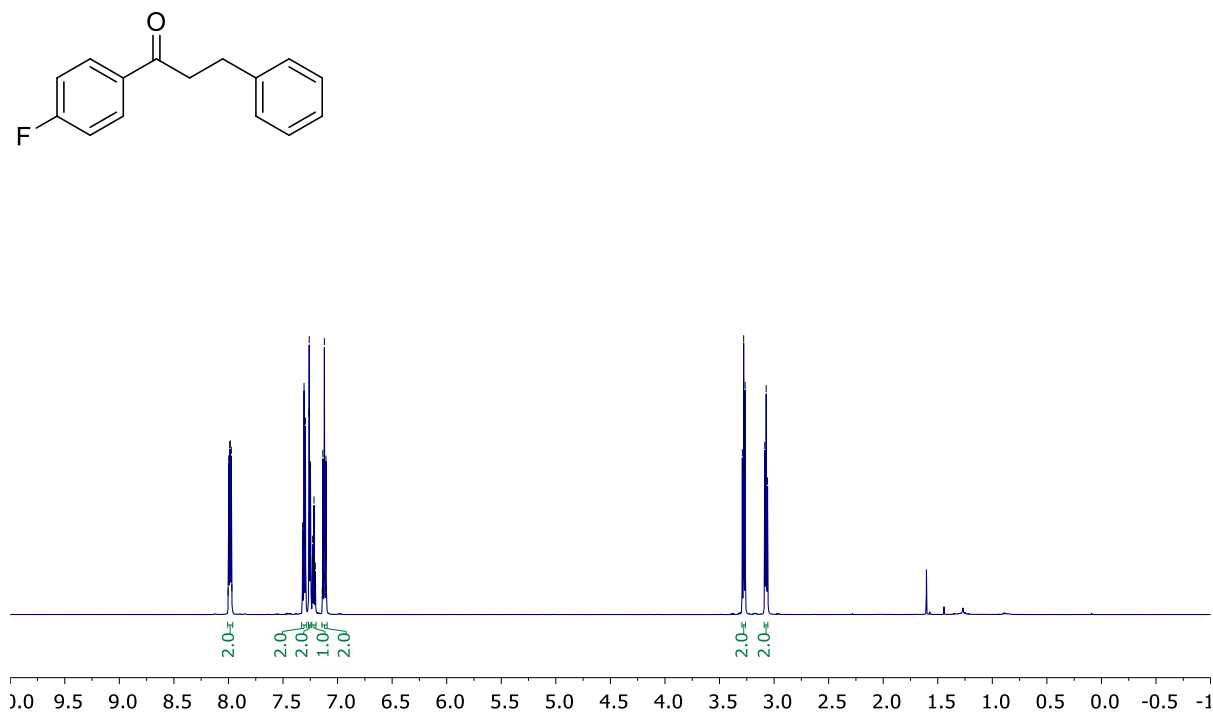
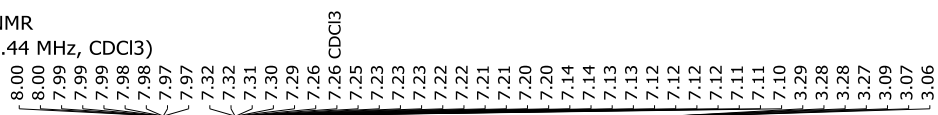


¹³C NMR
(151.00 MHz, CDCl₃)

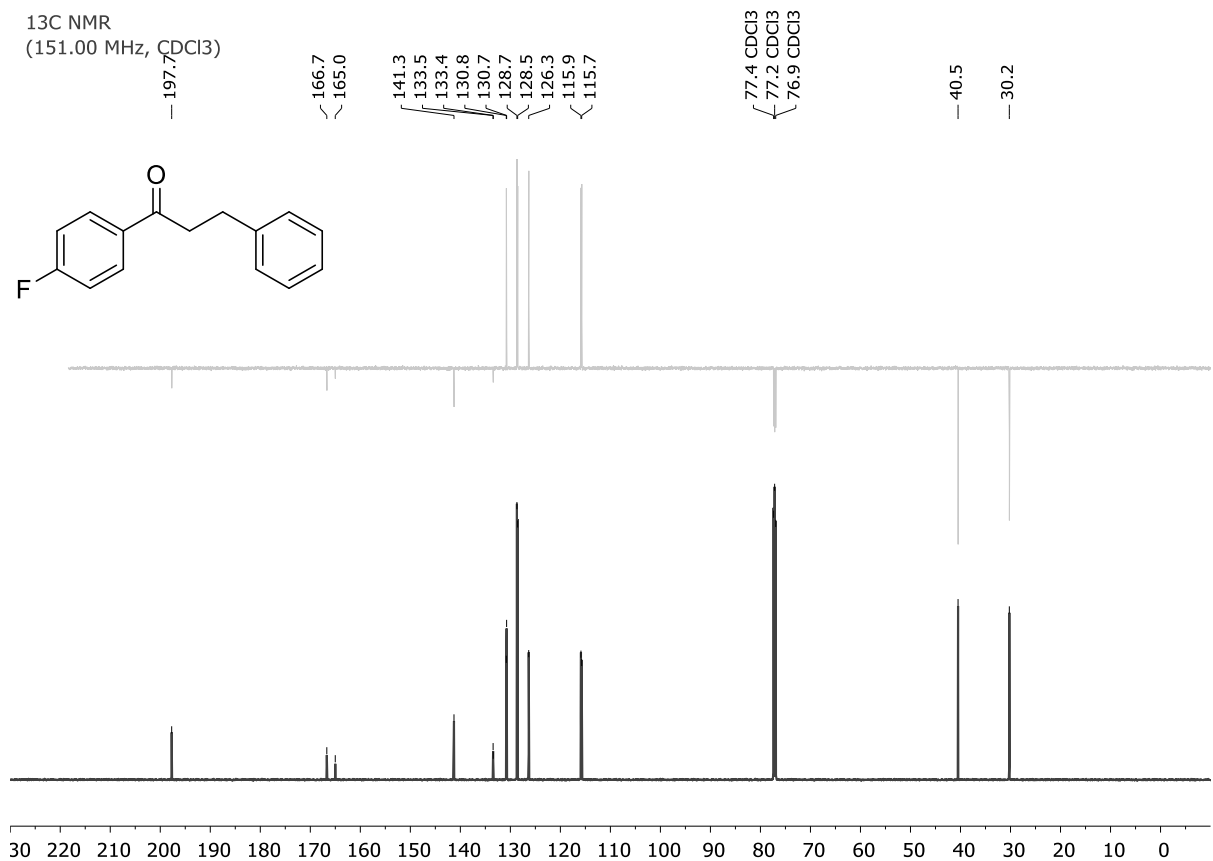


1-(4-fluorophenyl)-3-phenylpropan-1-one (2e)

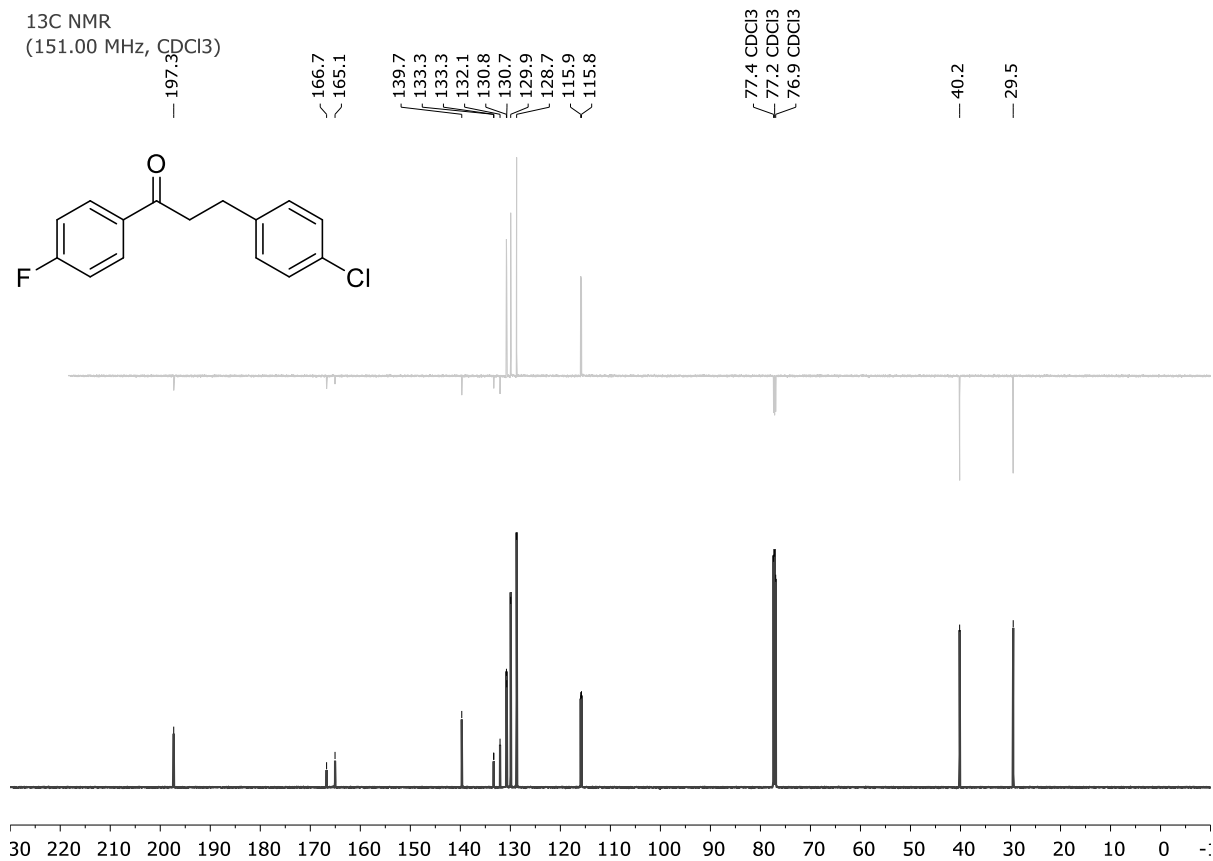
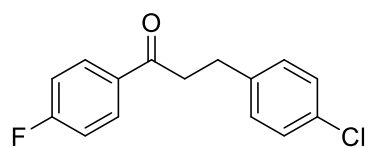
¹H NMR
(600.44 MHz, CDCl₃)



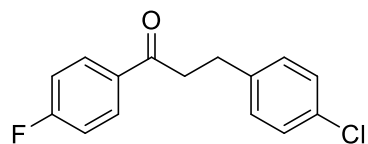
¹³C NMR
(151.00 MHz, CDCl₃)



¹³C NMR
(151.00 MHz, CDCl₃)

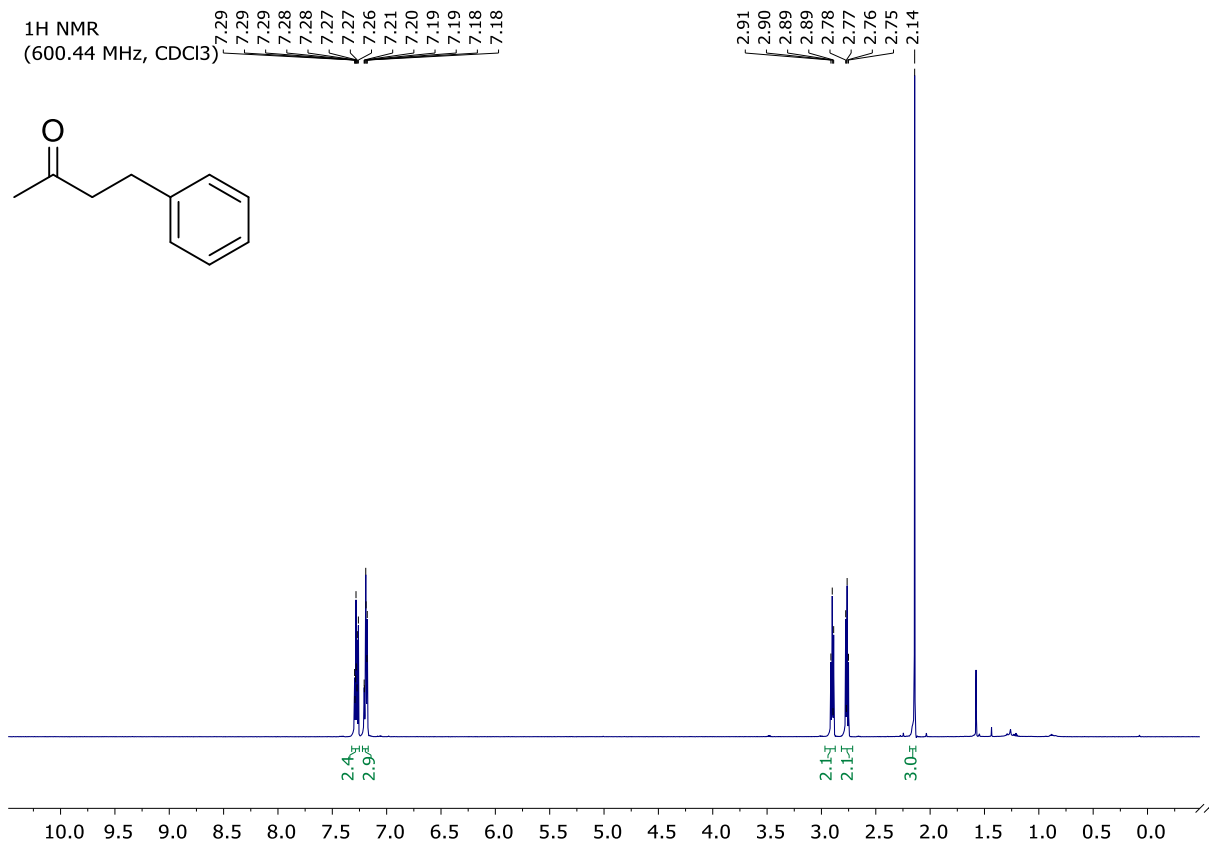
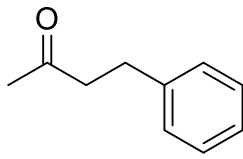


¹⁹F NMR
(564.92 MHz, CDCl₃)

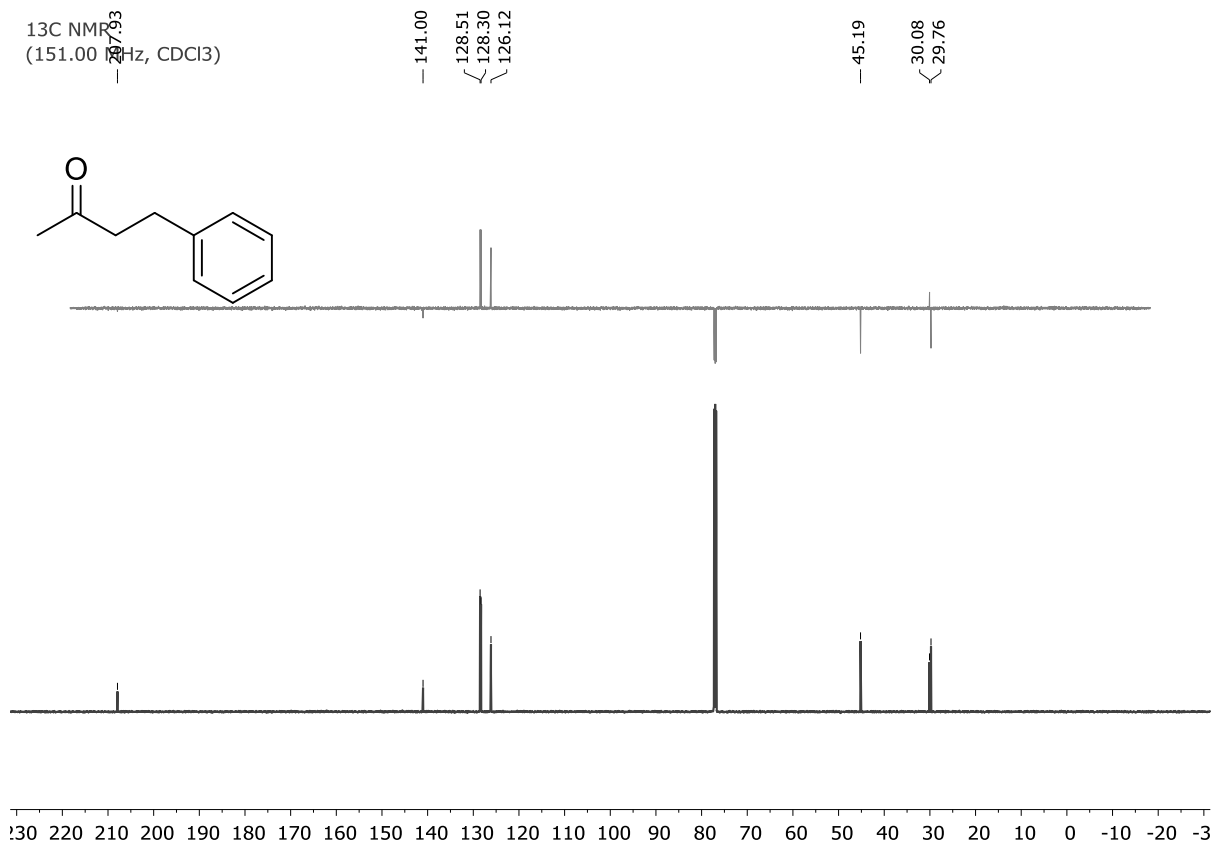
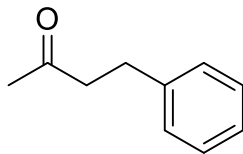


4-phenylbutan-2-one (2g)

¹H NMR
(600.44 MHz, CDCl₃)

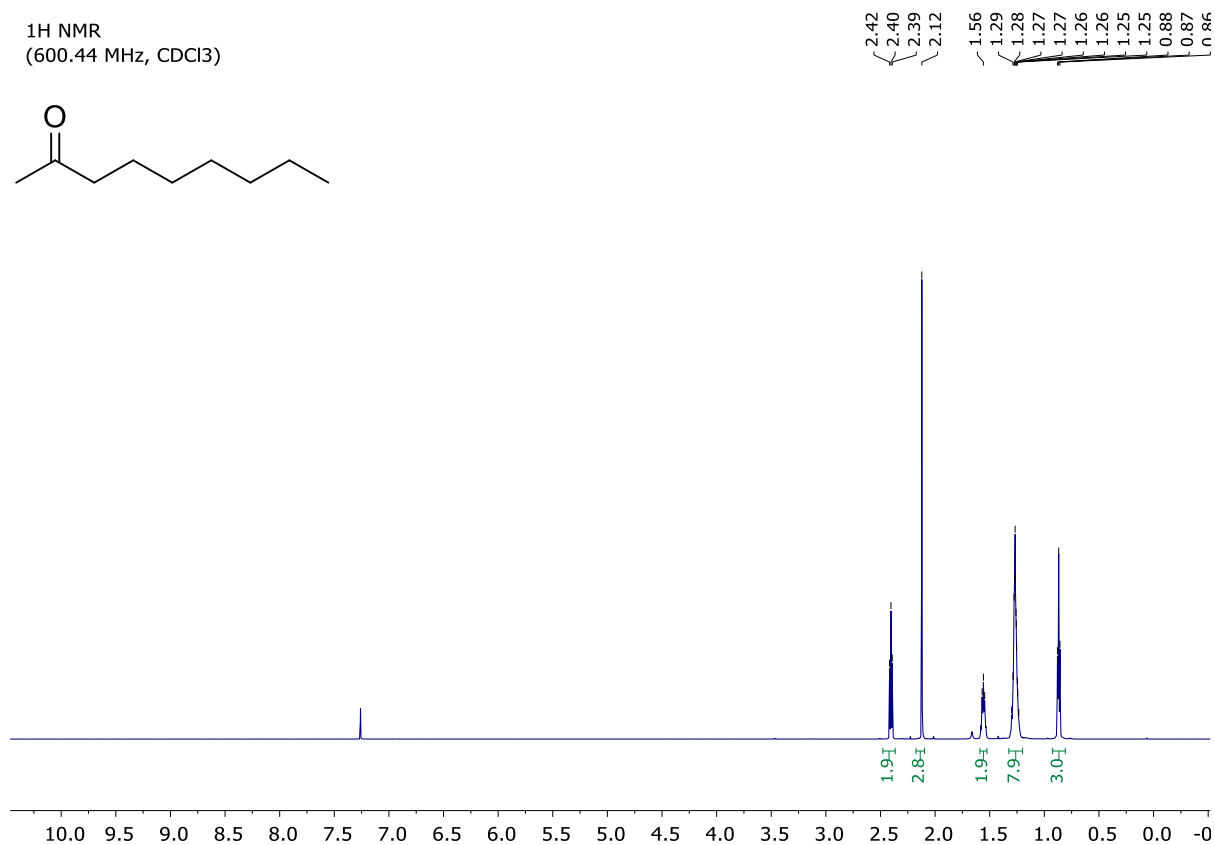
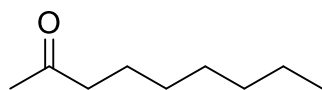


¹³C NMR
(151.00 MHz, CDCl₃)

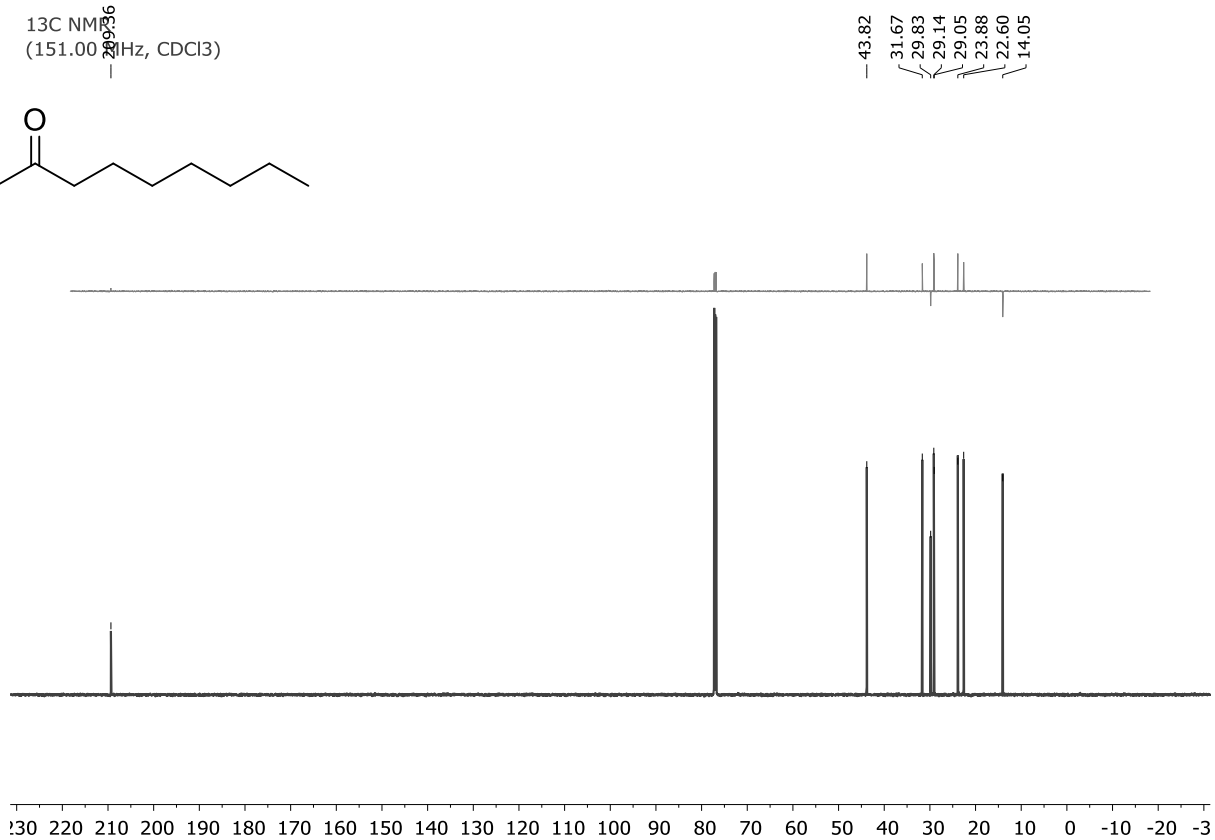
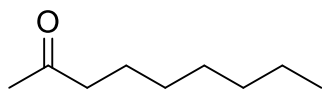


Nonan-2-one (2h)

¹H NMR
(600.44 MHz, CDCl₃)

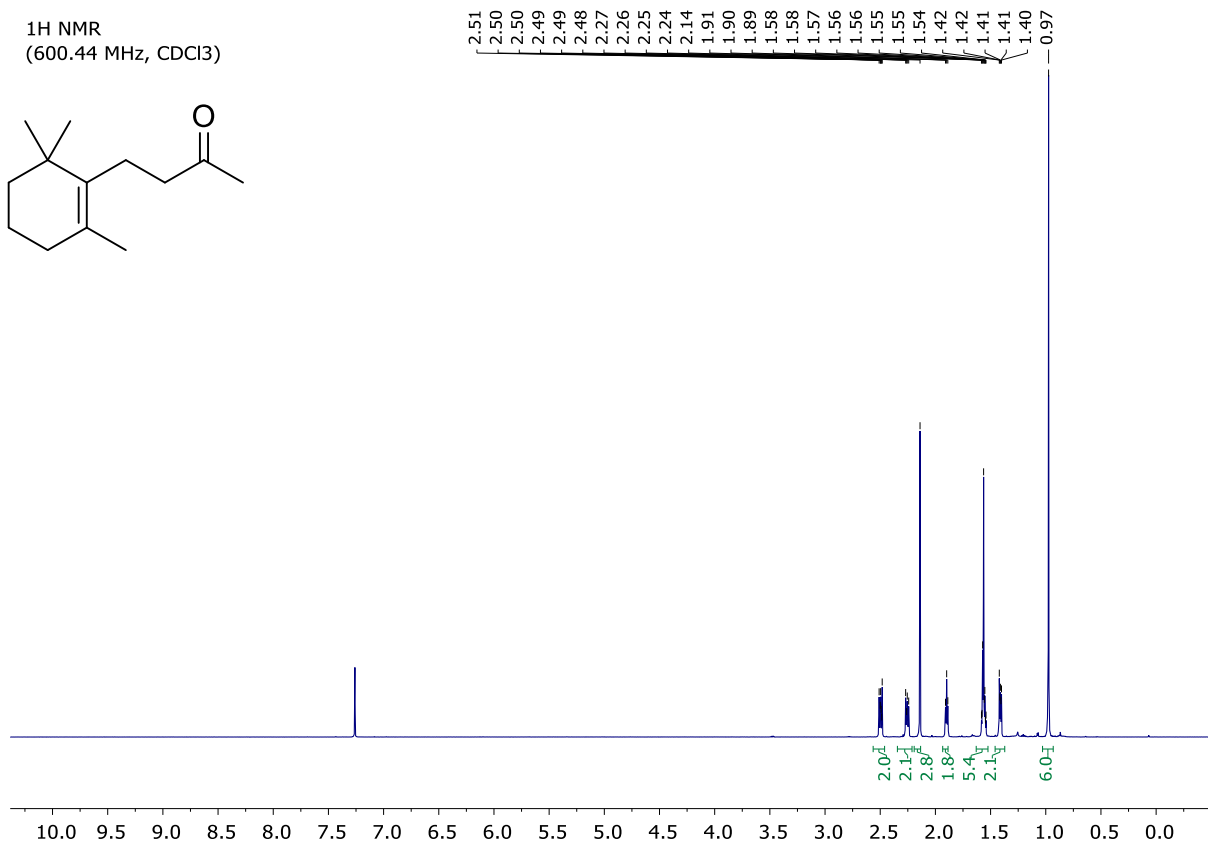
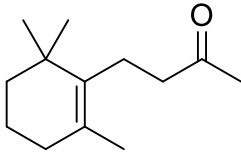


¹³C NMR
(151.00 MHz, CDCl₃)

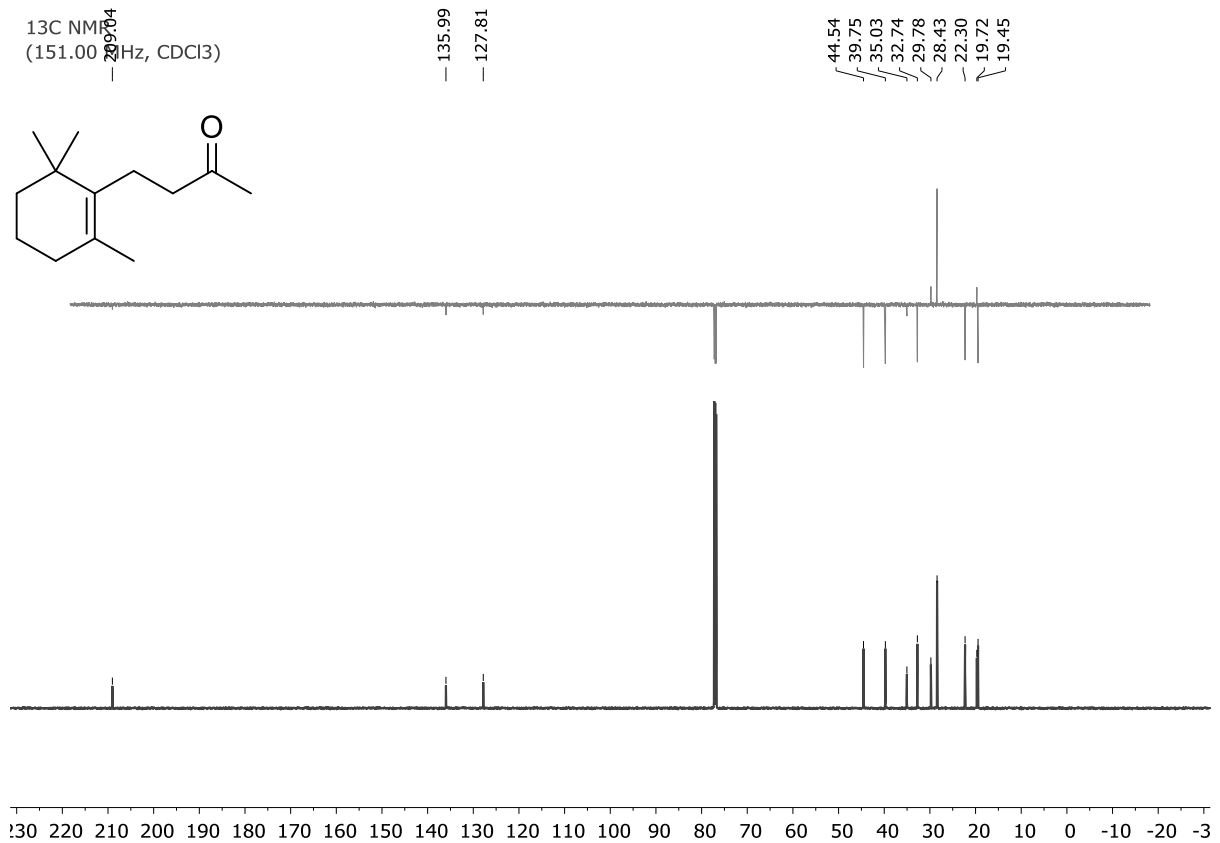
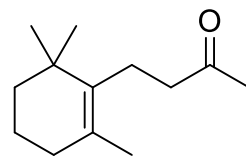


4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-one (2i)

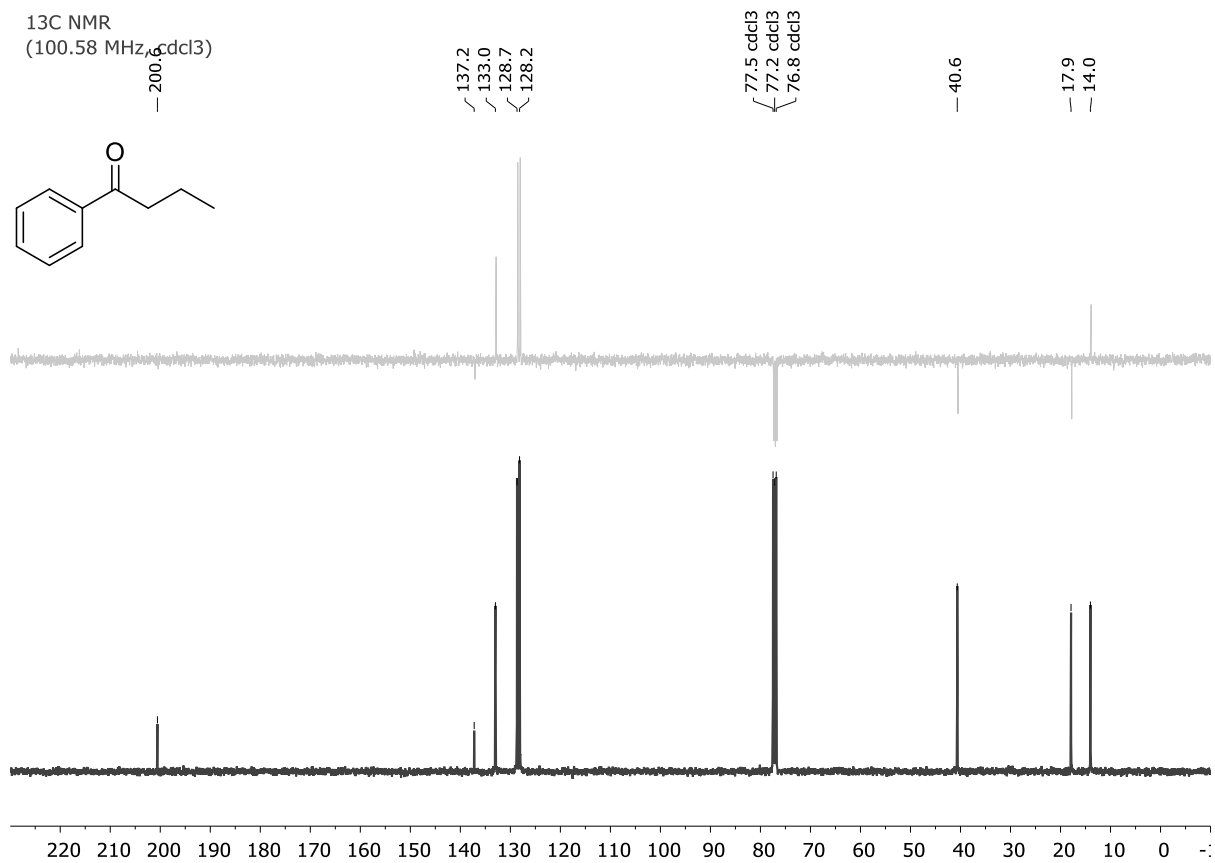
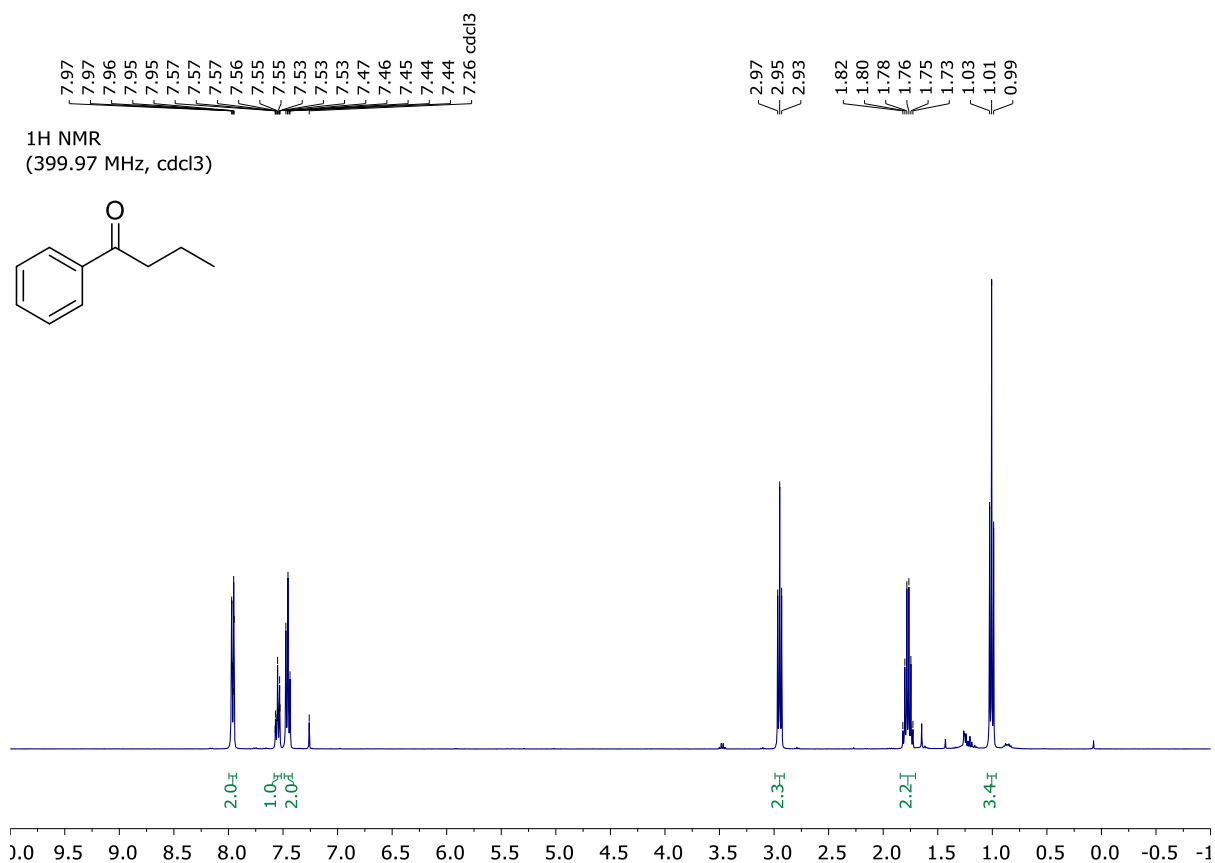
¹H NMR
(600.44 MHz, CDCl₃)



¹³C NMR
(151.00 MHz, CDCl₃)

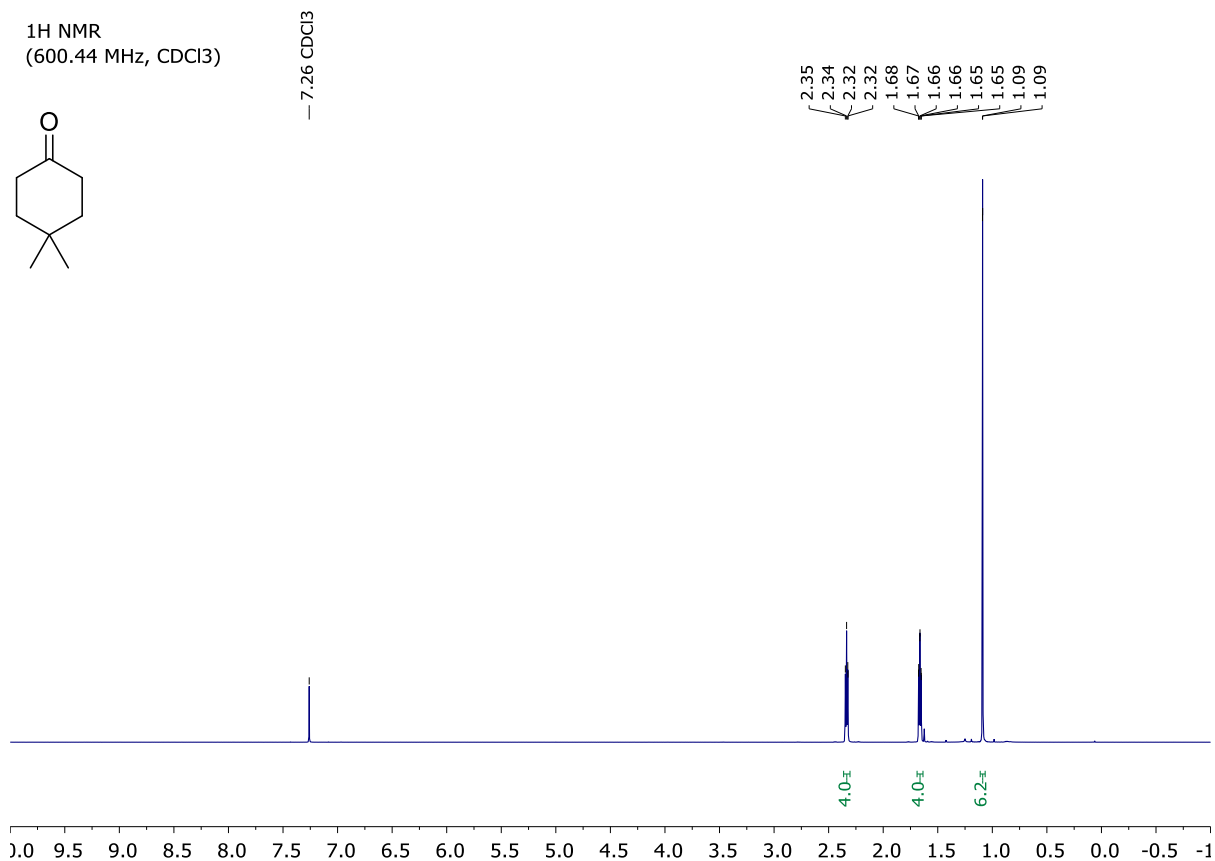
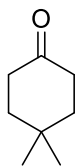


1-phenylbutan-1-one (2j)

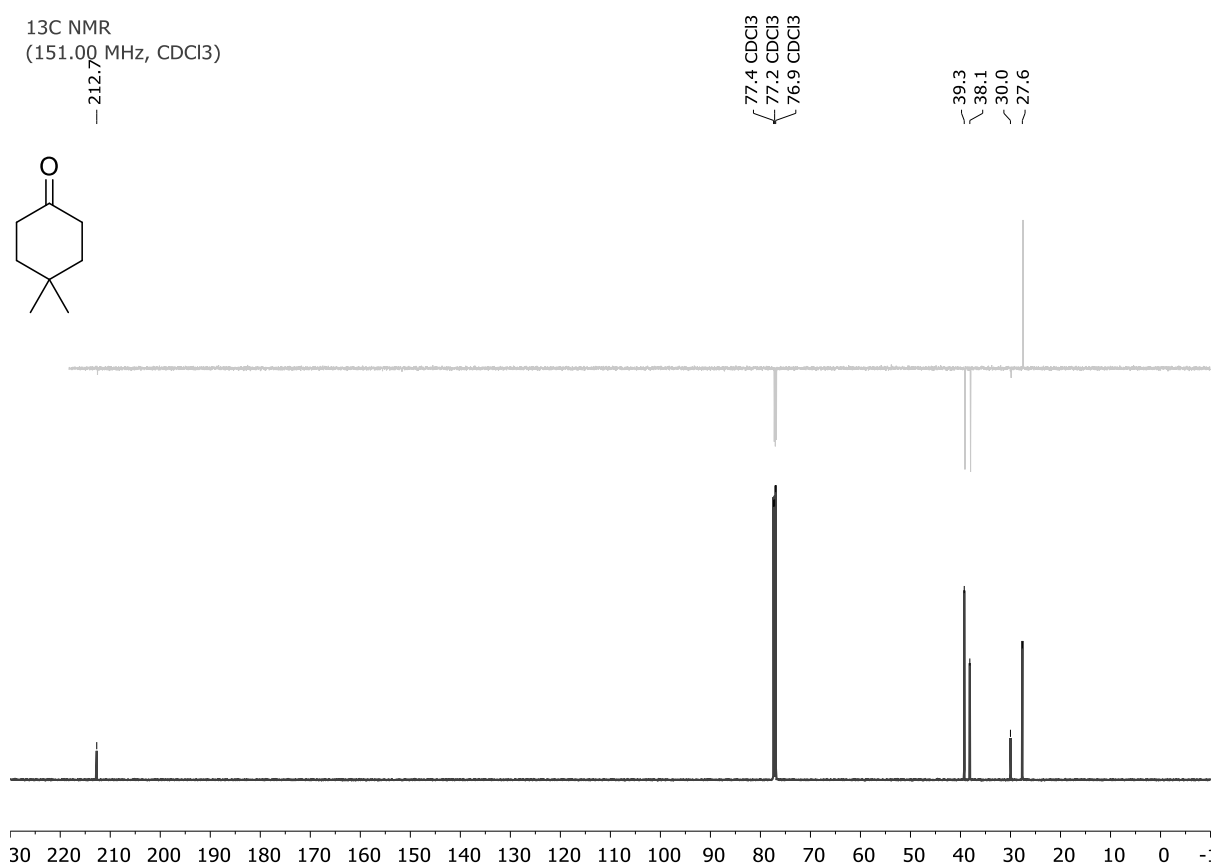
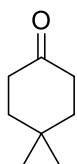


4,4-dimethylcyclohexan-1-one (2k)

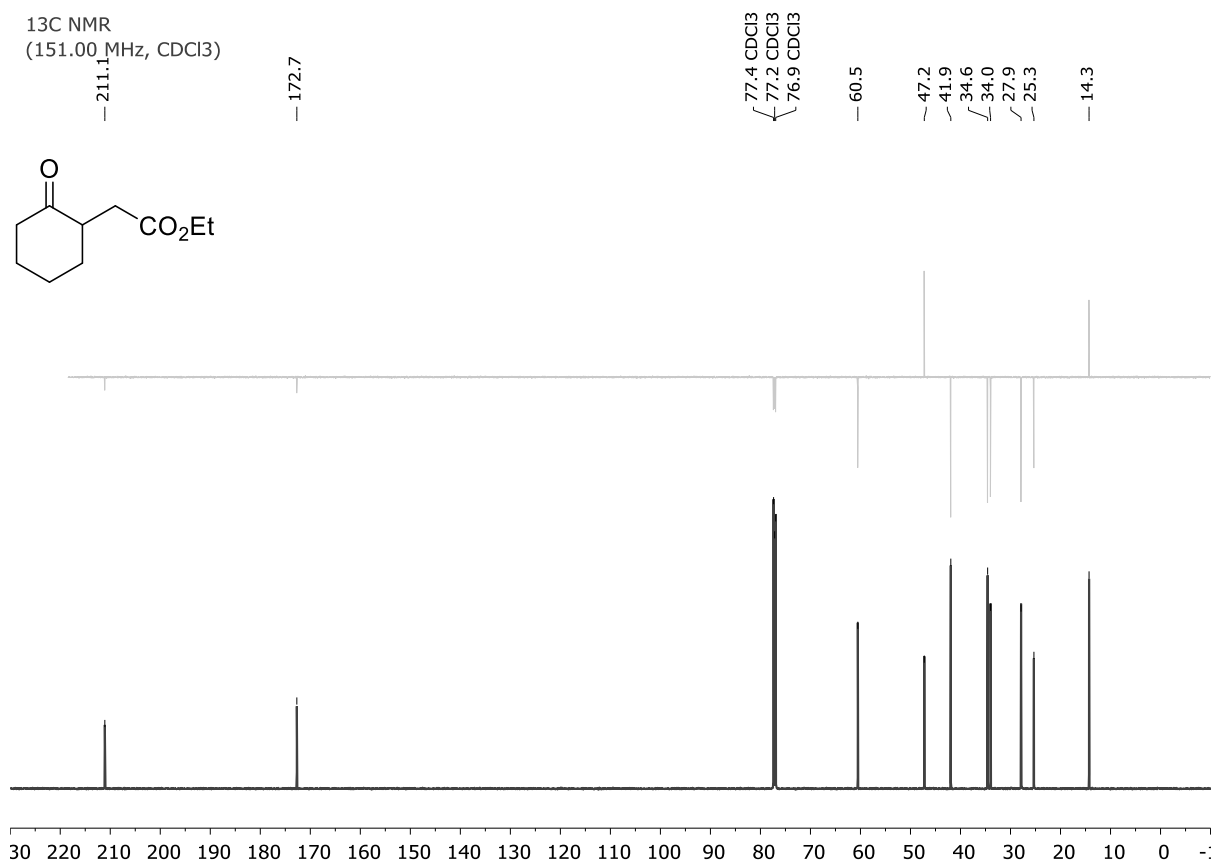
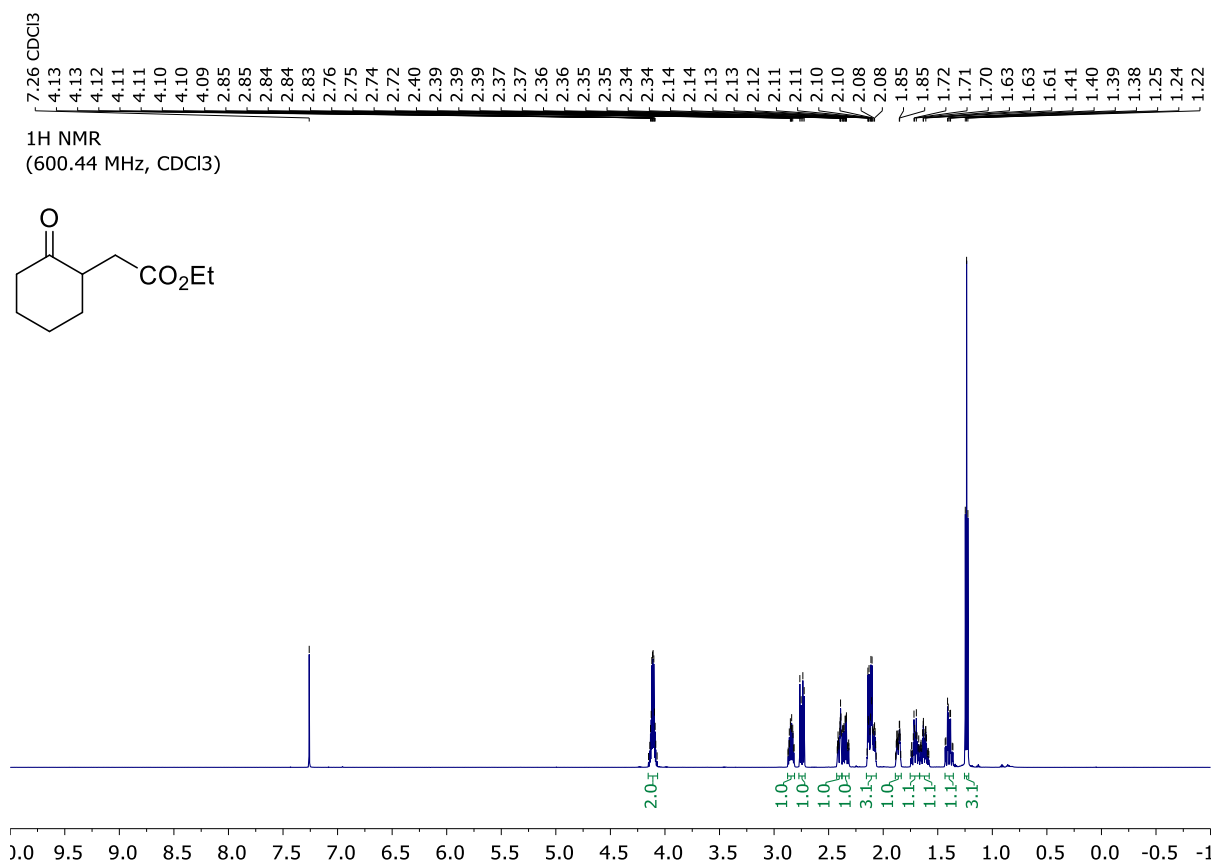
¹H NMR
(600.44 MHz, CDCl₃)



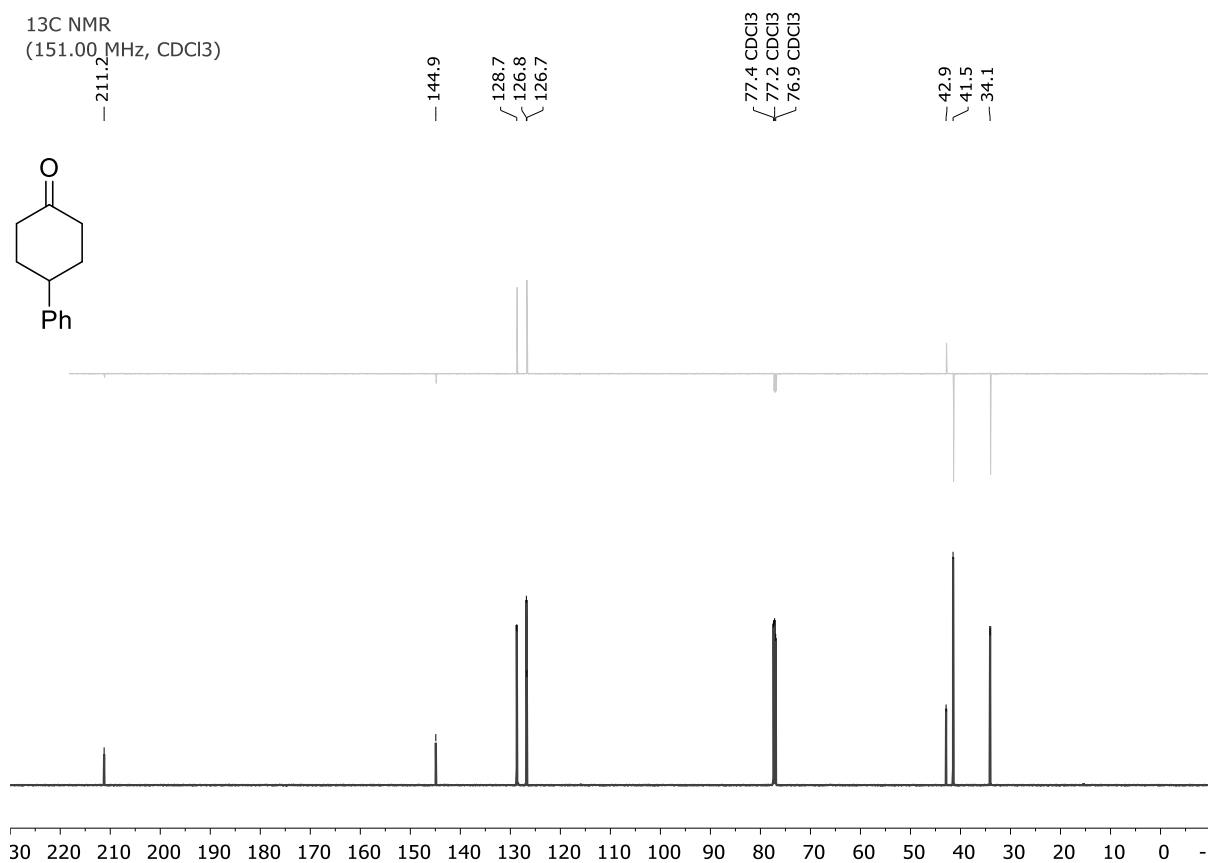
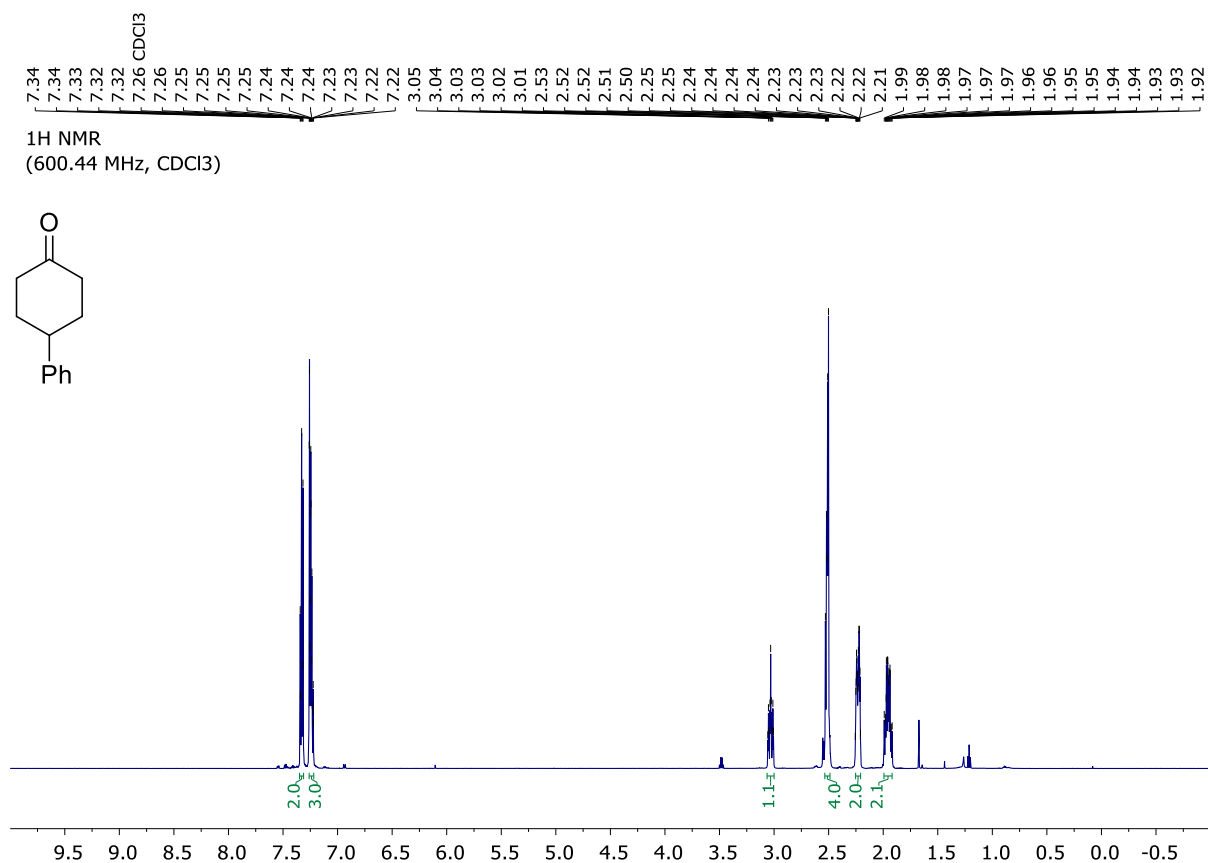
¹³C NMR
(151.00 MHz, CDCl₃)



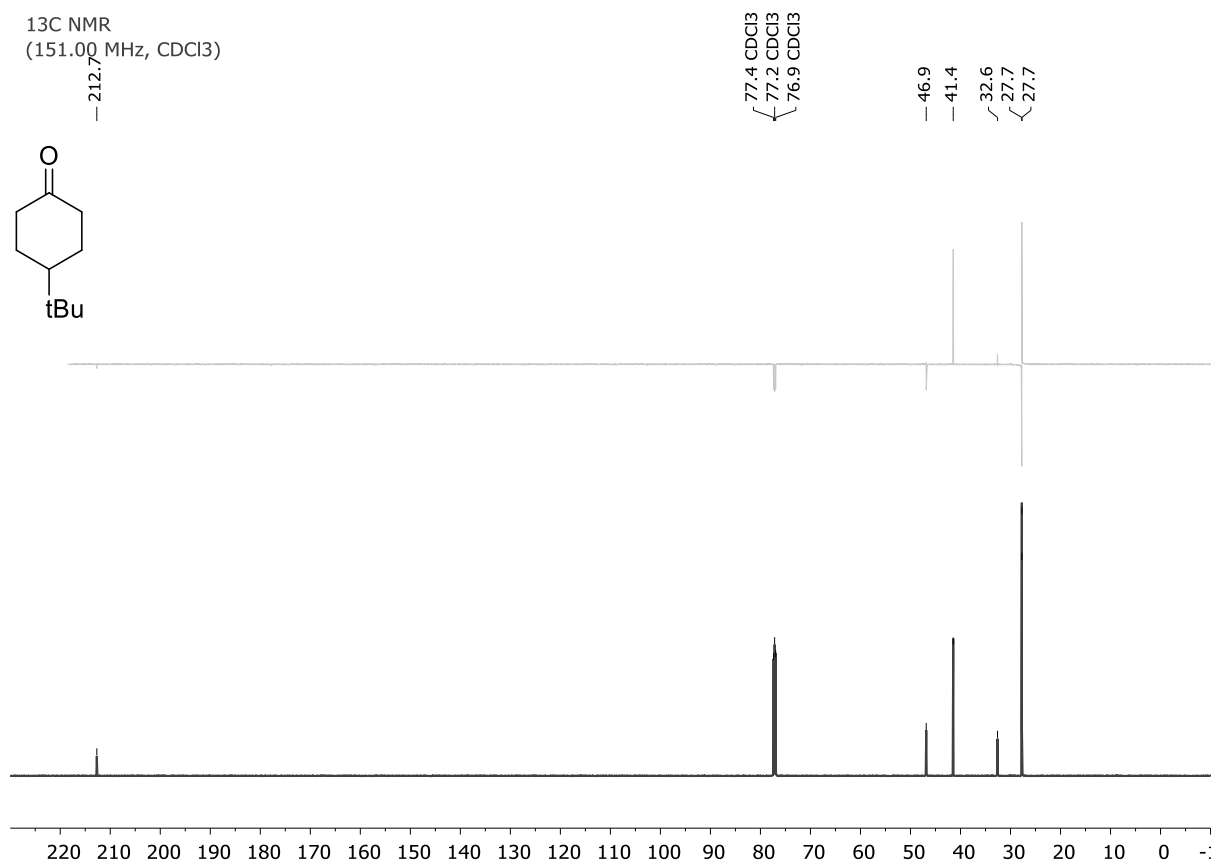
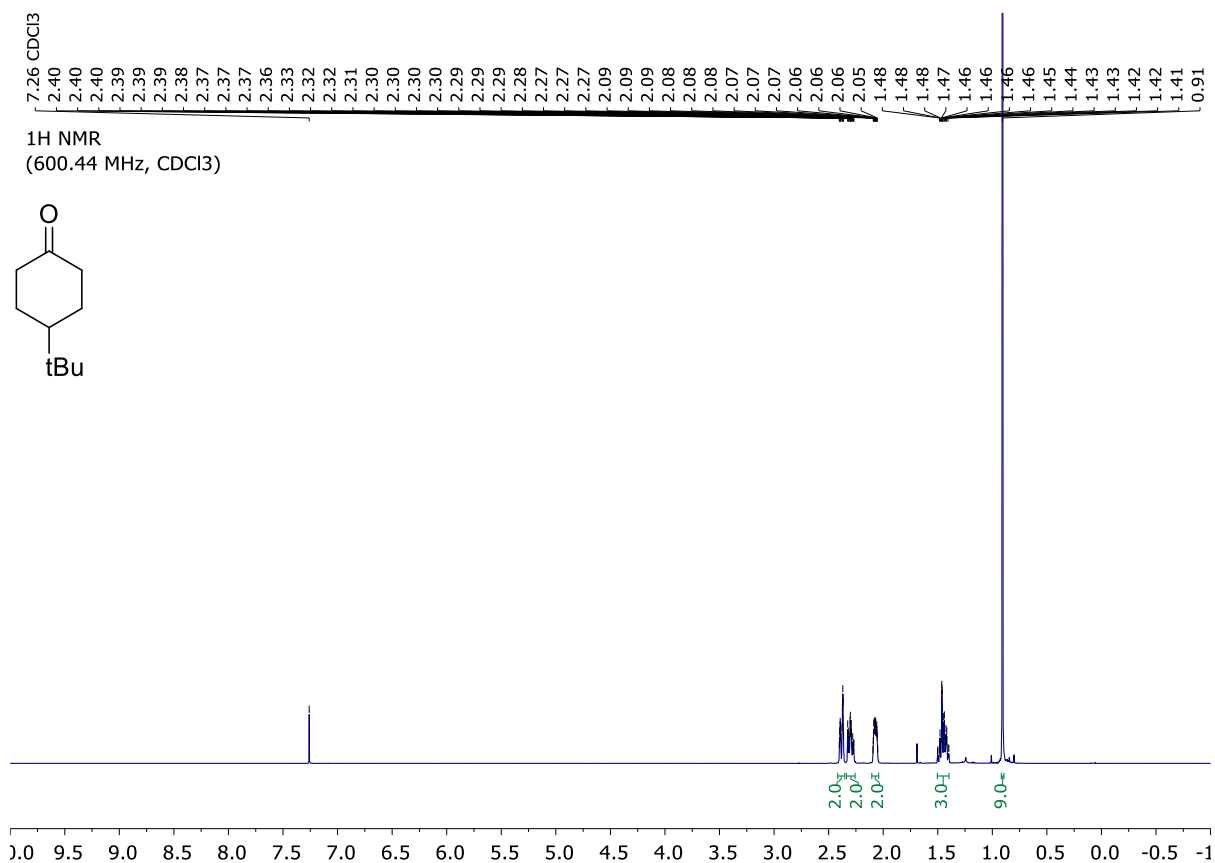
ethyl 2-(2-oxocyclohexyl)acetate (2l)



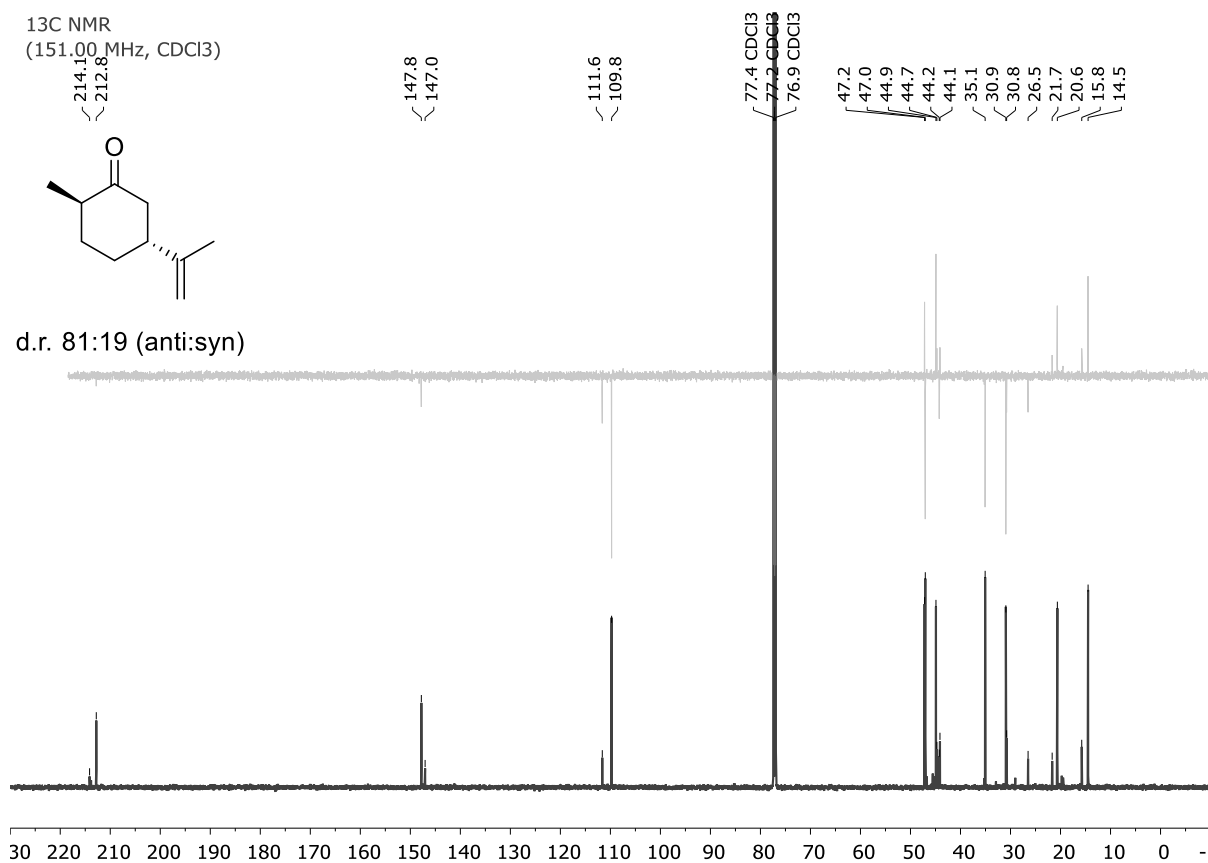
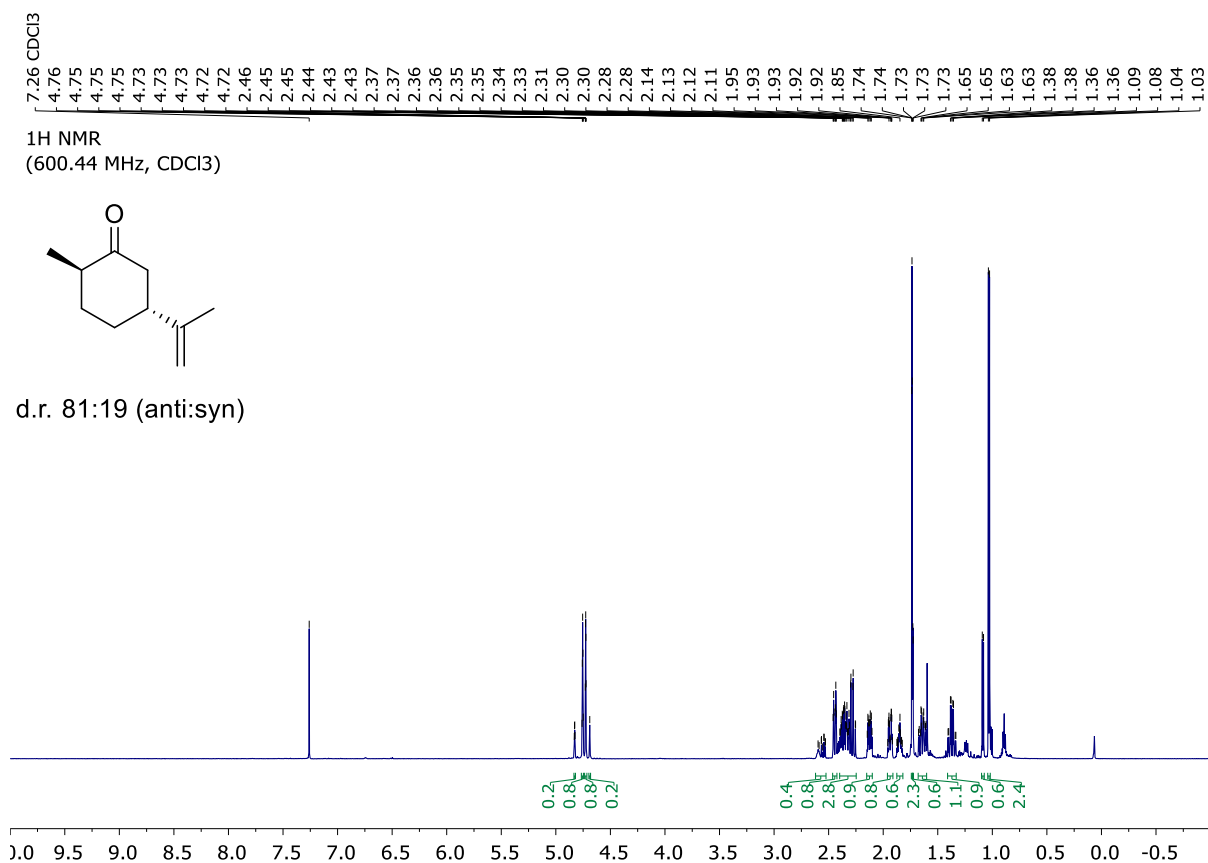
4-phenylcyclohexan-1-one (2m)



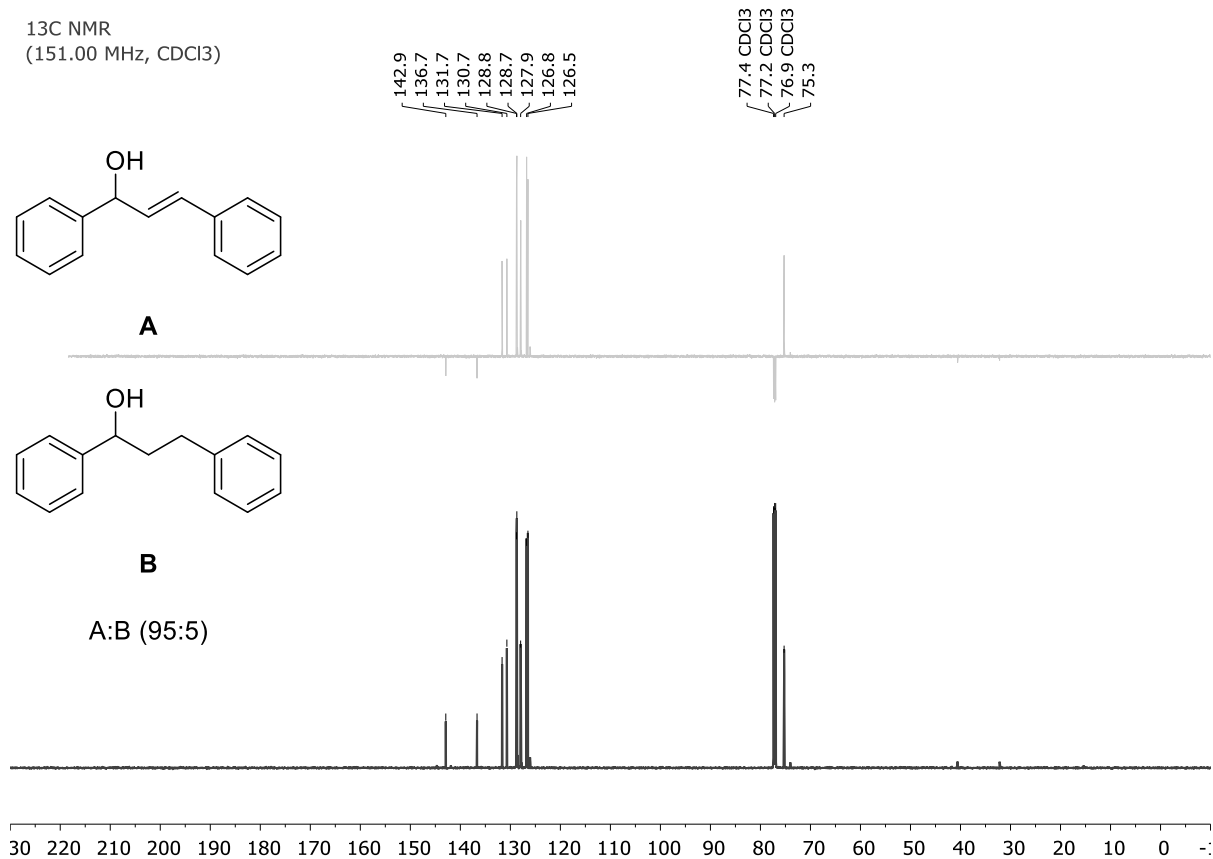
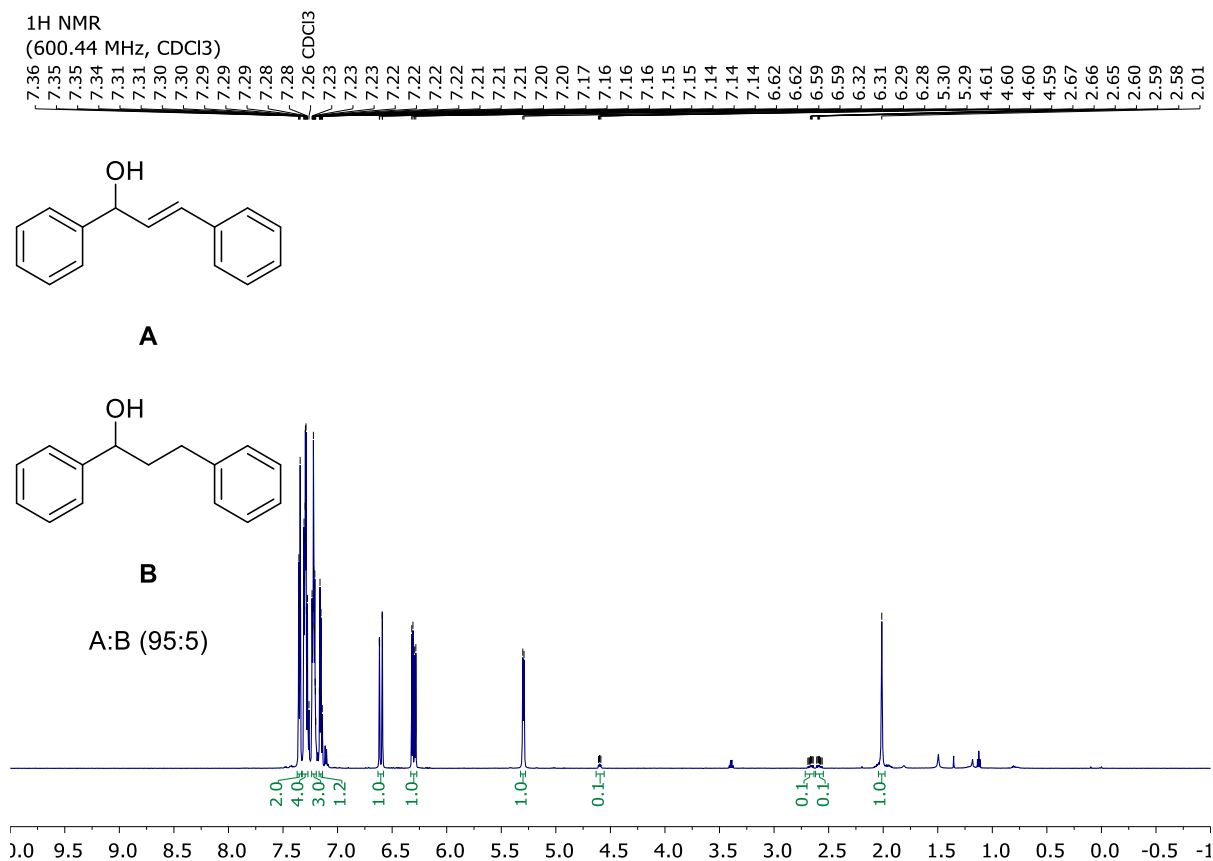
4-(tert-butyl)cyclohexan-1-one (2n)



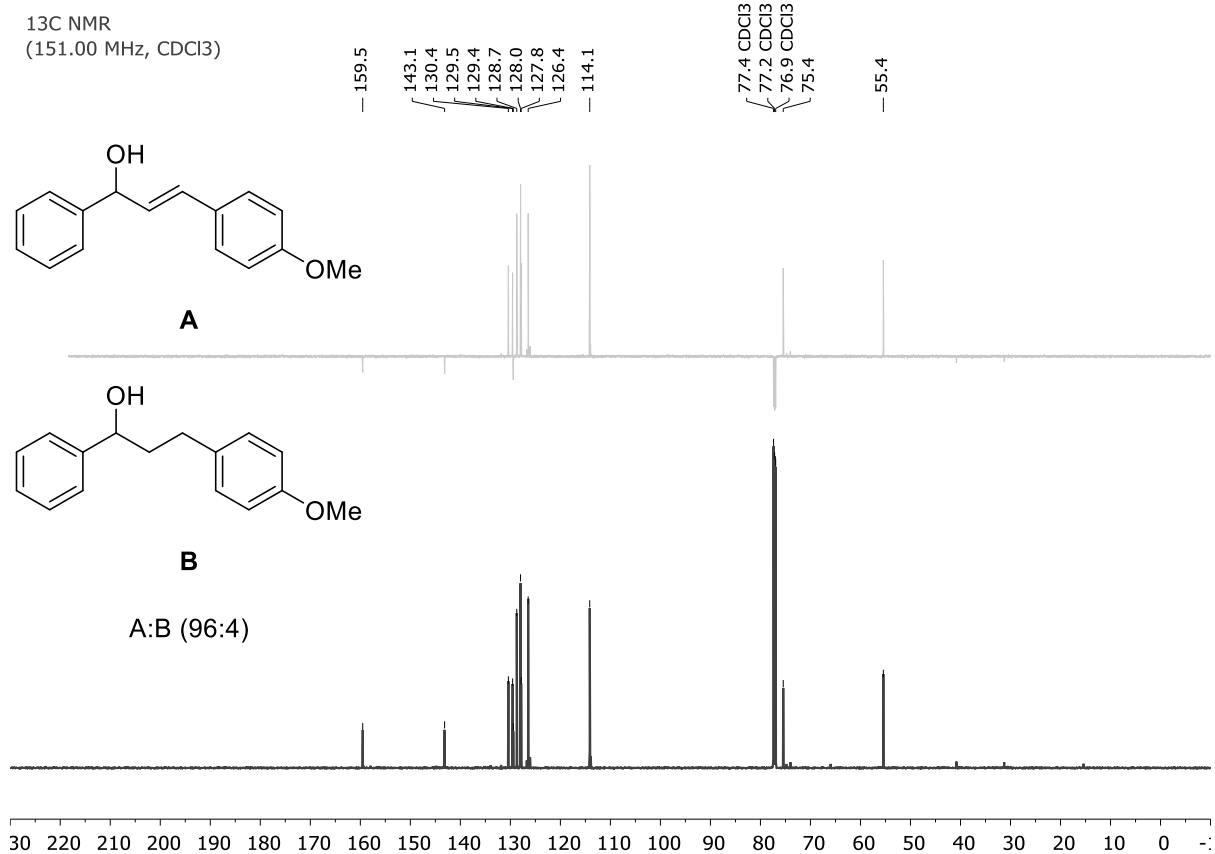
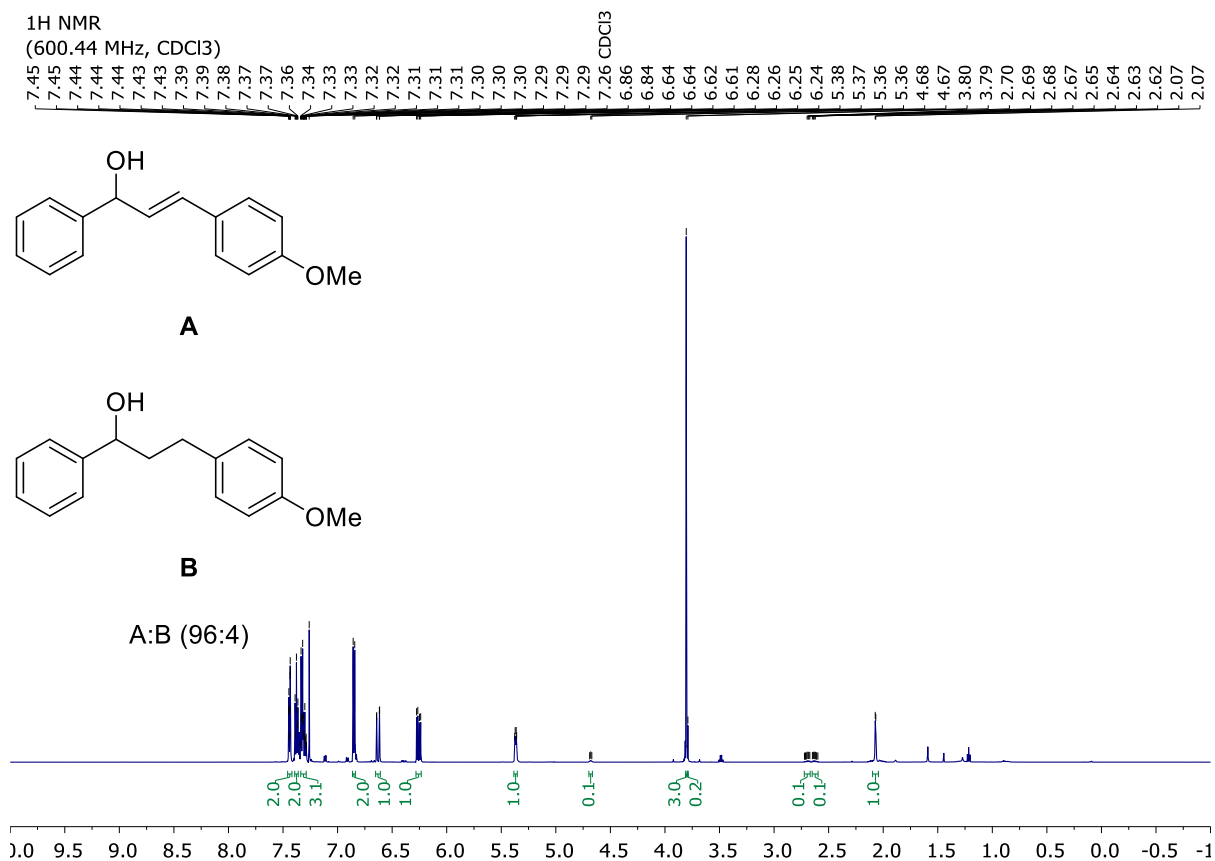
(2R,5R)-2-methyl-5-(prop-1-en-2-yl)cyclohexan-1-one (2o)



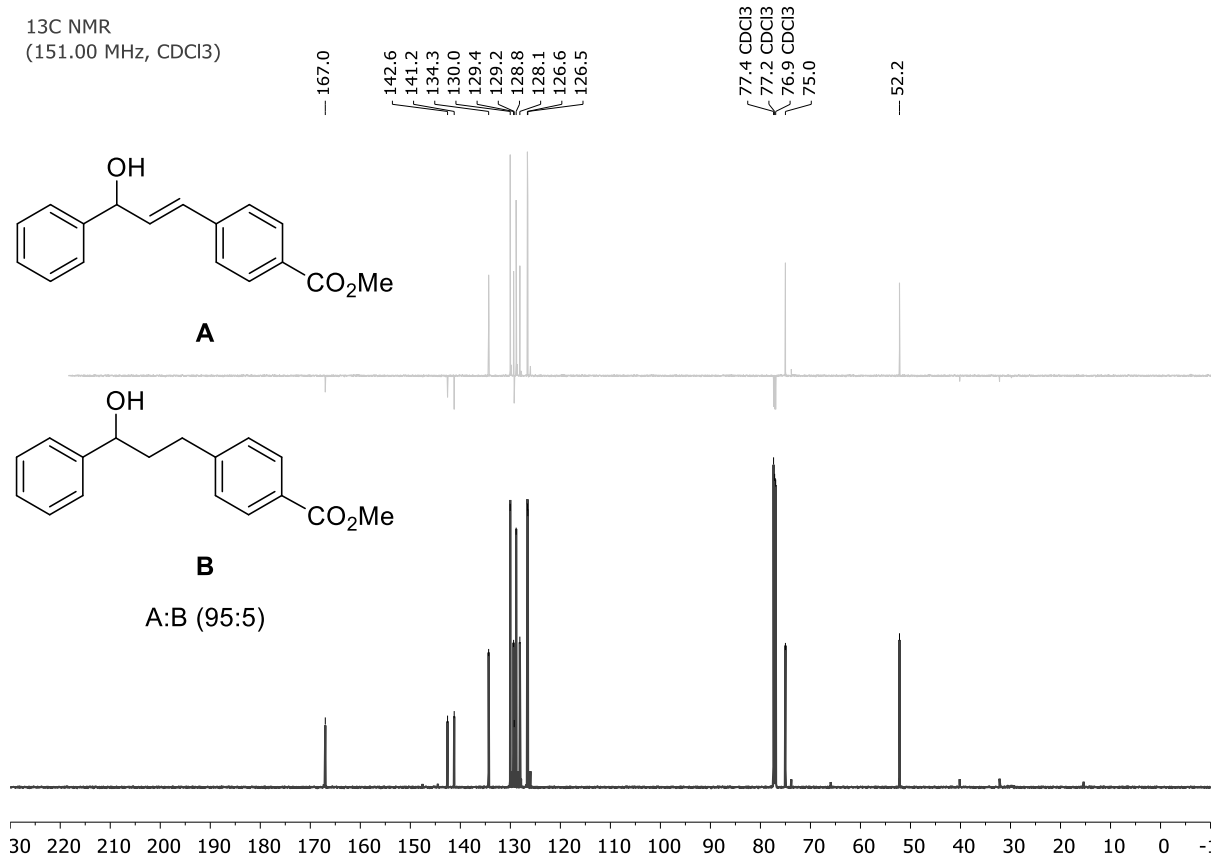
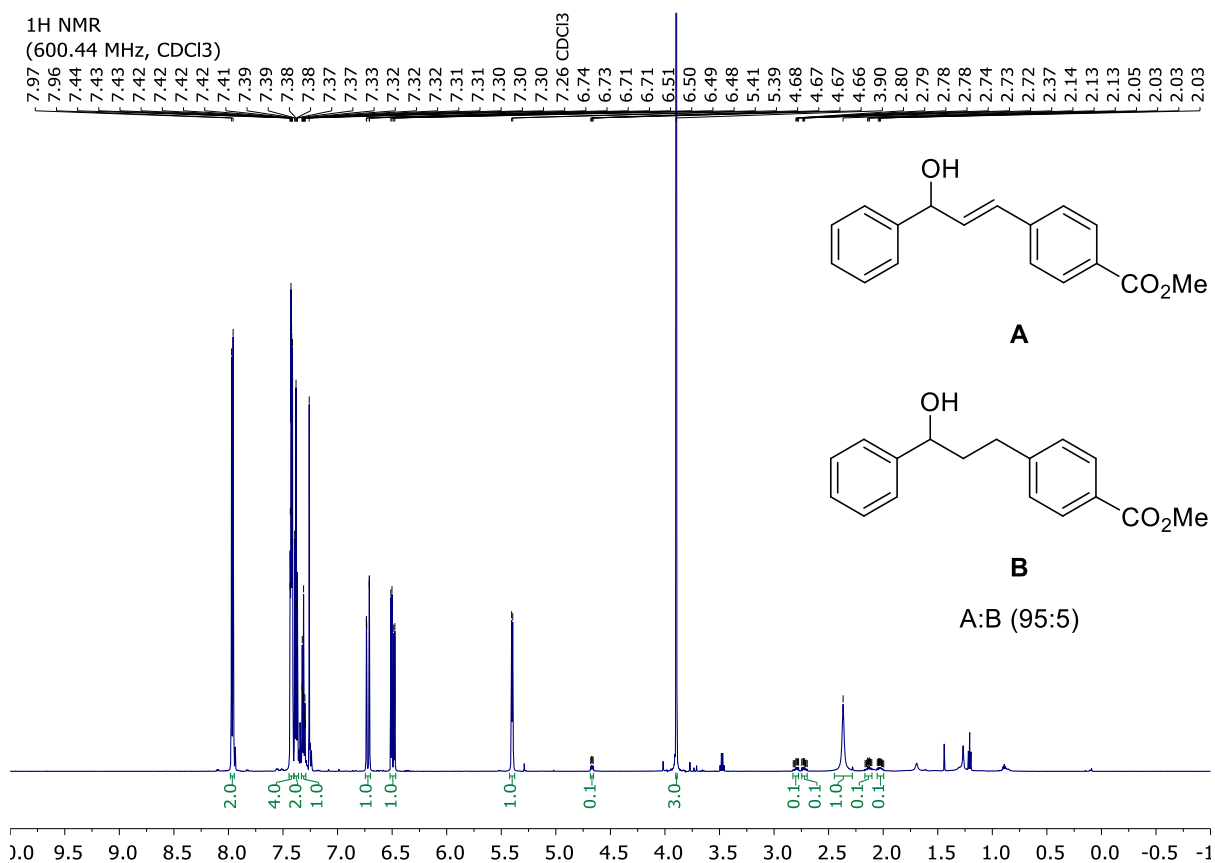
(E)-1,3-diphenylprop-2-en-1-ol (3a)



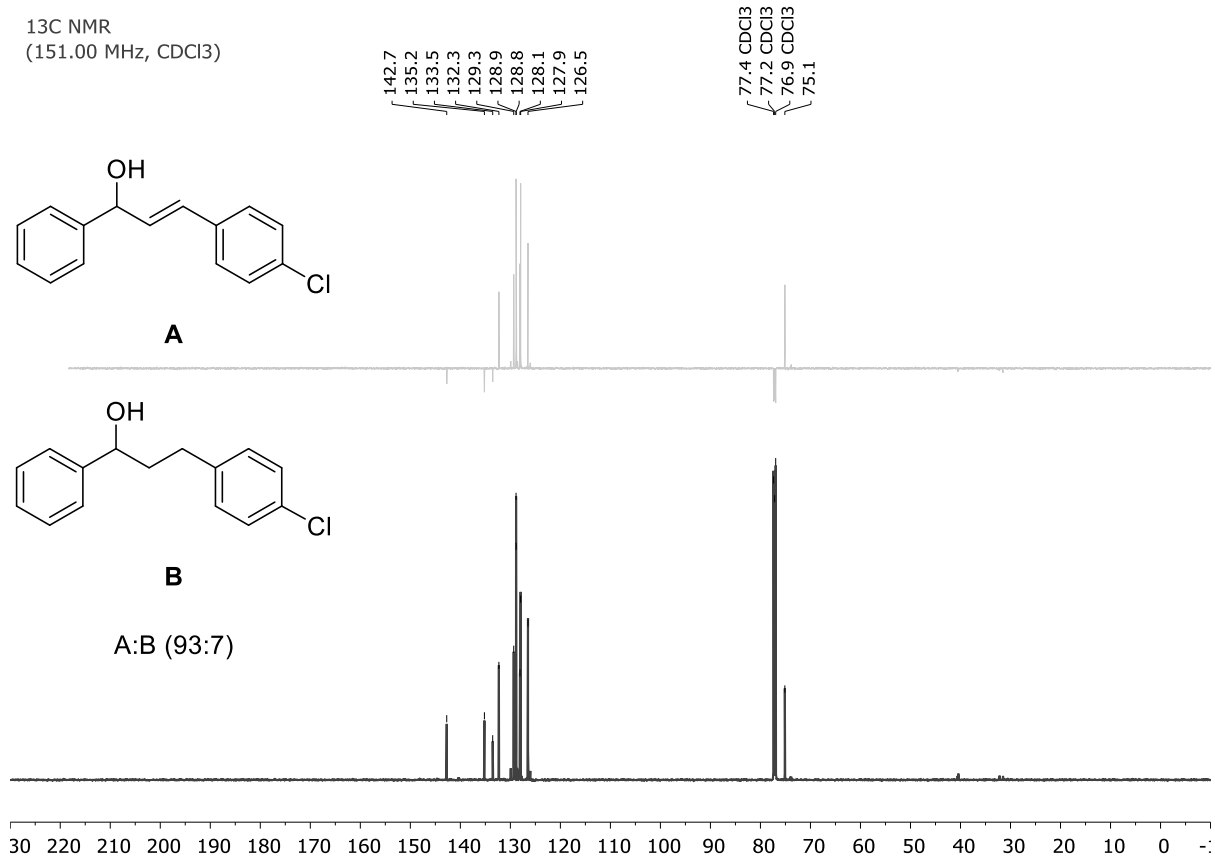
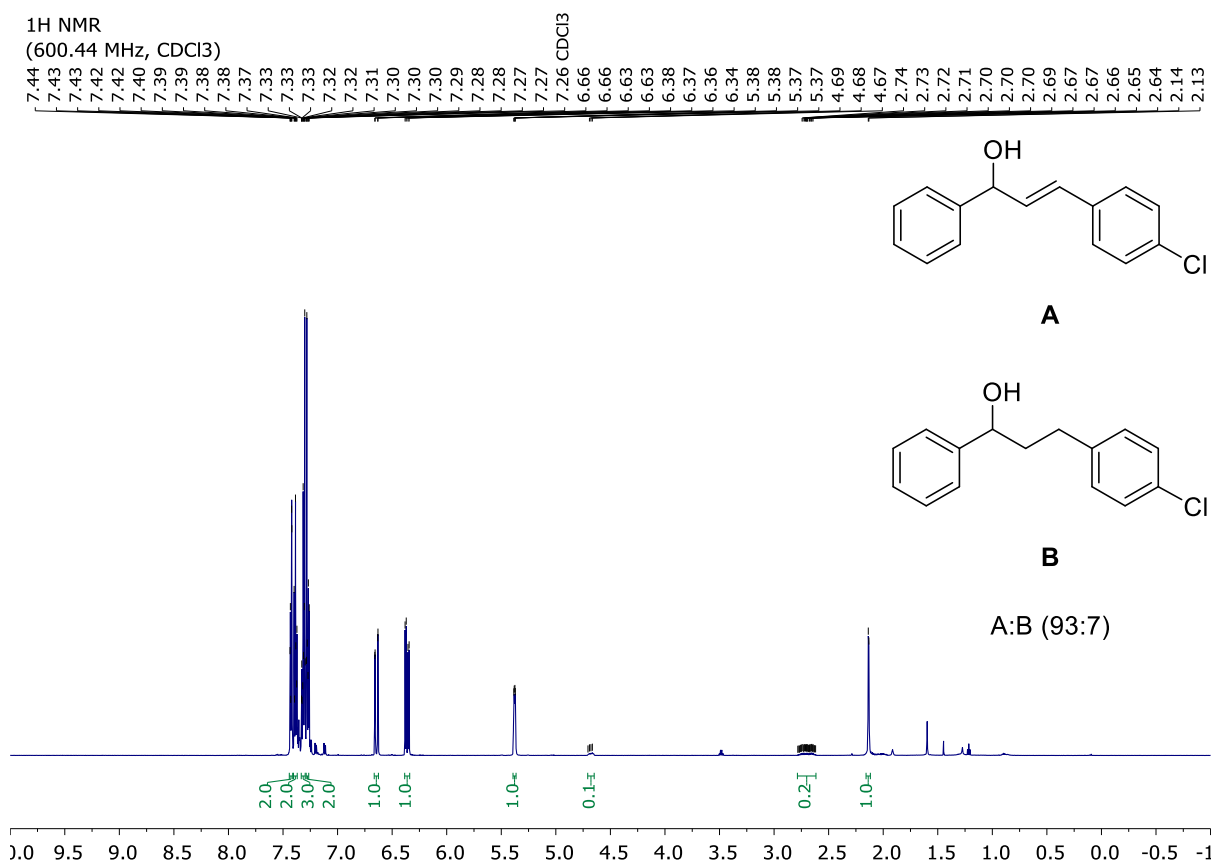
(E)-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-ol (3b)



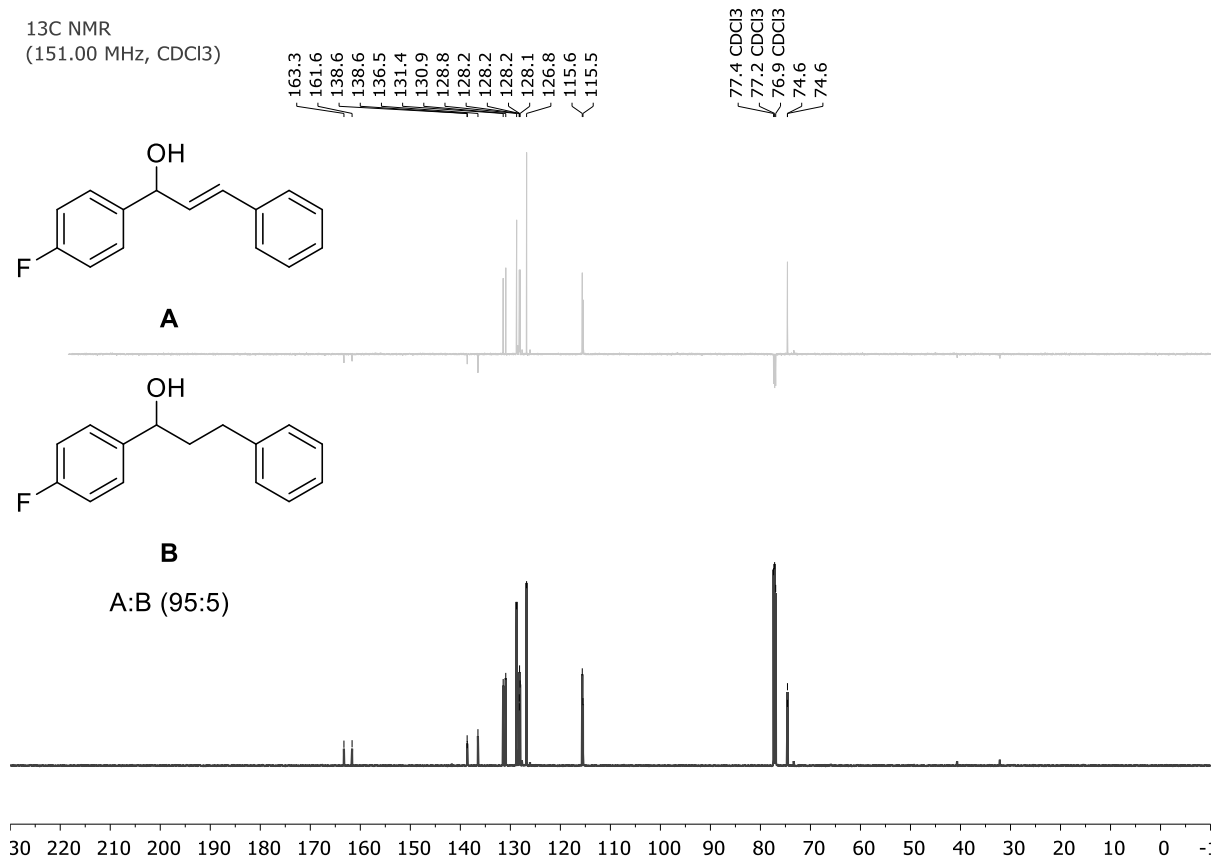
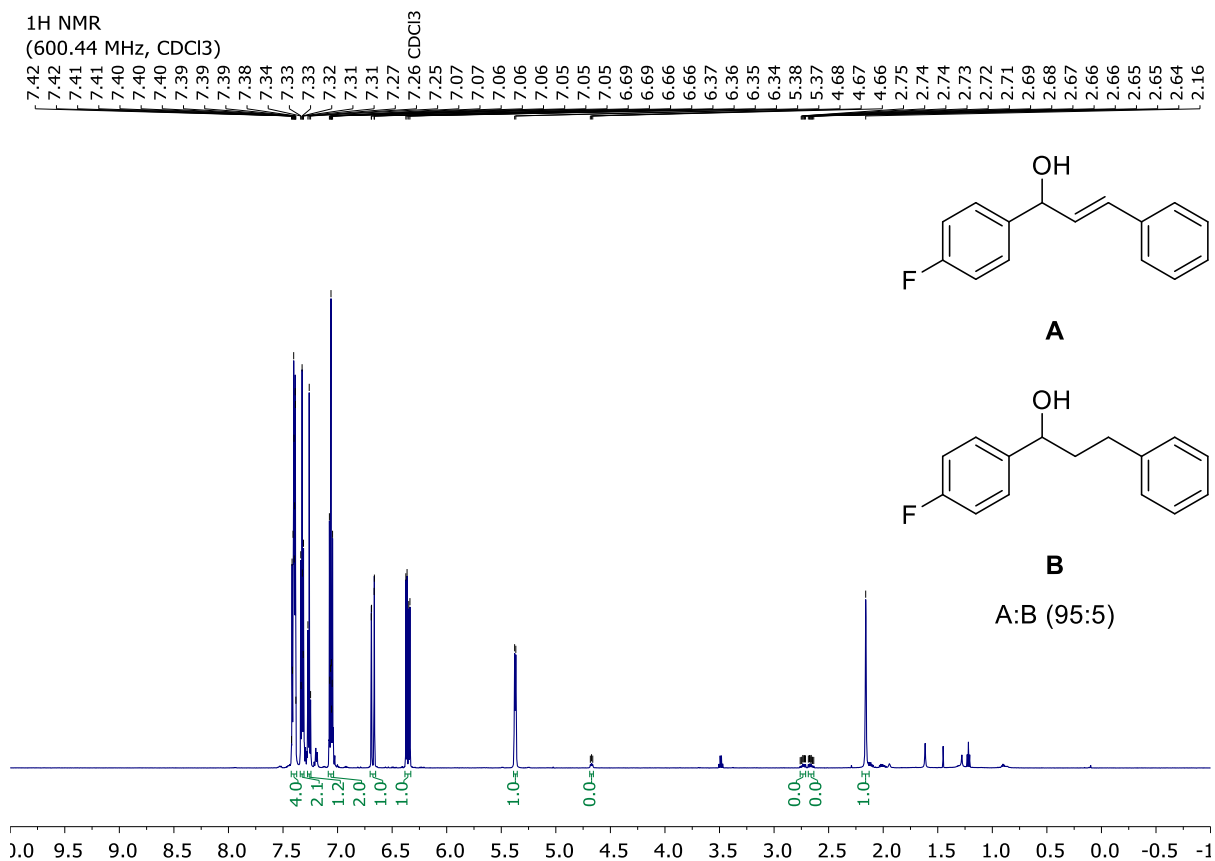
methyl (E)-4-(3-hydroxy-3-phenylprop-1-en-1-yl)benzoate (3c)



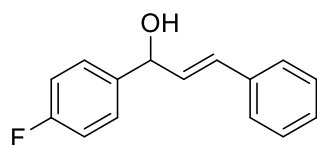
(E)-3-(4-chlorophenyl)-1-phenylprop-2-en-1-ol (3d)



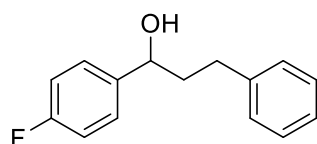
(E)-1-(4-fluorophenyl)-3-phenylprop-2-en-1-ol (3e)



19F NMR
(564.92 MHz, CDCl3)



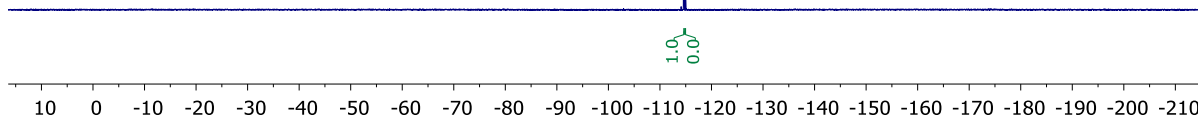
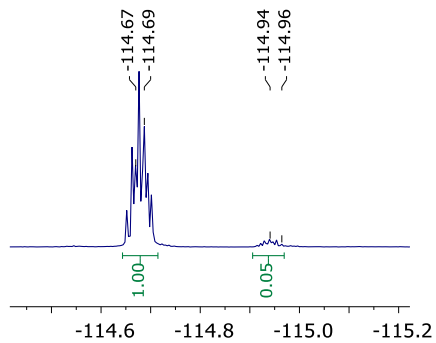
A



B

A:B (95:5)

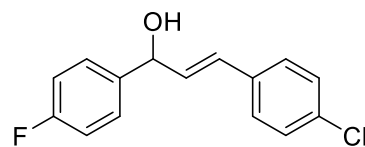
-114.67
-114.69
-114.94
-114.96



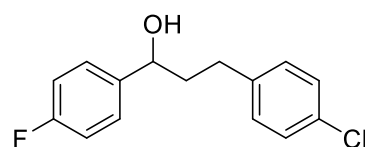
(E)-3-(4-chlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-ol (3f)

1H NMR
(600.44 MHz, CDCl3)

7.40
7.40
7.39
7.39
7.38
7.38
7.31
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.26 CDCl3
7.07
7.07
7.06
7.06
7.06
7.05
7.05
6.64
6.64
6.62
6.61
6.34
6.33
6.32
6.30
5.37
5.37
5.36
5.36
5.36
4.67
4.66
4.66
4.65
4.65
4.64
2.72
2.71
2.70
2.69
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2.65
2.64
2.64
2.63
2.63
2.08
2.07

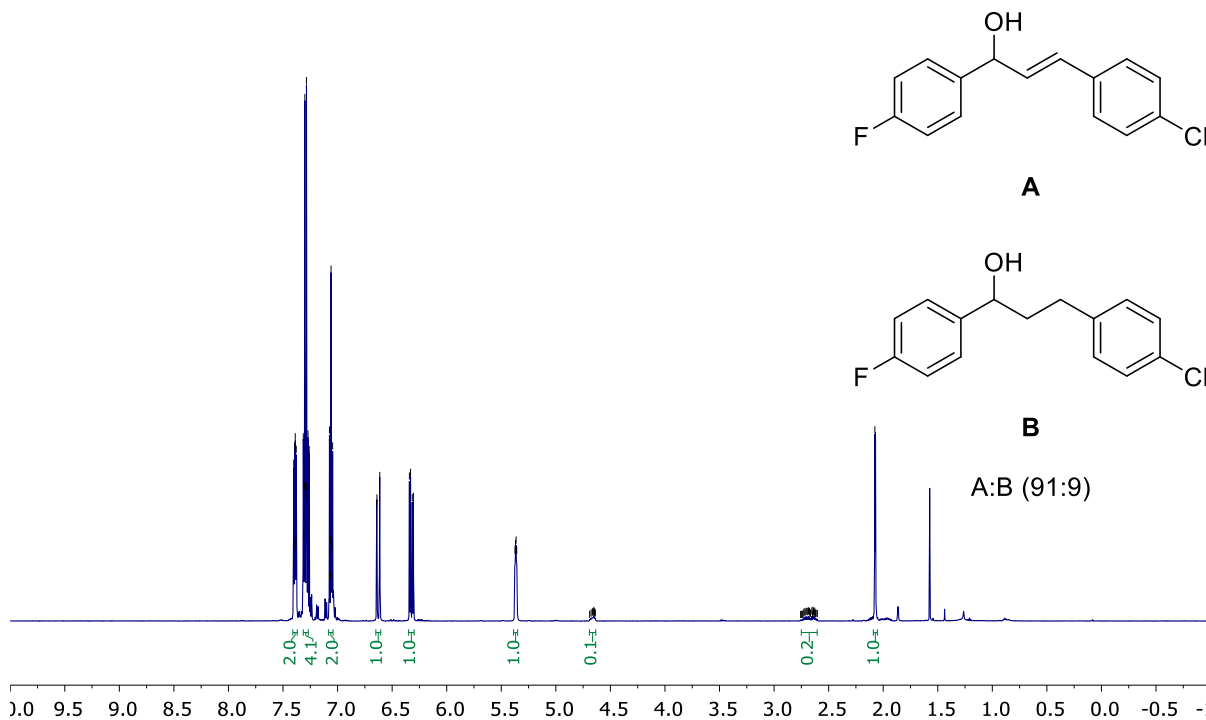


A



B

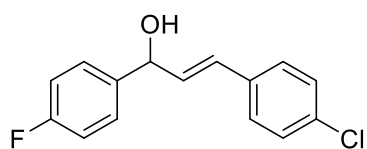
A:B (91:9)



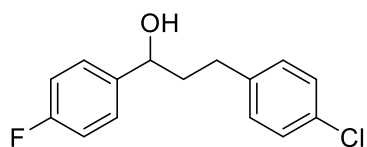
¹³C NMR
(151.00 MHz, CDCl₃)

163.3
161.7
138.5
138.4
135.0
133.7
132.1
129.6
128.9
128.2
128.2
128.0
115.7
115.6

77.4 CDCl₃
77.2 CDCl₃
76.9 CDCl₃
74.5

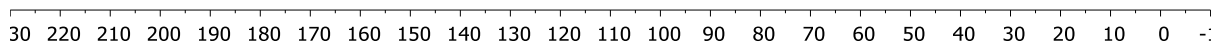


A



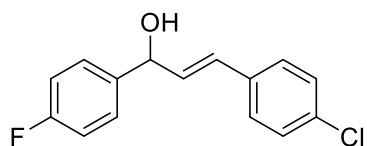
B

A:B (91:9)

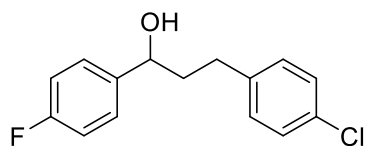


¹⁹F NMR
(564.92 MHz, CDCl₃)

-114.42
-114.44
-114.72
-114.73
-114.75

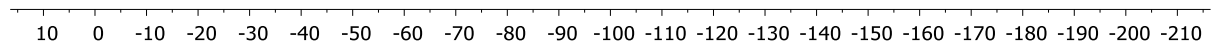
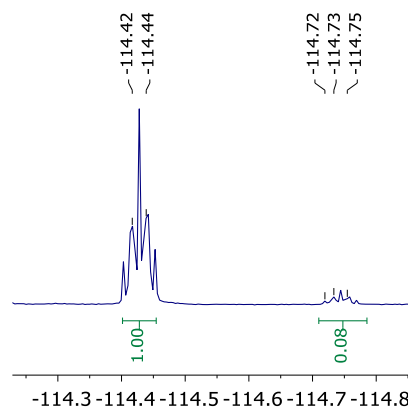


A

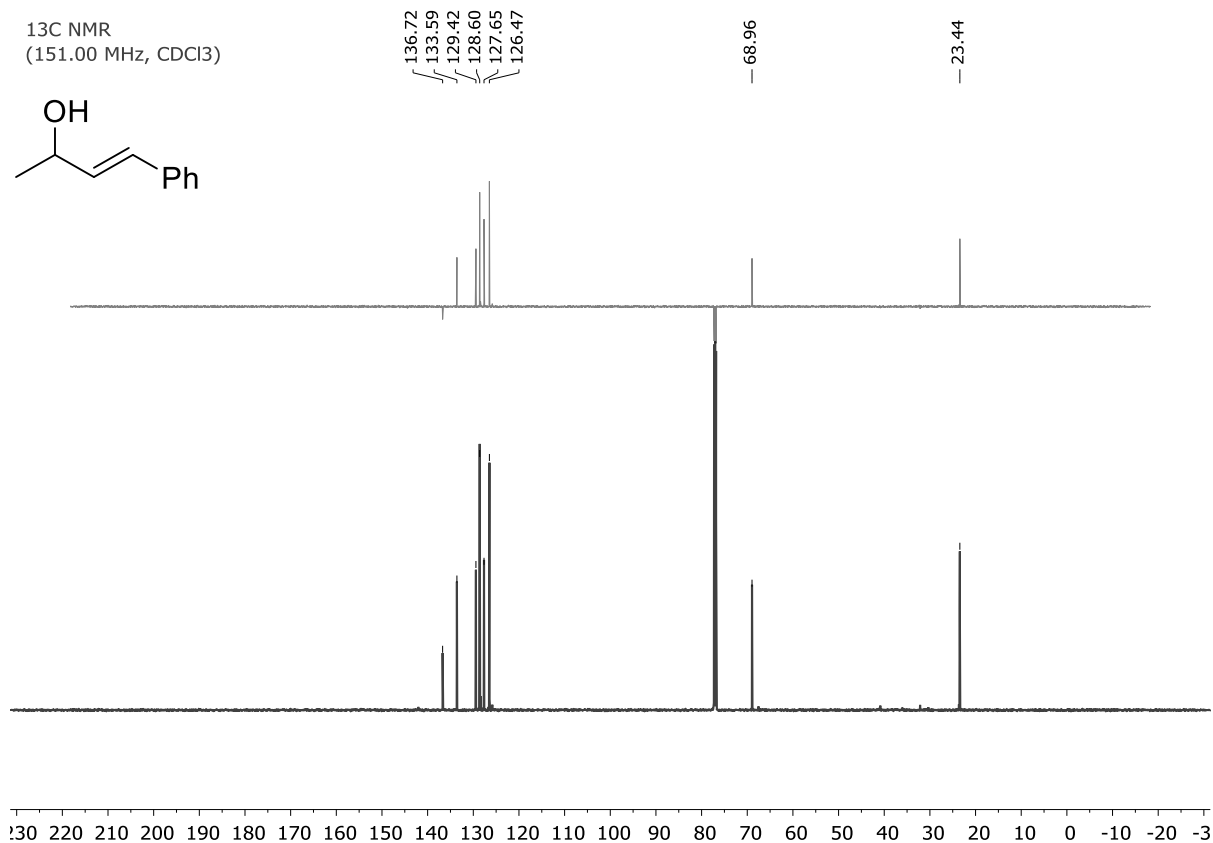
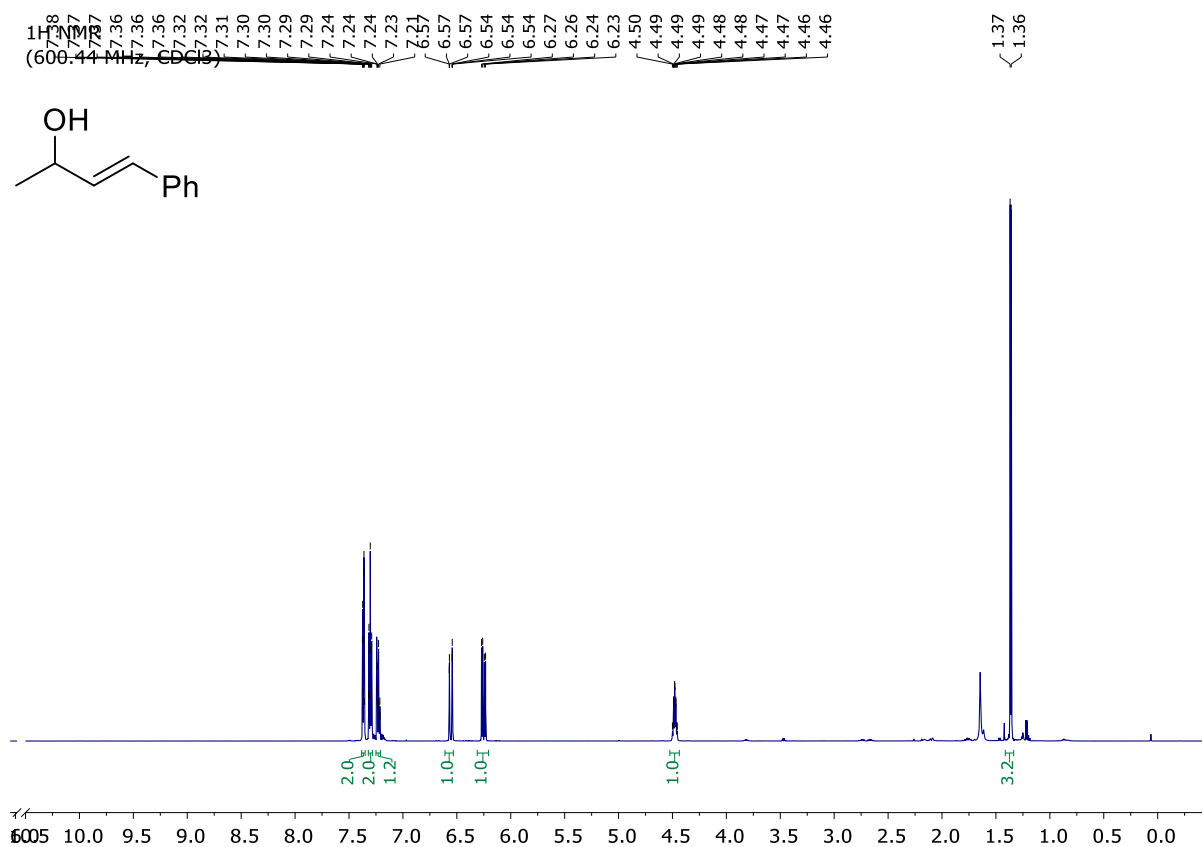


B

A:B (91:9)

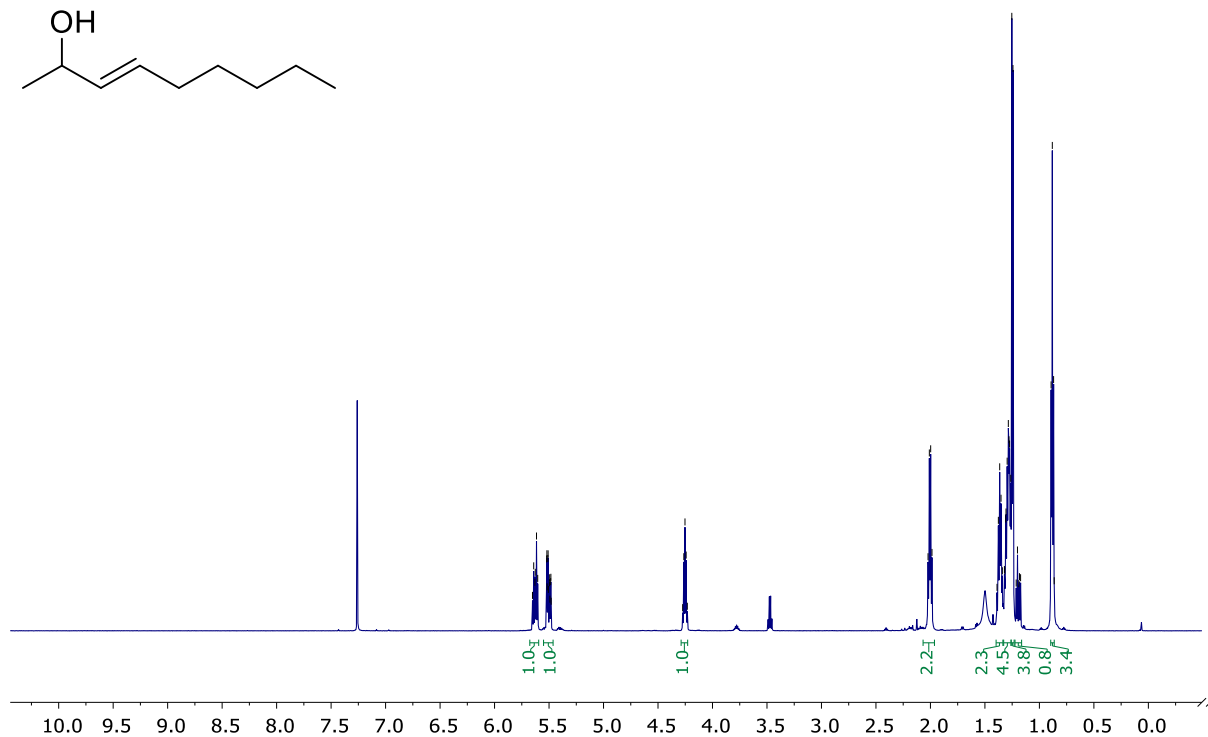
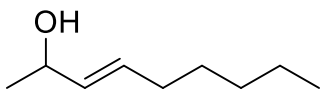


(E)-4-phenylbut-3-en-2-ol (3g)

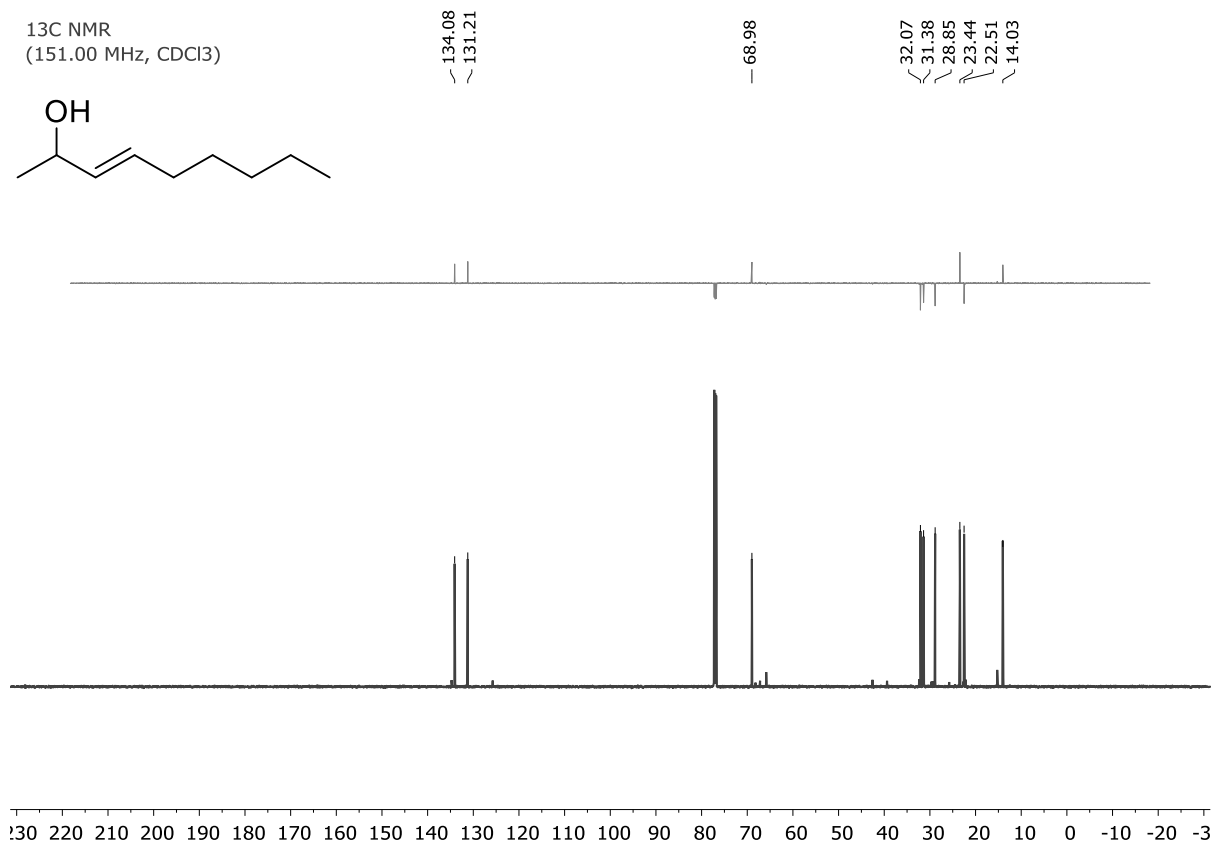
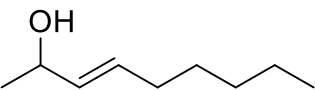


(E)-non-3-en-2-ol (3h)

¹H NMR (600.44 MHz, CDCl₃)

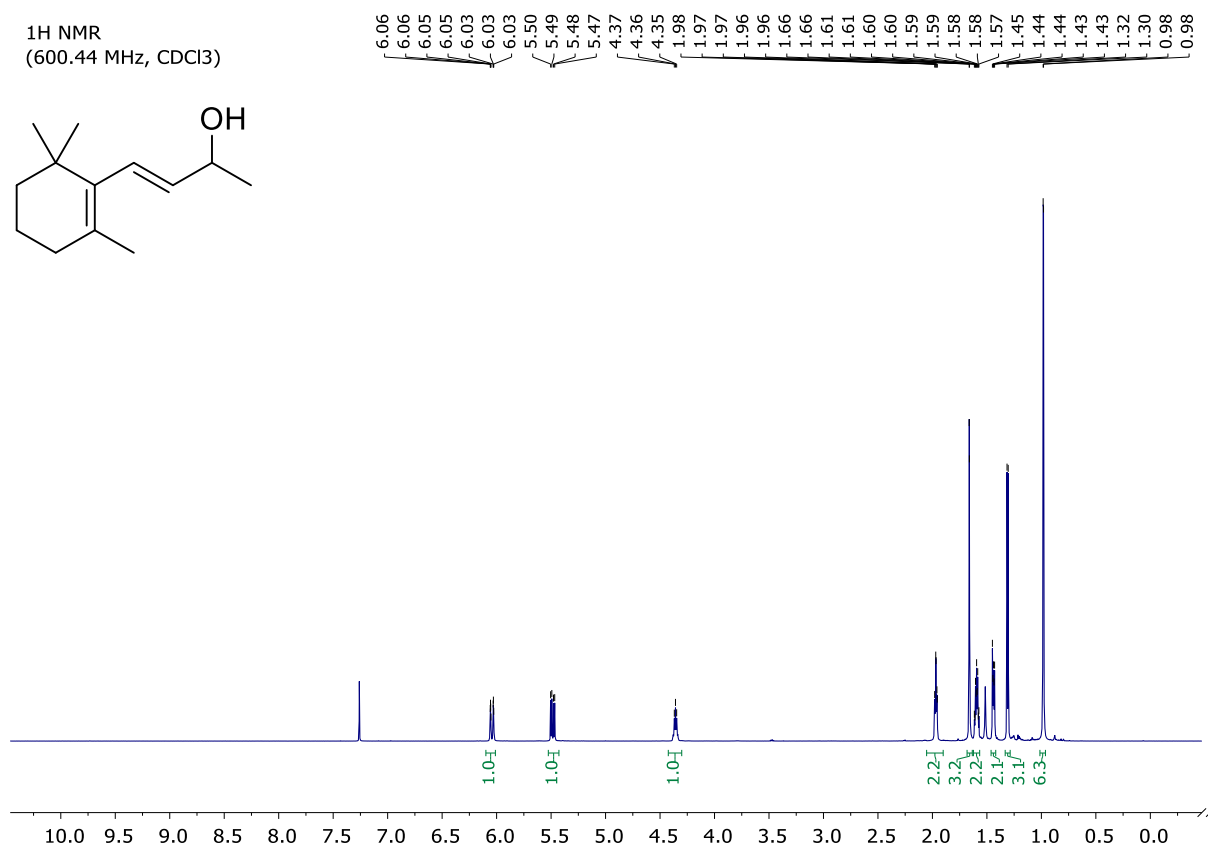
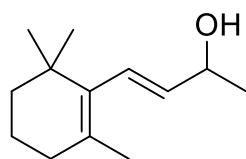


¹³C NMR (151.00 MHz, CDCl₃)

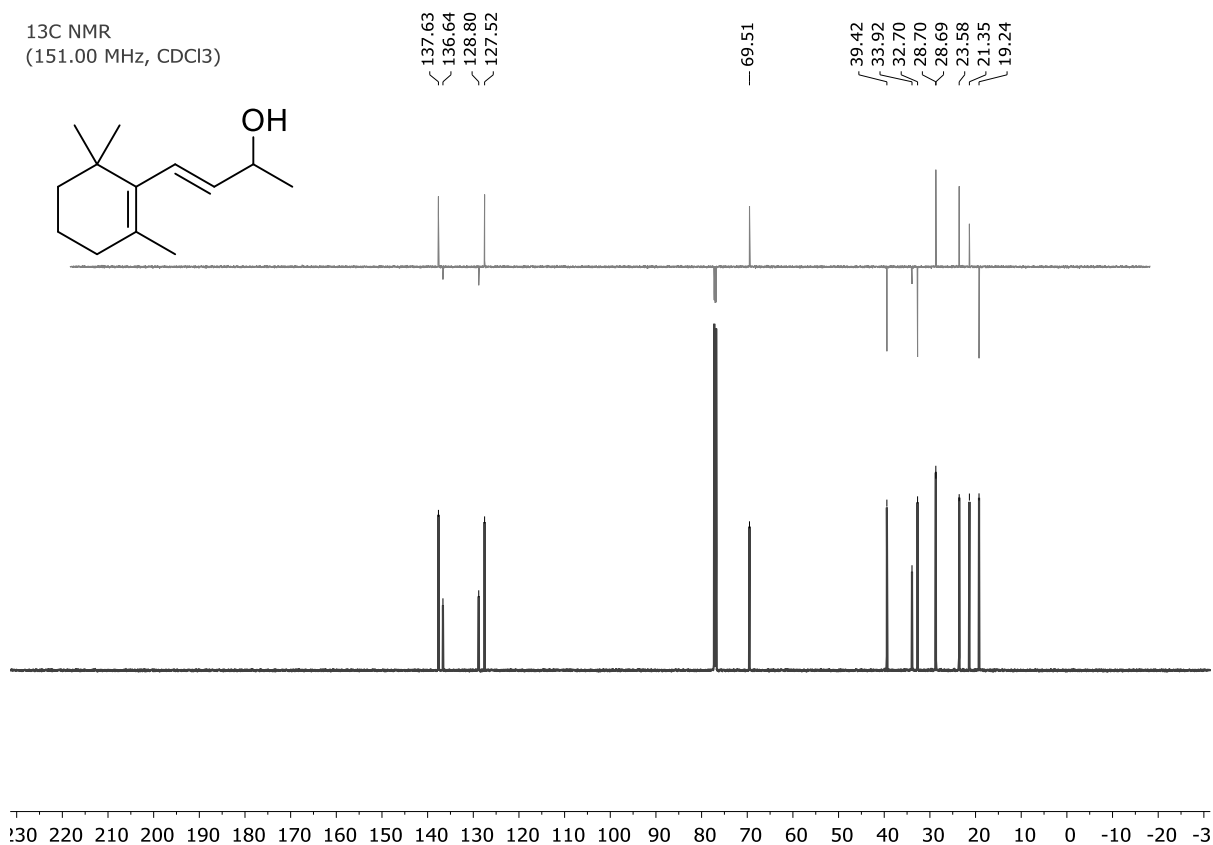
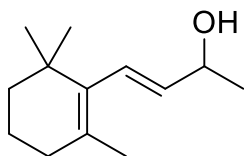


(E)-4-(2,6,6-trimethylcyclohex-1-en-1-yl)but-3-en-2-ol (3i)

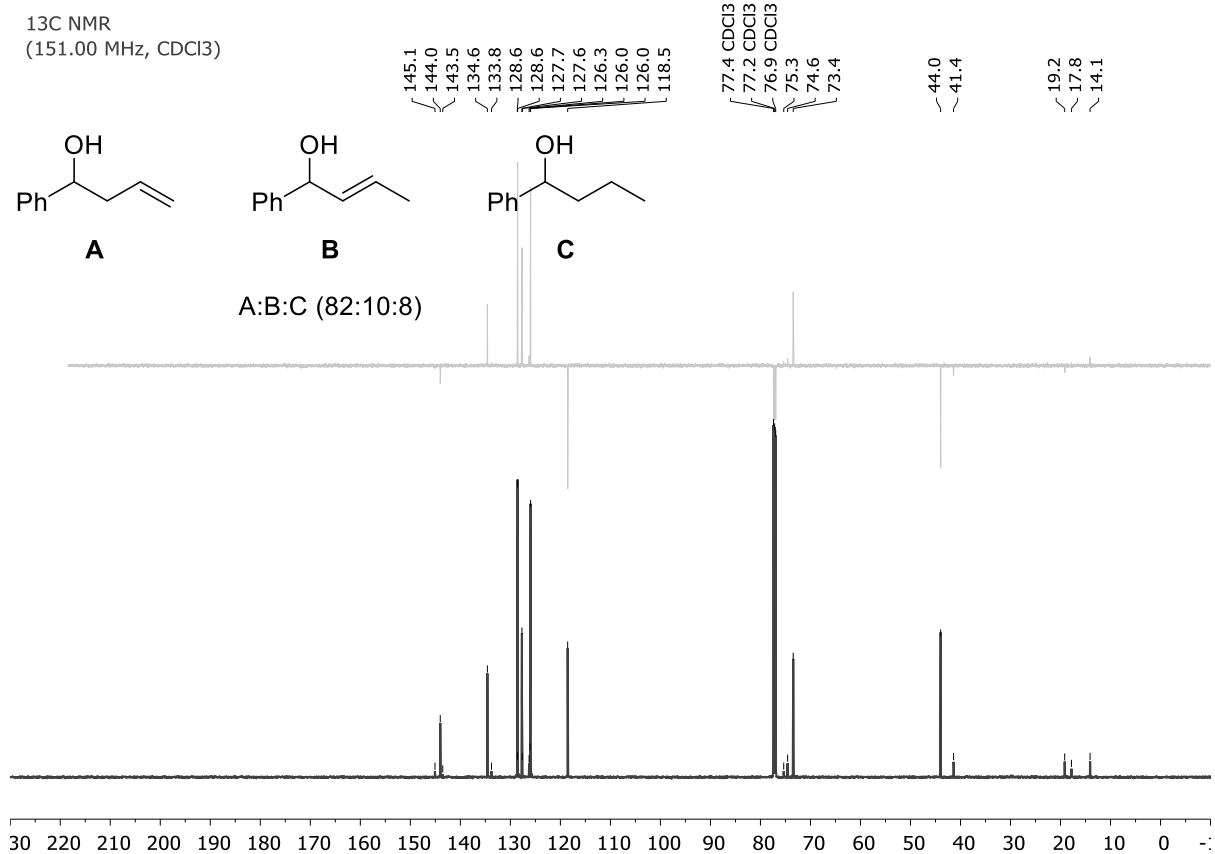
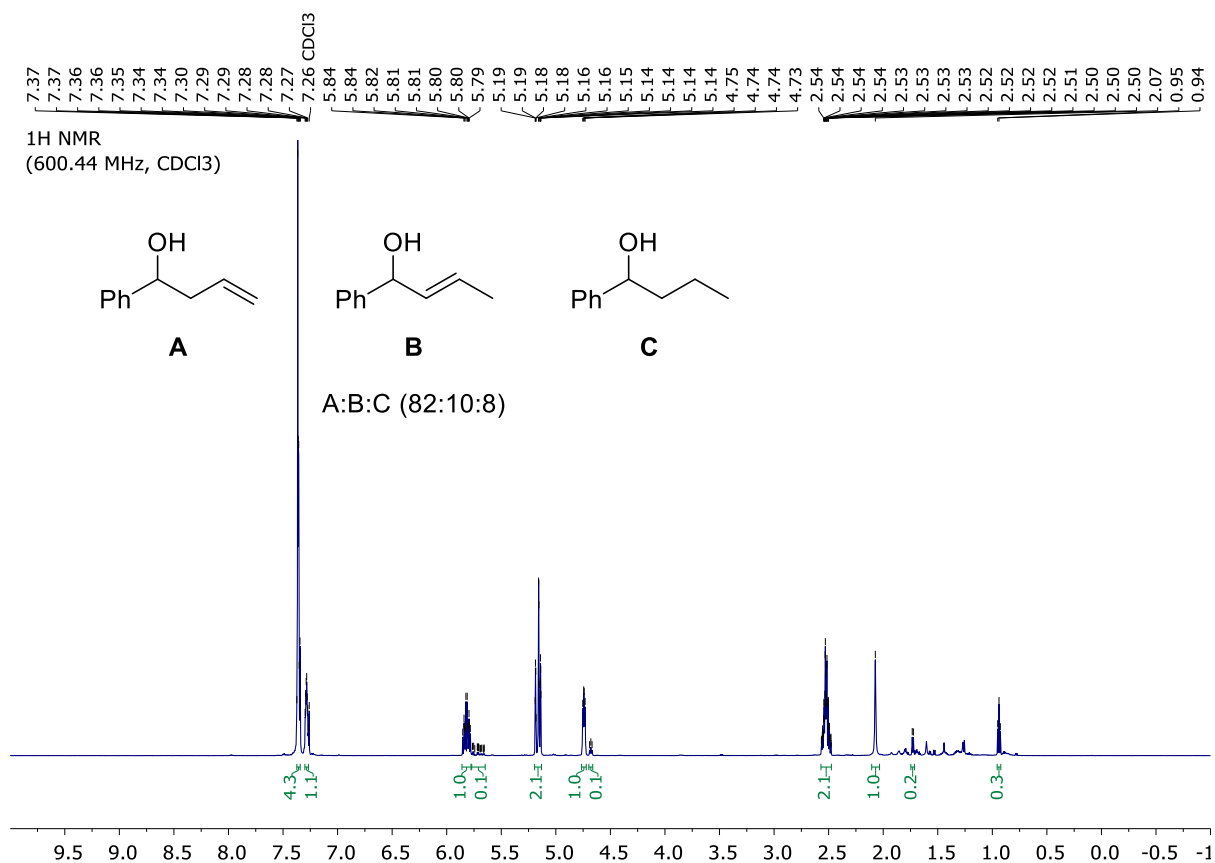
¹H NMR
(600.44 MHz, CDCl₃)



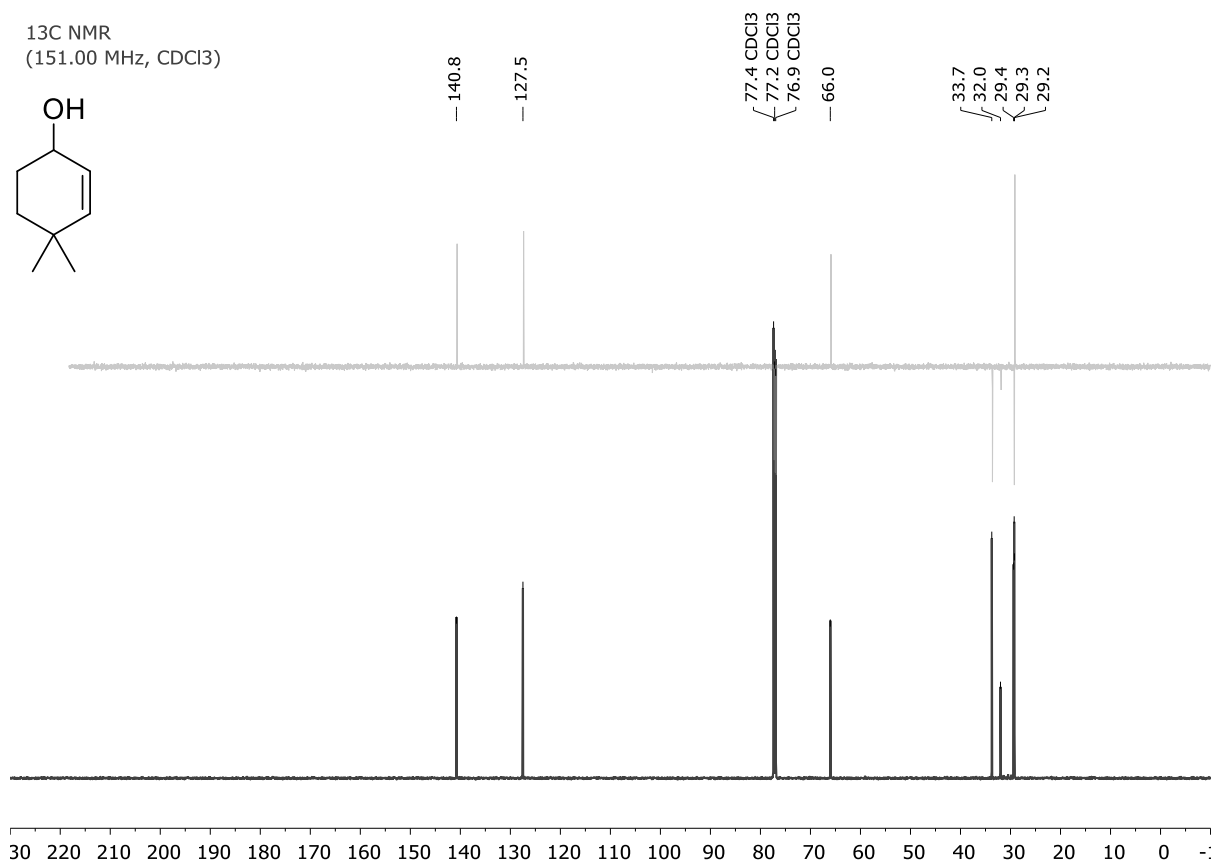
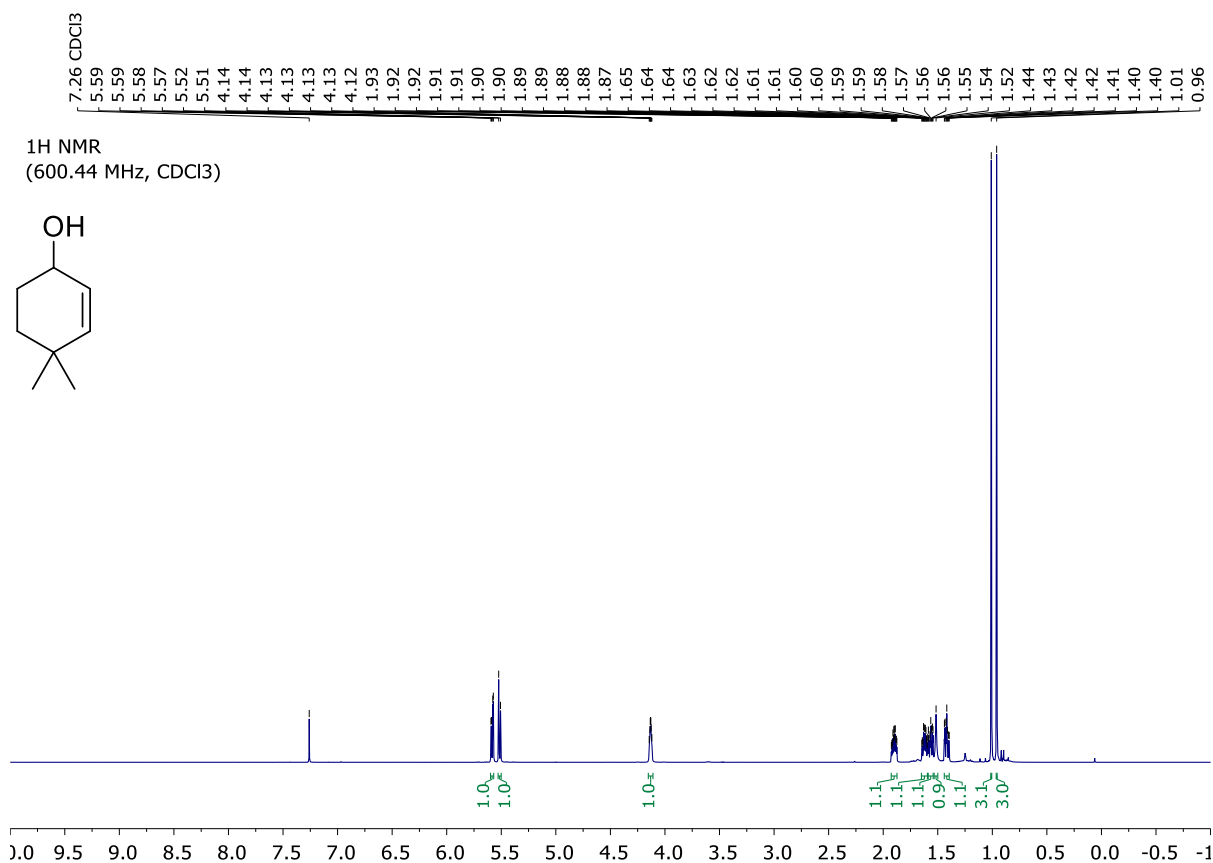
¹³C NMR
(151.00 MHz, CDCl₃)



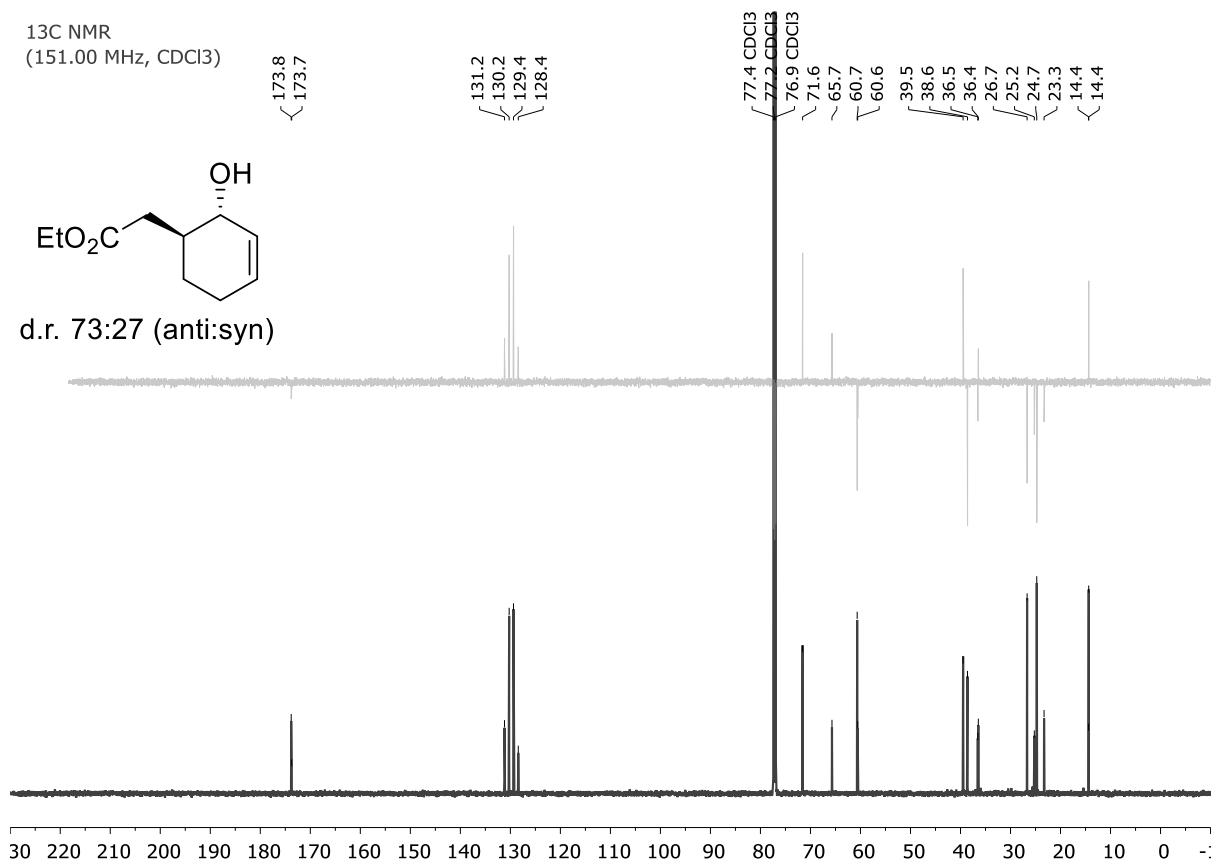
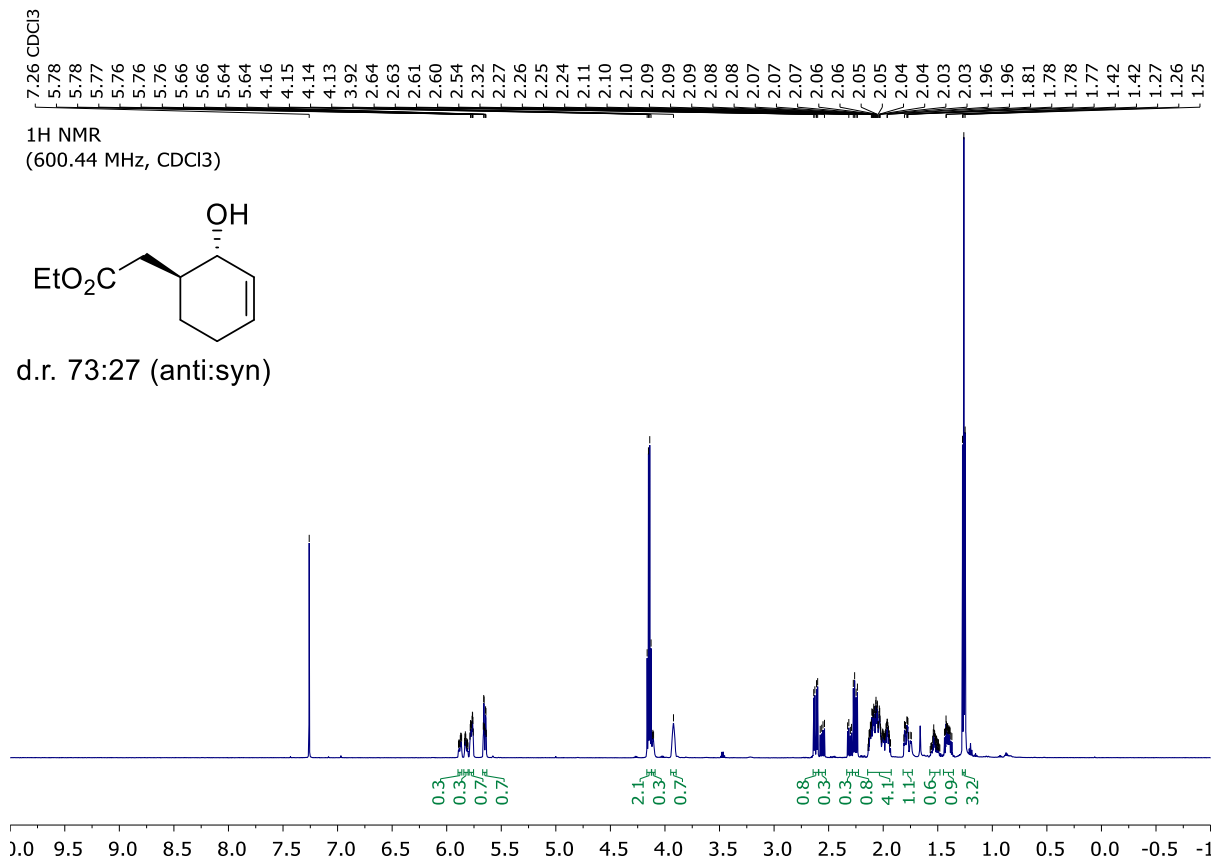
1-phenylbut-3-en-1-ol (3j)



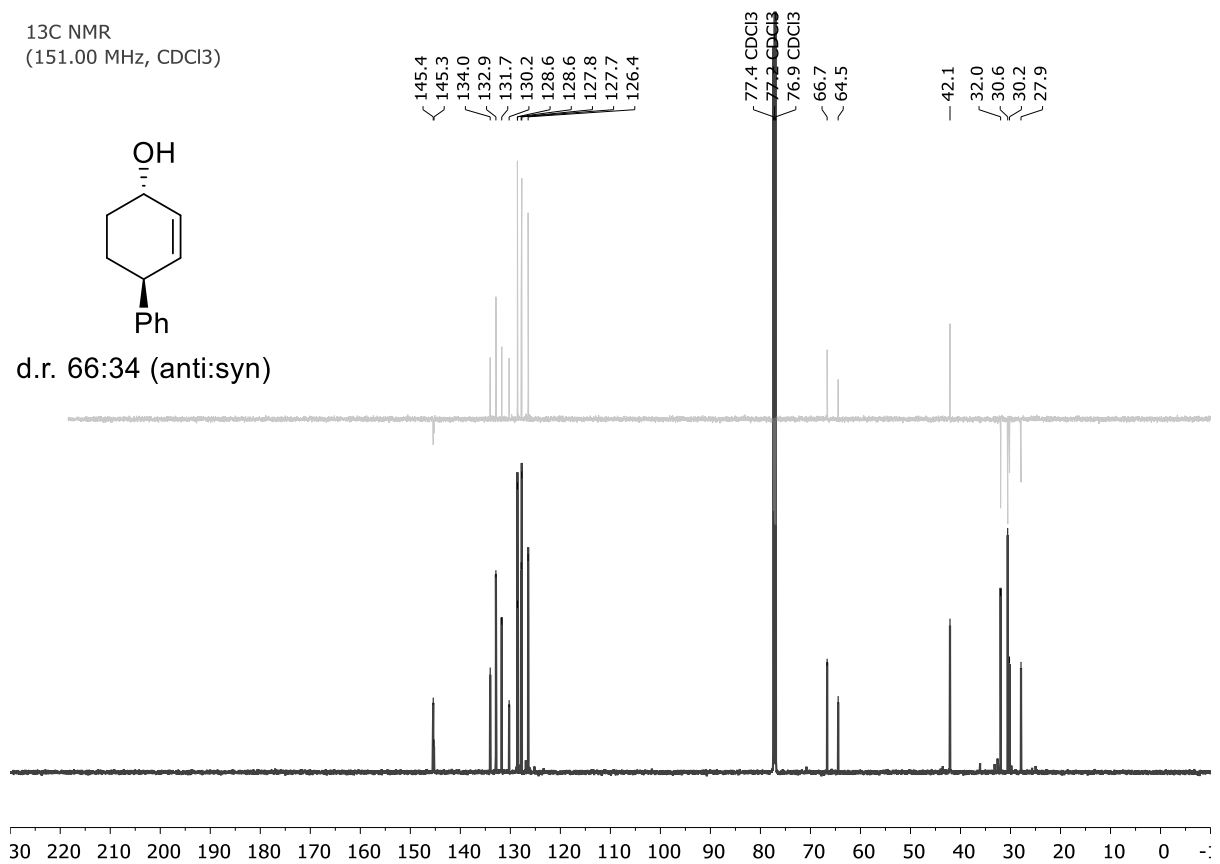
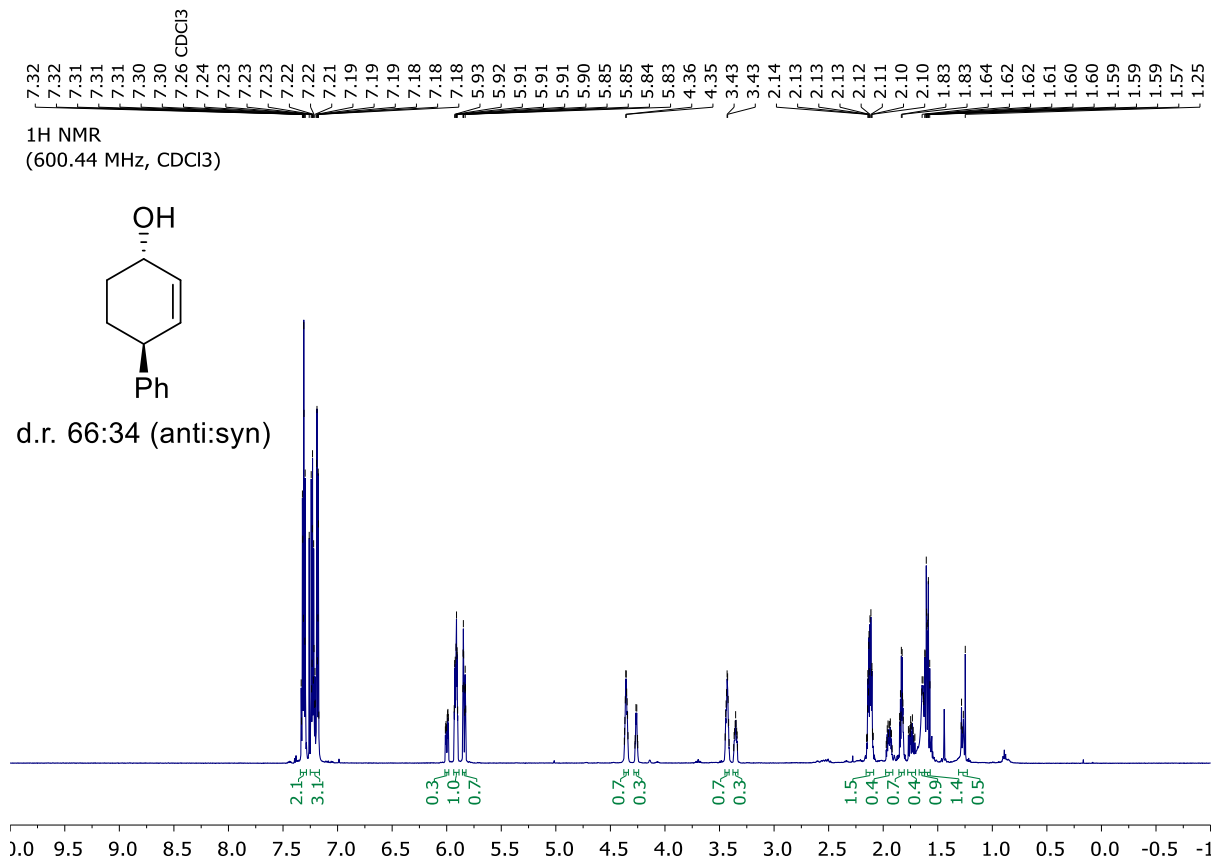
4,4-dimethylcyclohex-2-en-1-ol (3k)



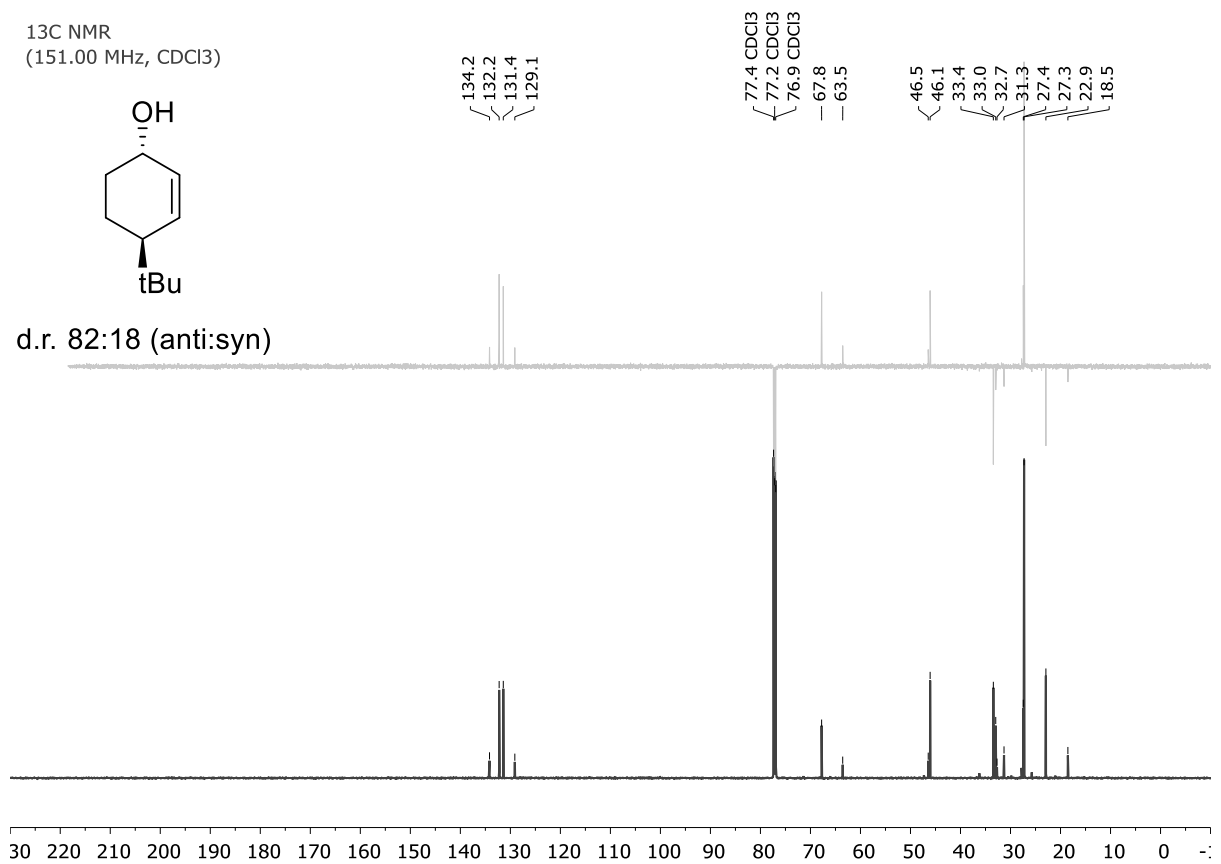
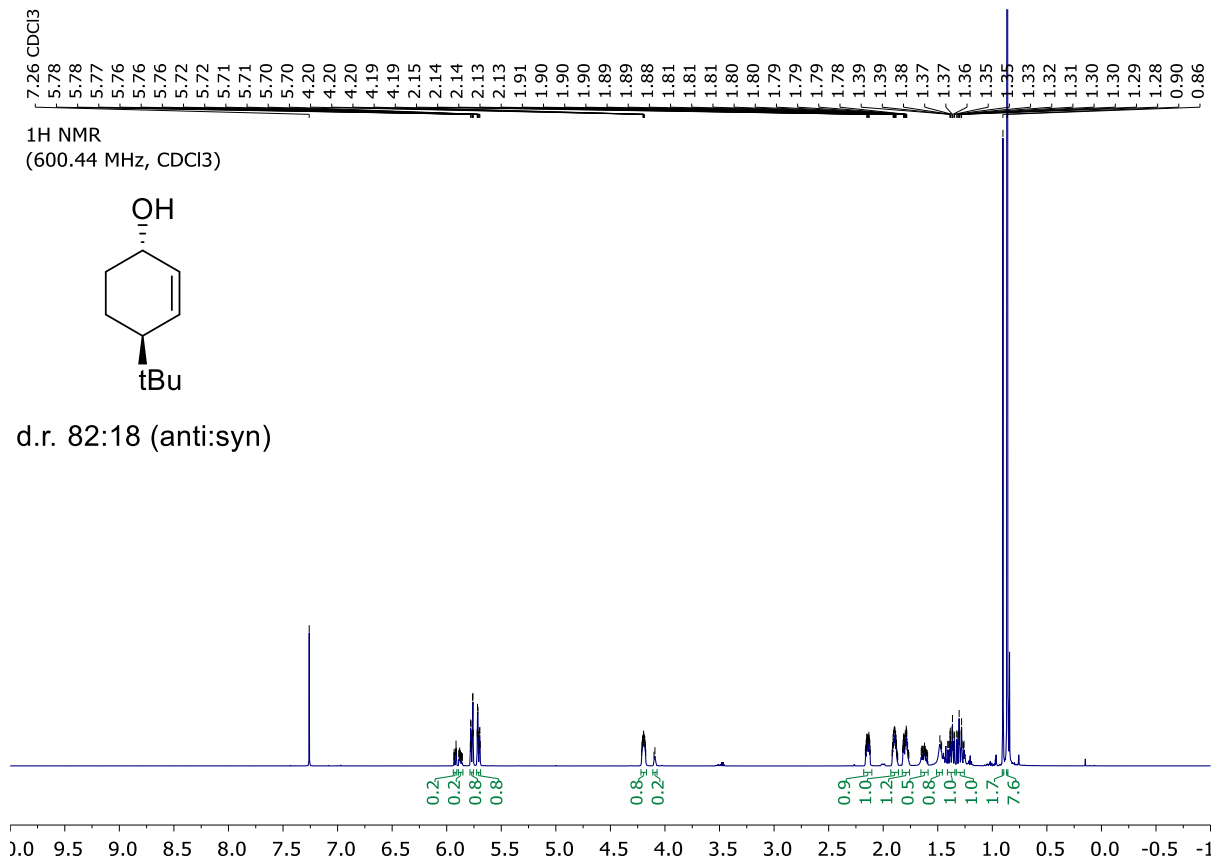
ethyl 2-((1R,2R)-2-hydroxycyclohex-3-en-1-yl)acetate (3l)



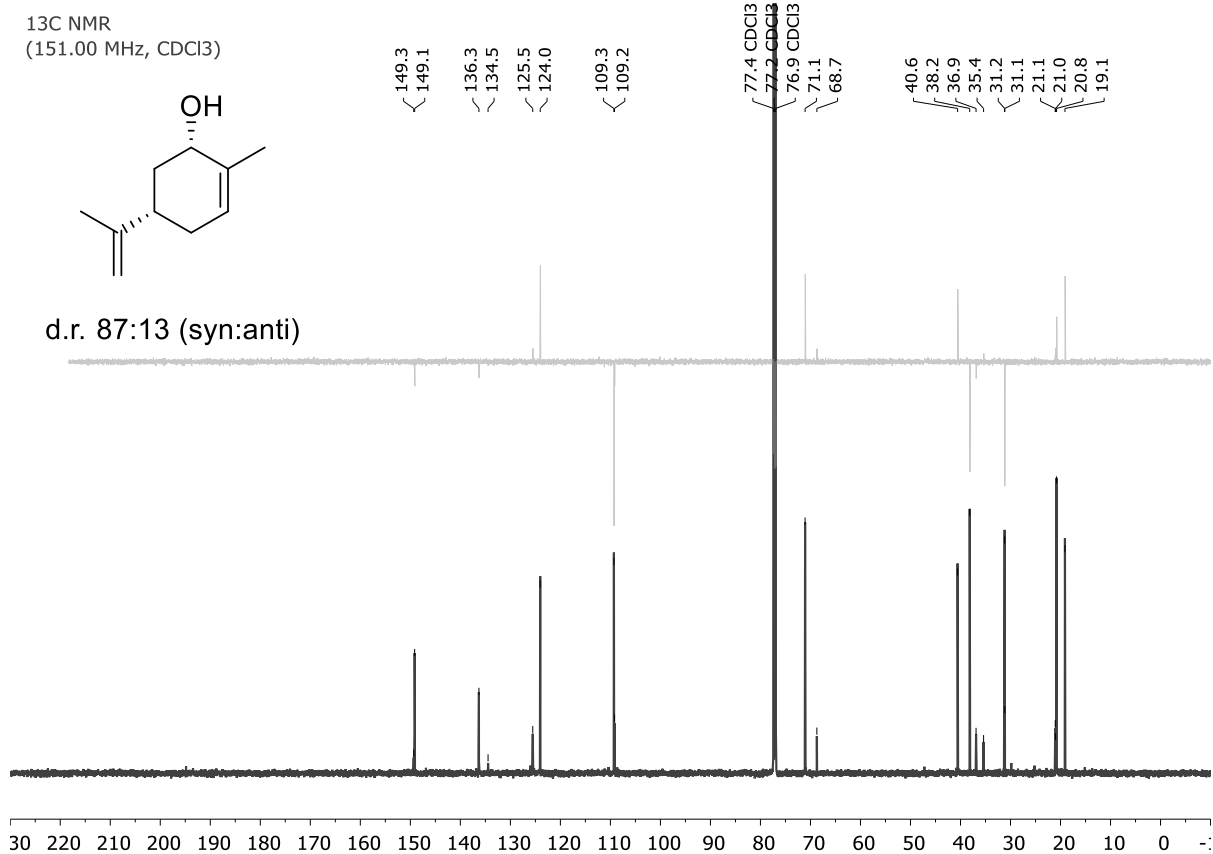
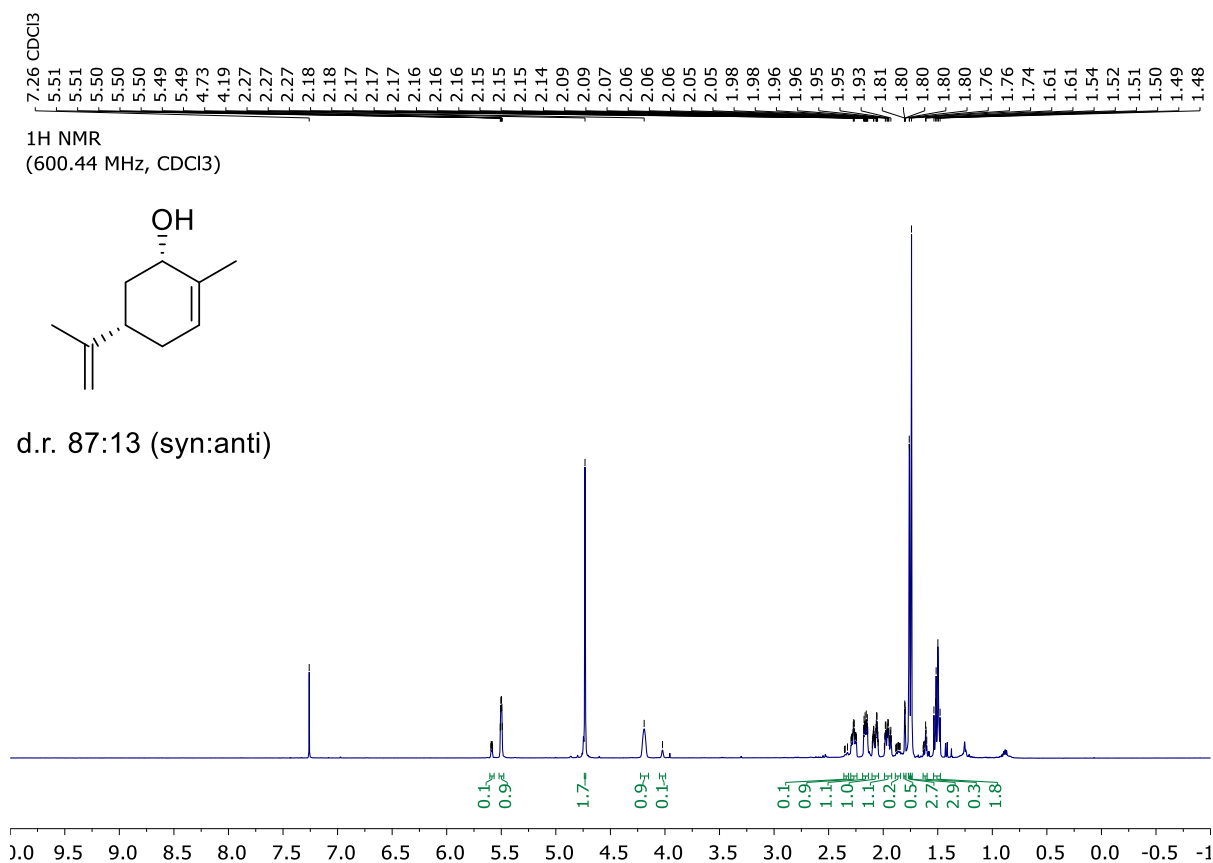
(1S,4S)-1,2,3,4-tetrahydro-[1,1'-biphenyl]-4-ol (3m)



(1R,4R)-4-(tert-butyl)cyclohex-2-en-1-ol (3n)

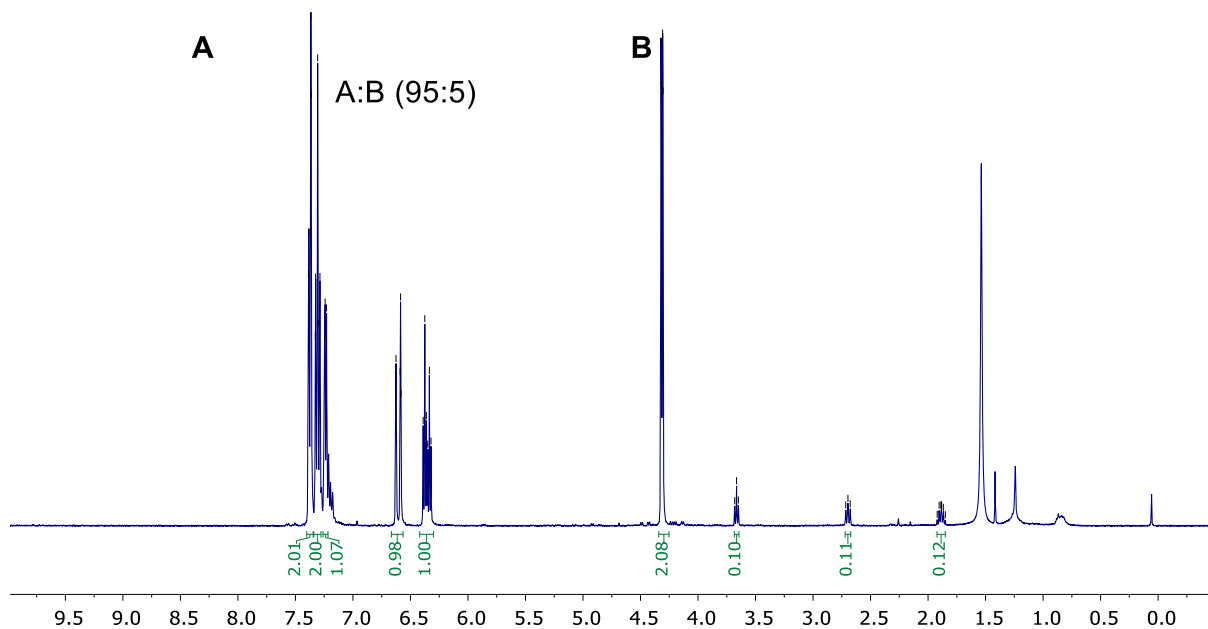
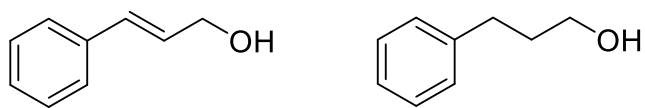


(1R,5R)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-ol (3o)

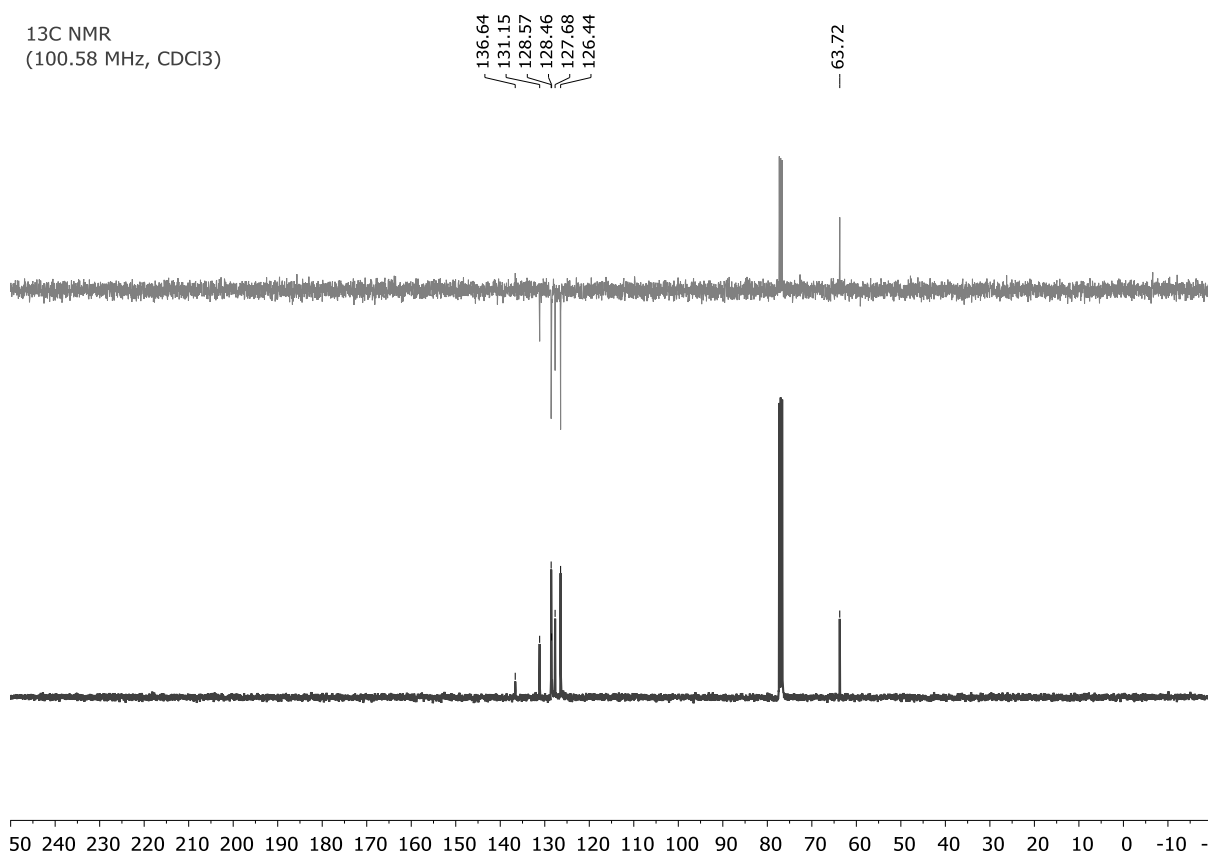


(E)-3-phenylprop-2-en-1-ol (3p)

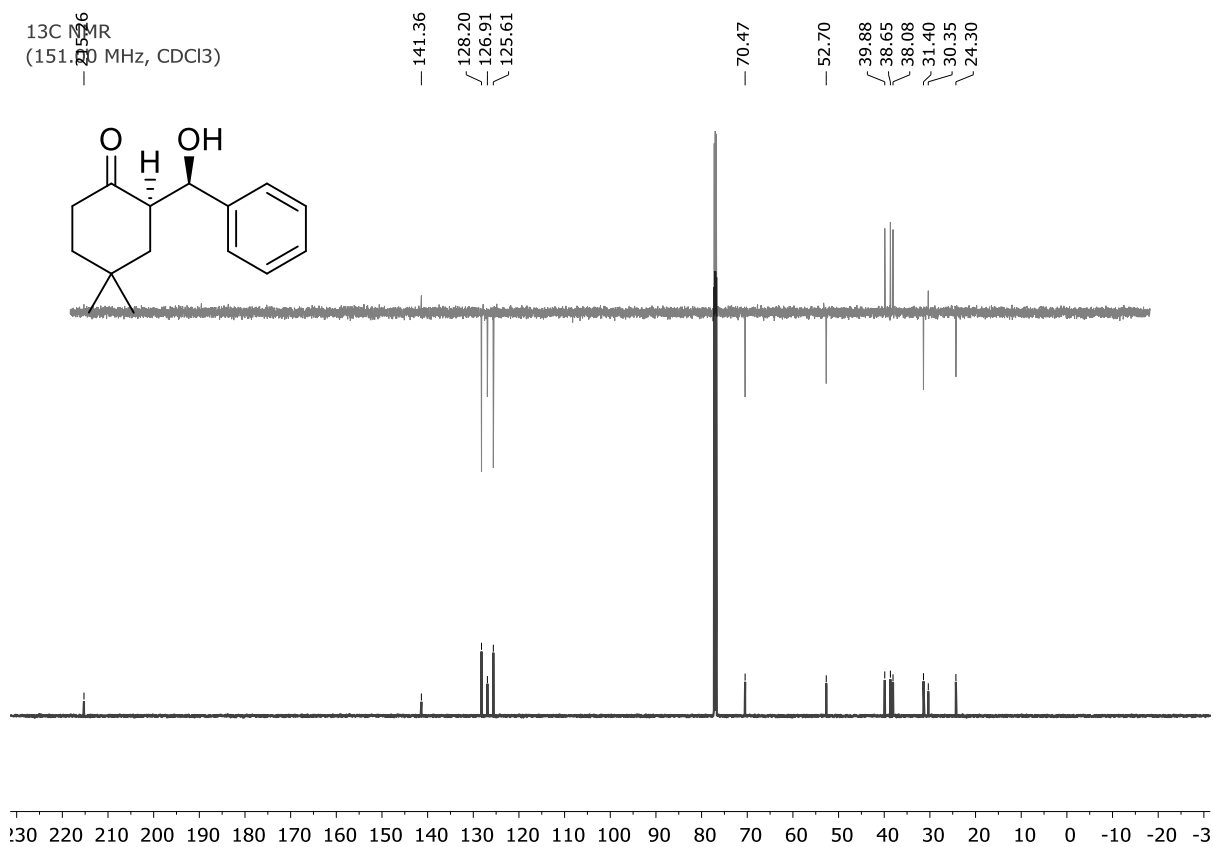
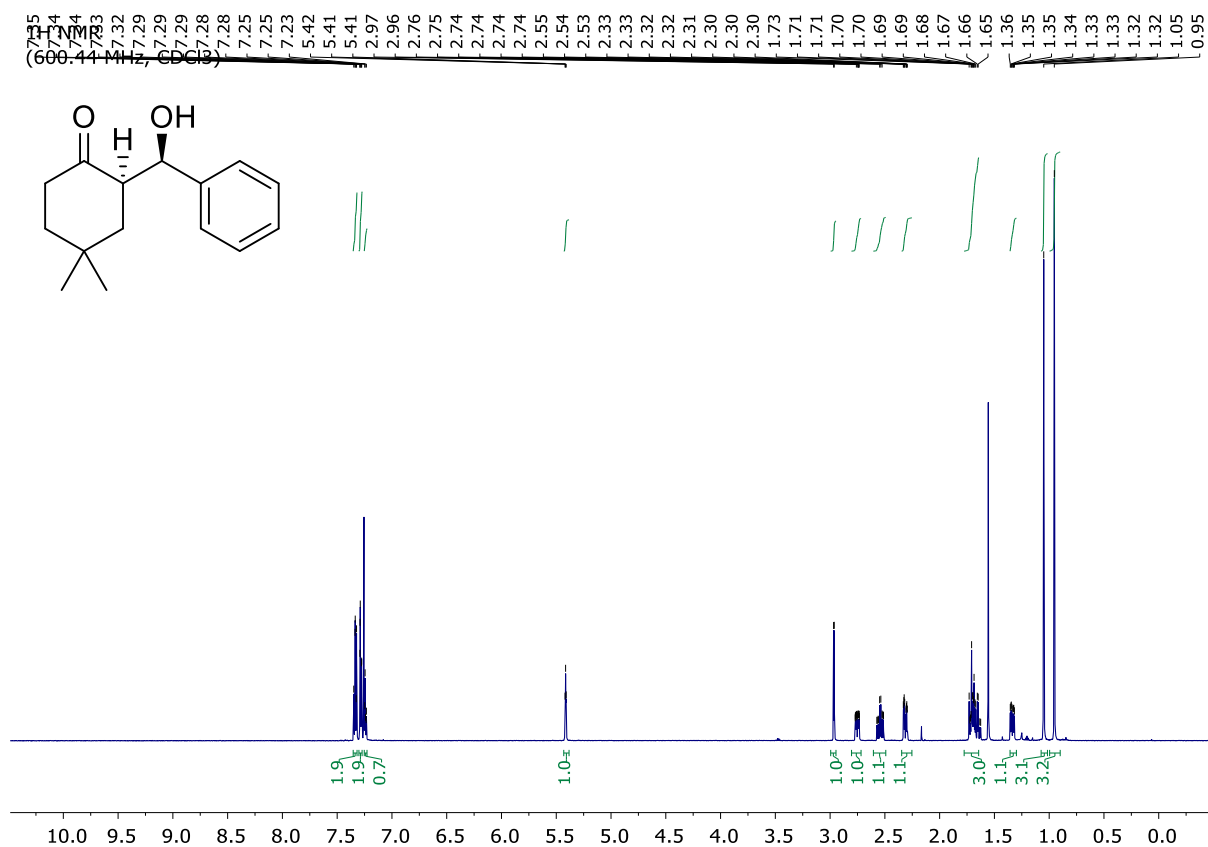
¹H NMR (399.97 MHz, CDCl₃)



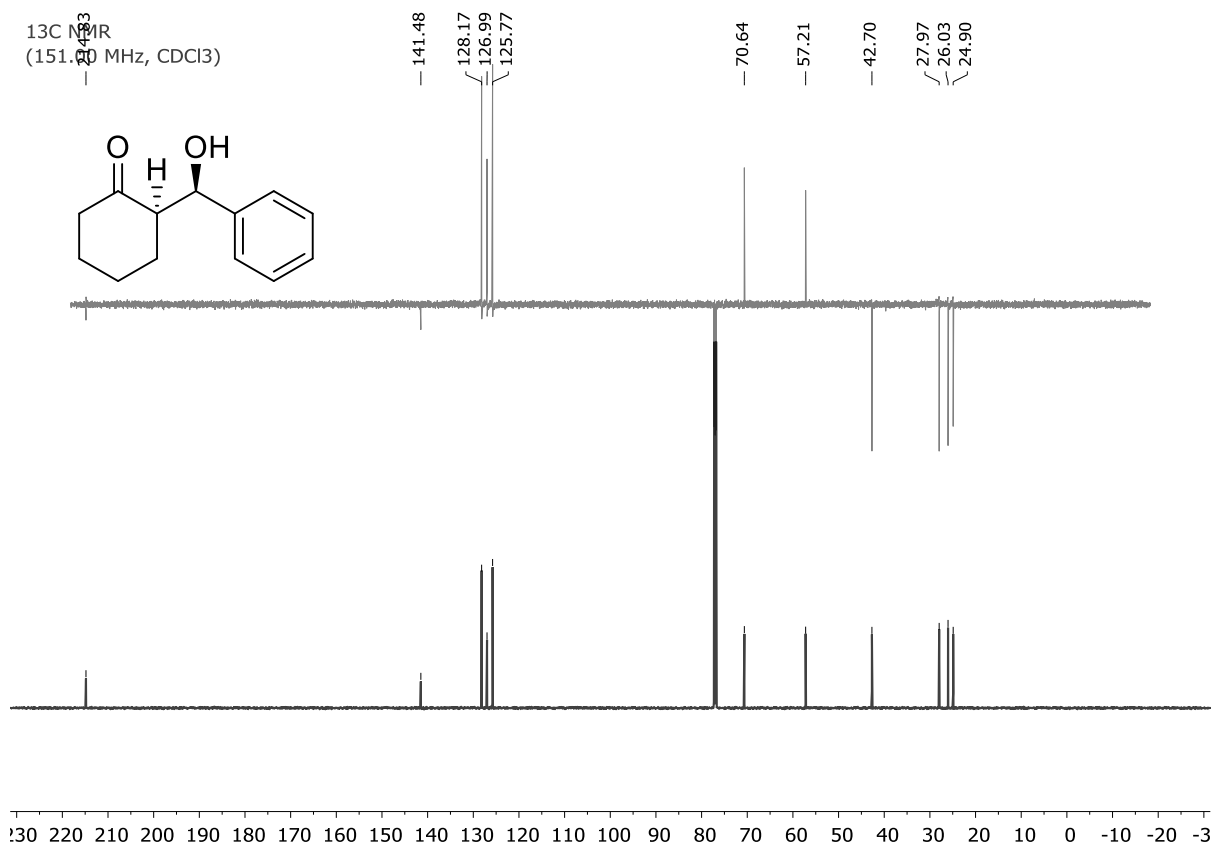
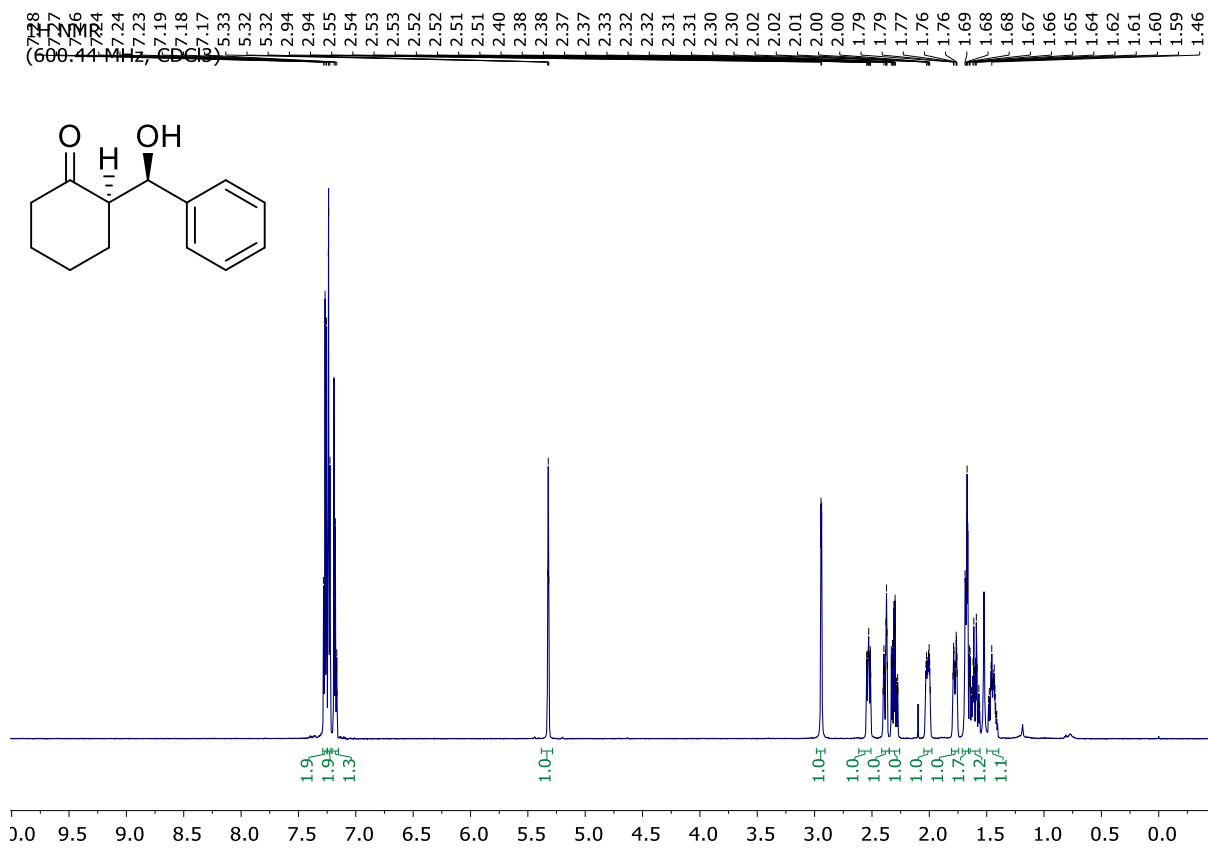
¹³C NMR (100.58 MHz, CDCl₃)



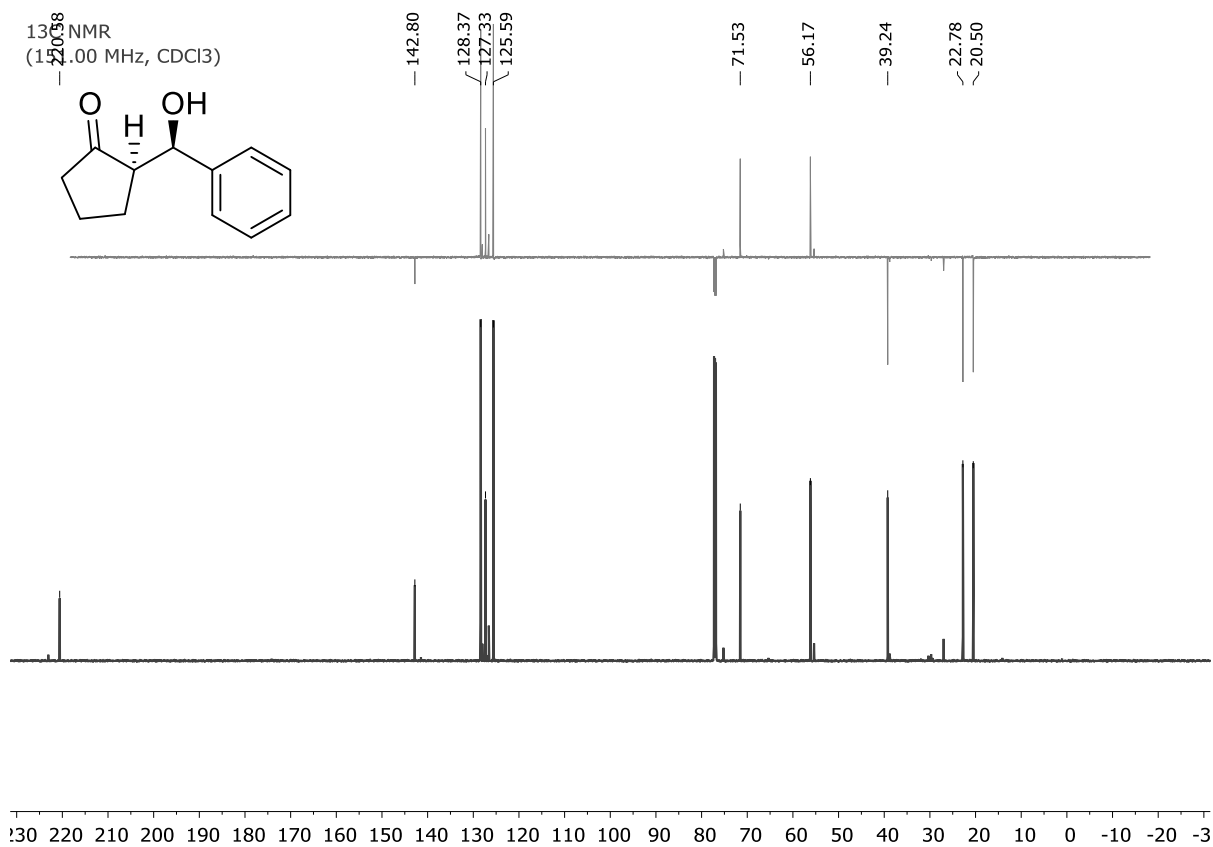
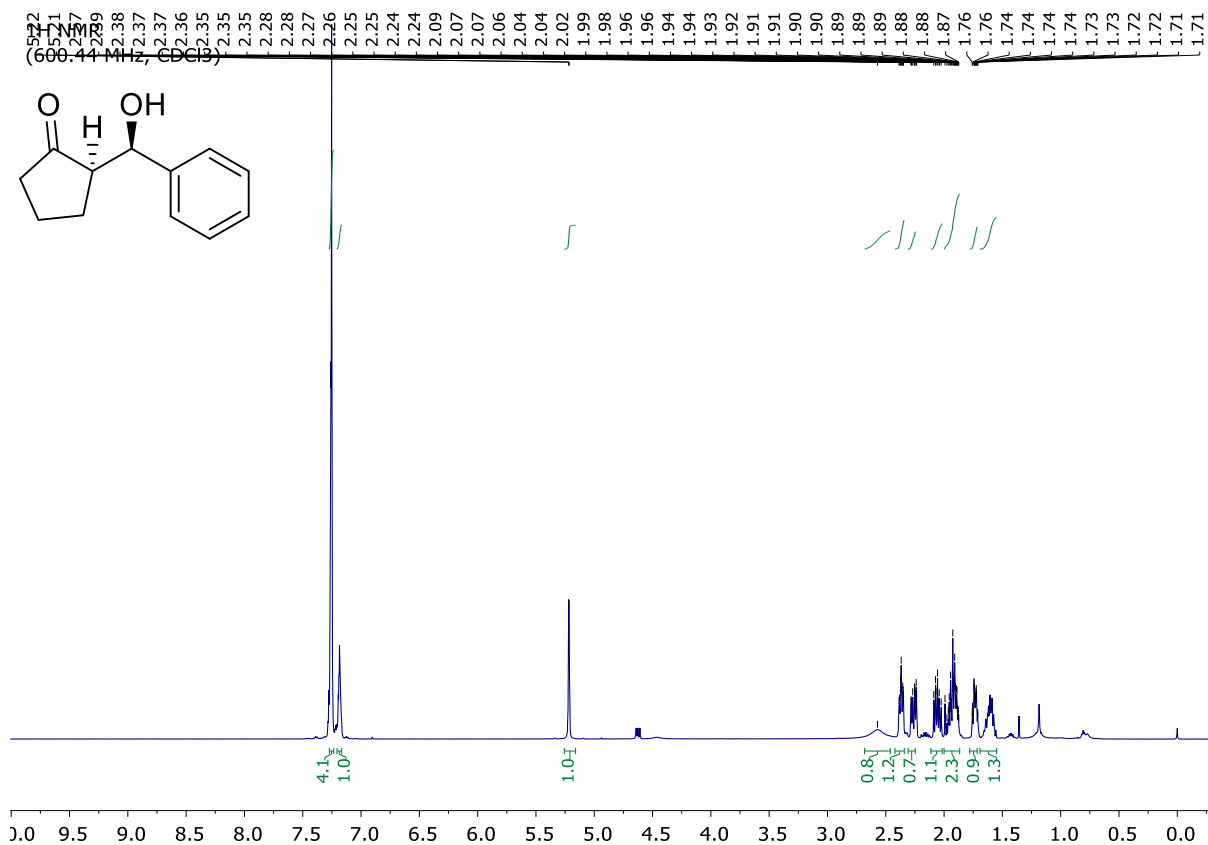
2-(hydroxy(phenyl)methyl)-4,4-dimethylcyclohexan-1-one (4a)



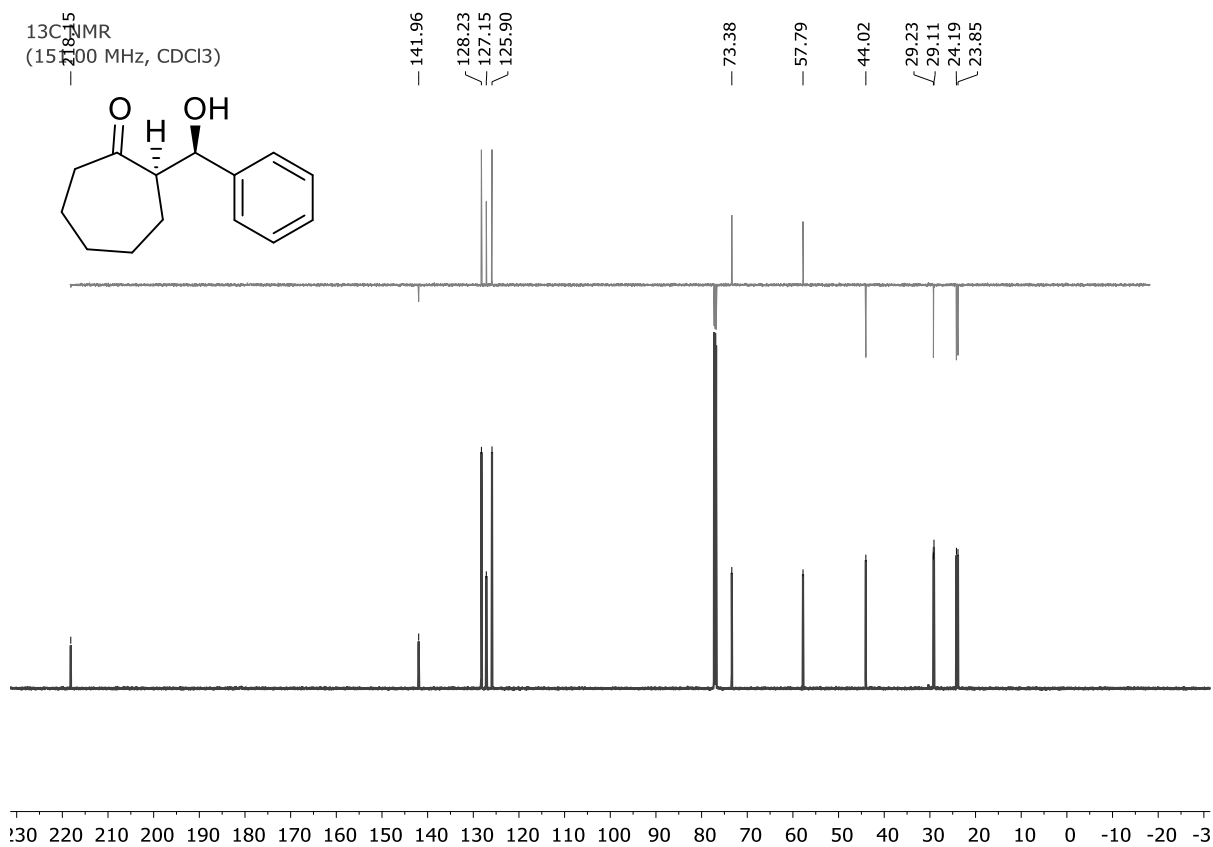
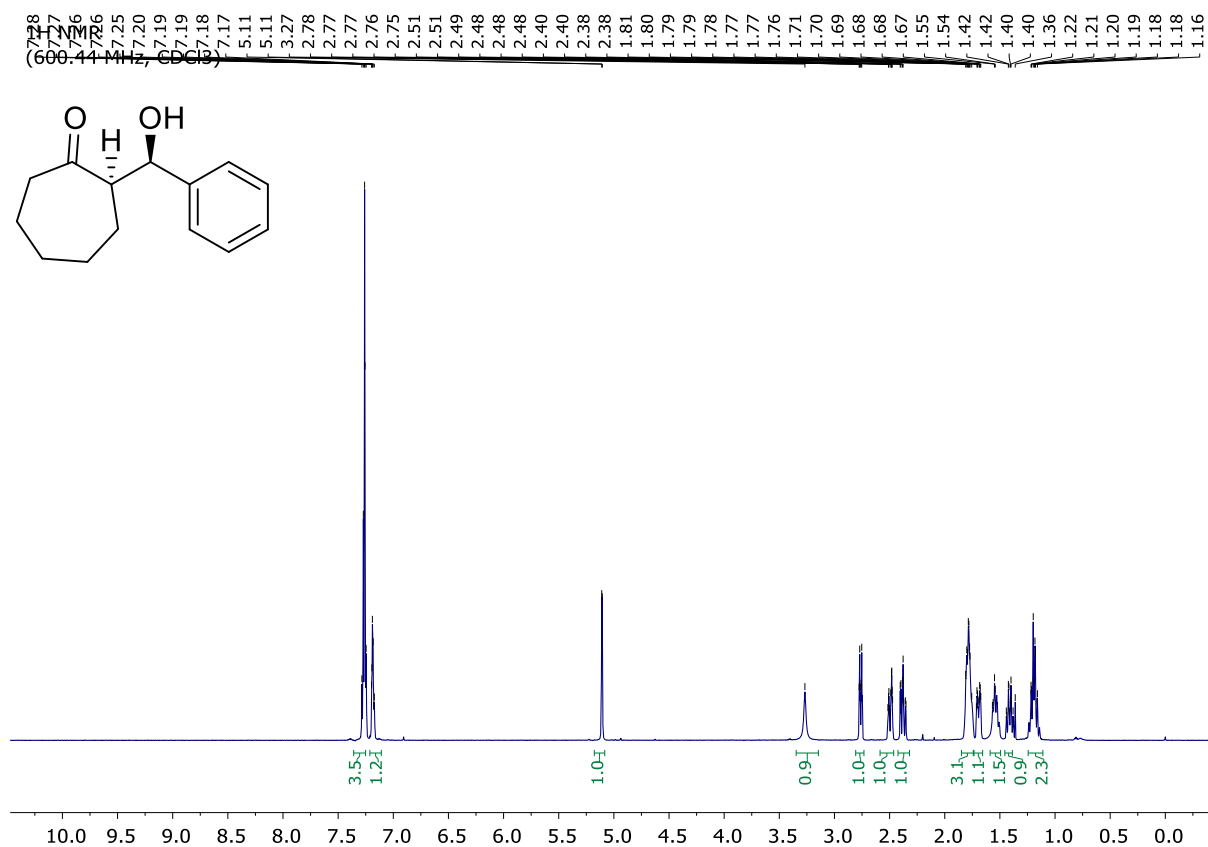
2-(hydroxy(phenyl)methyl)cyclohexan-1-one (4b)



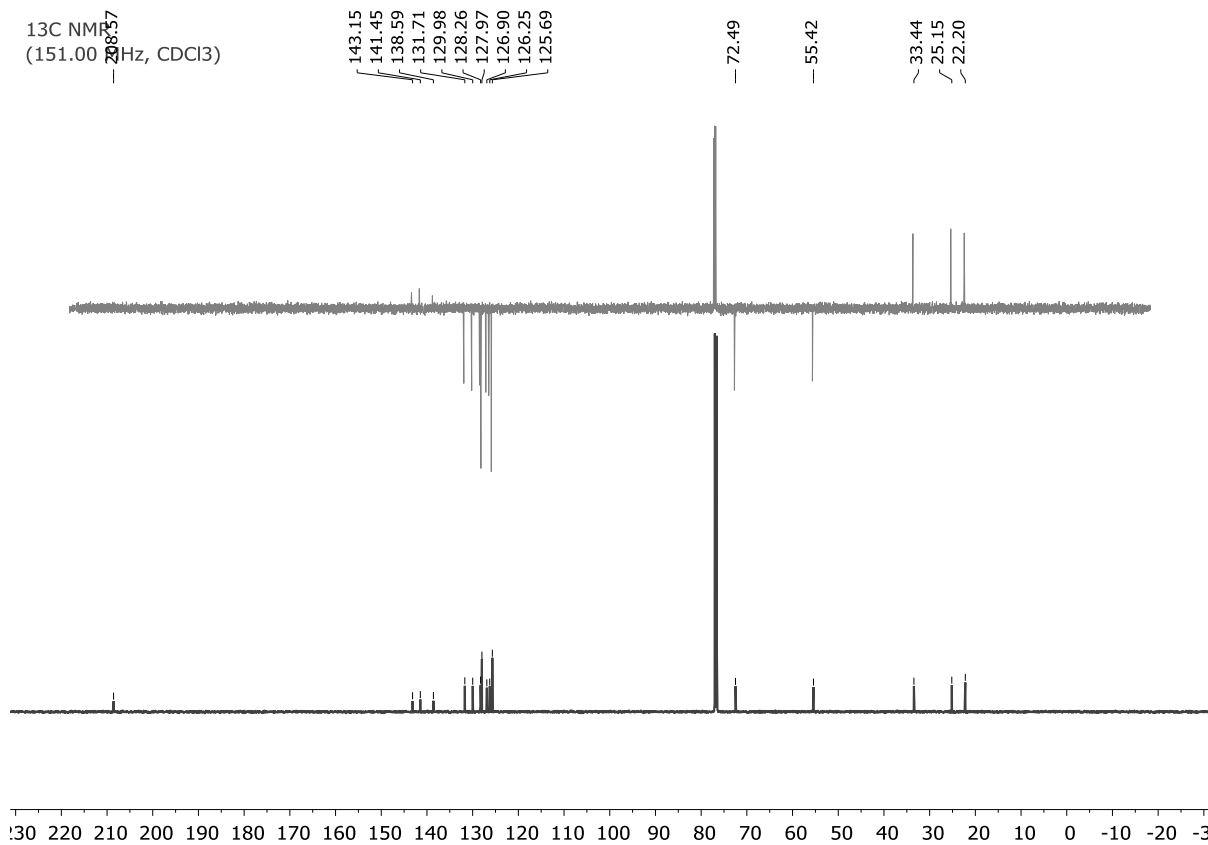
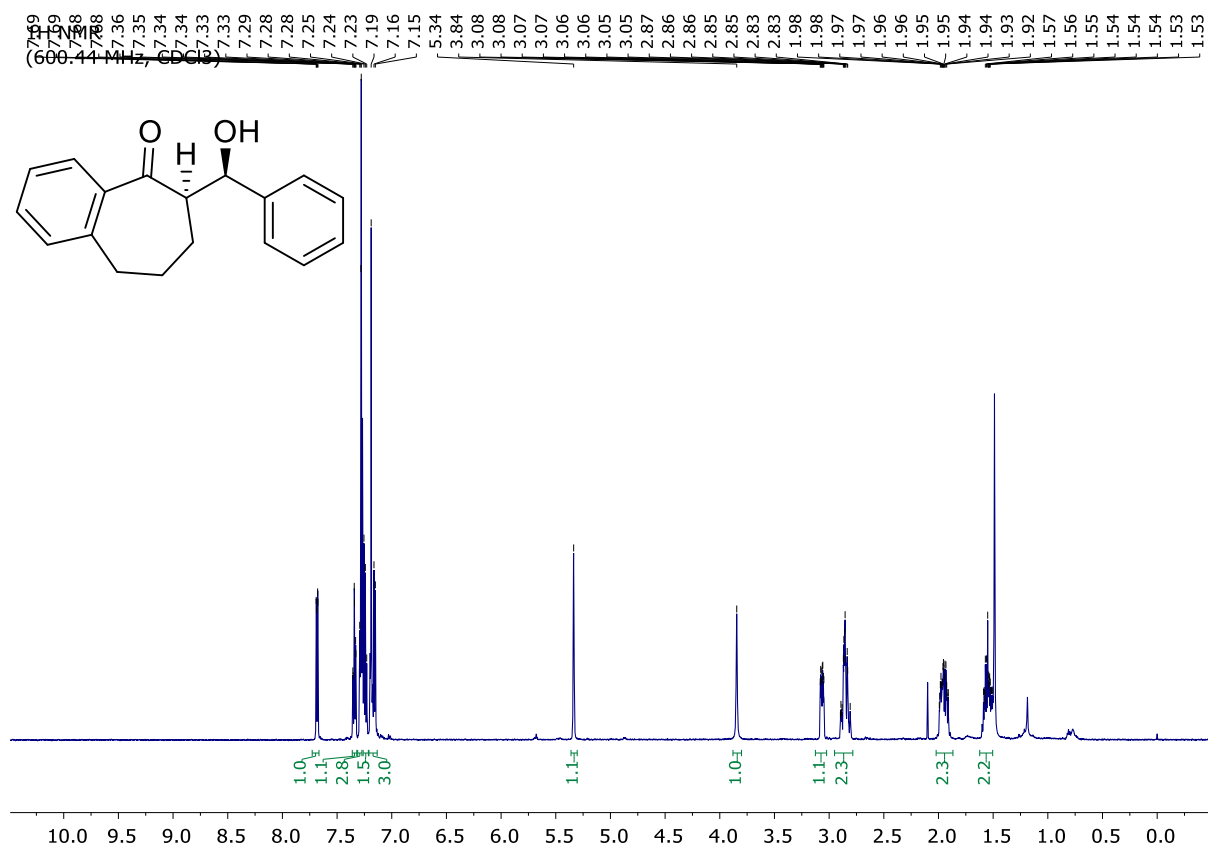
2-(hydroxy(phenyl)methyl)cyclopentan-1-one (4c)



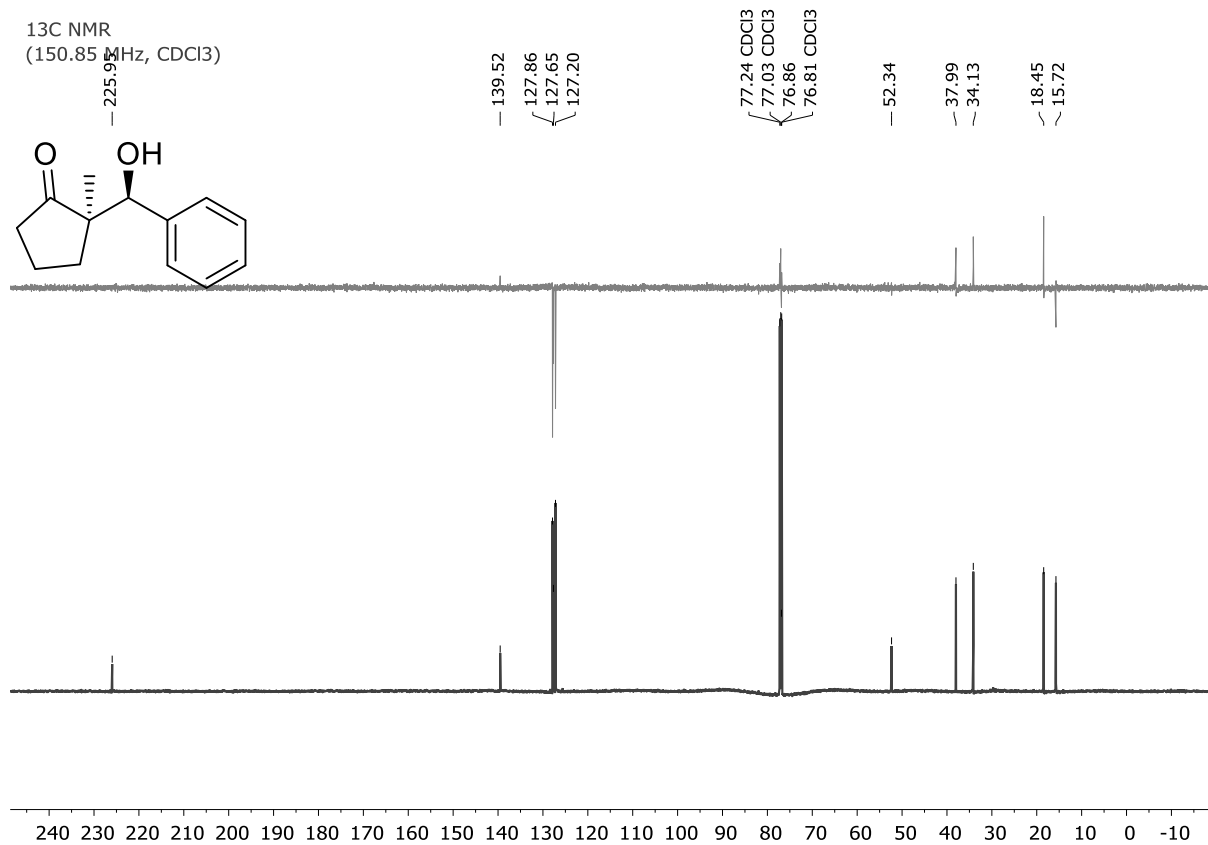
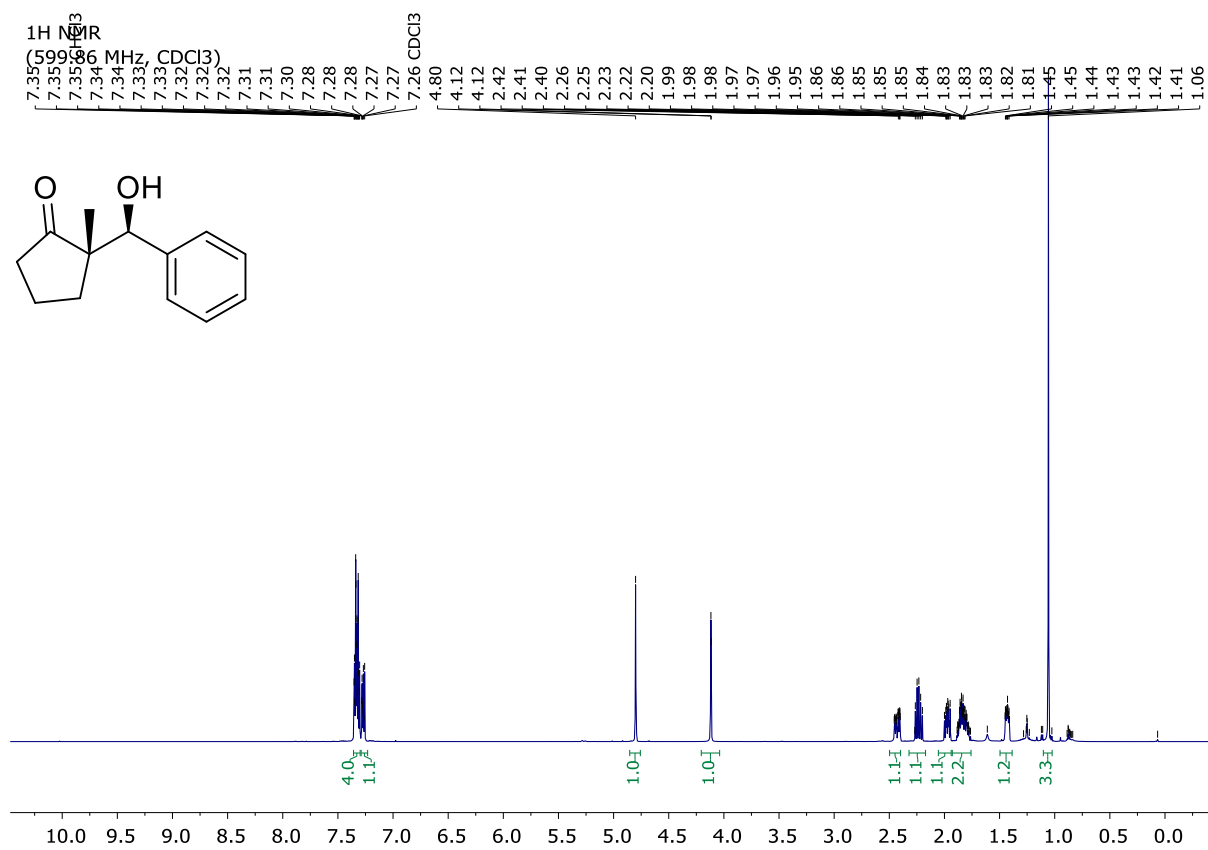
2-(hydroxy(phenyl)methyl)cycloheptan-1-one (4d)



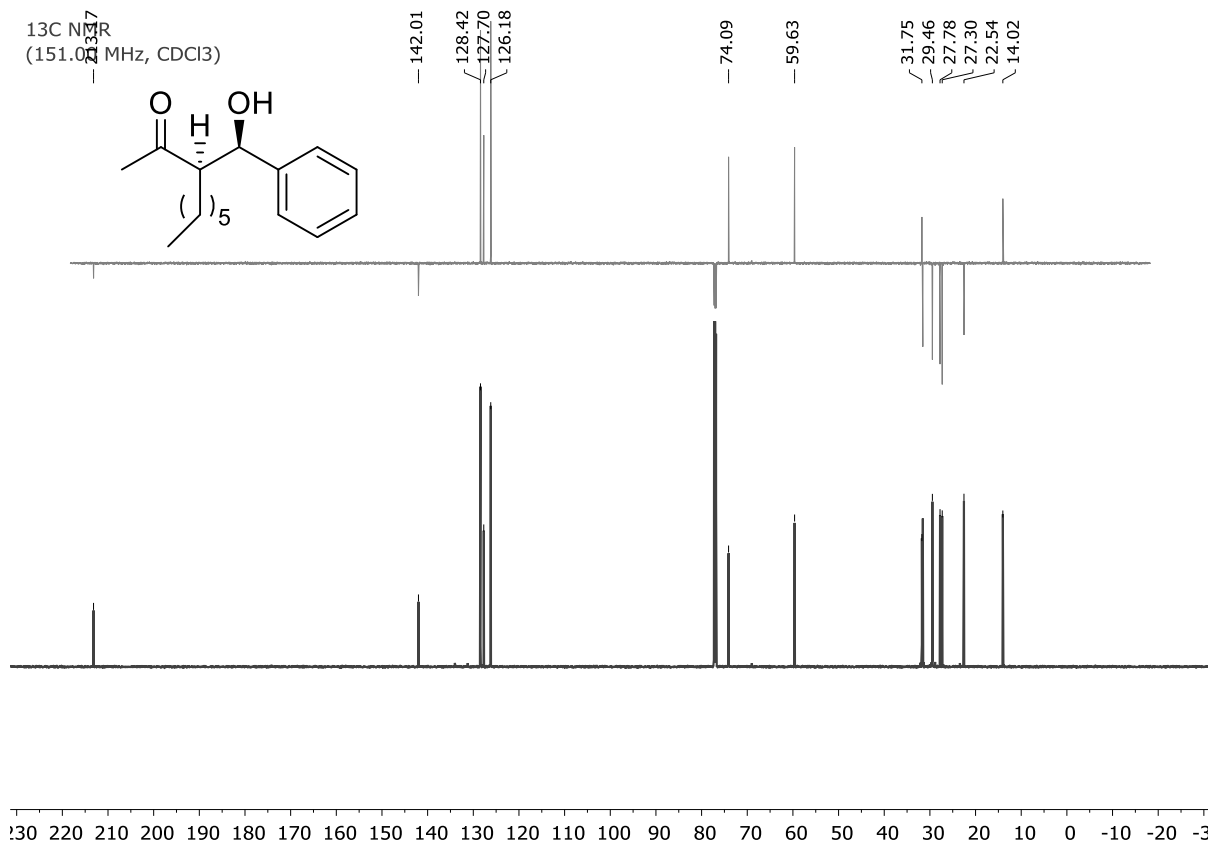
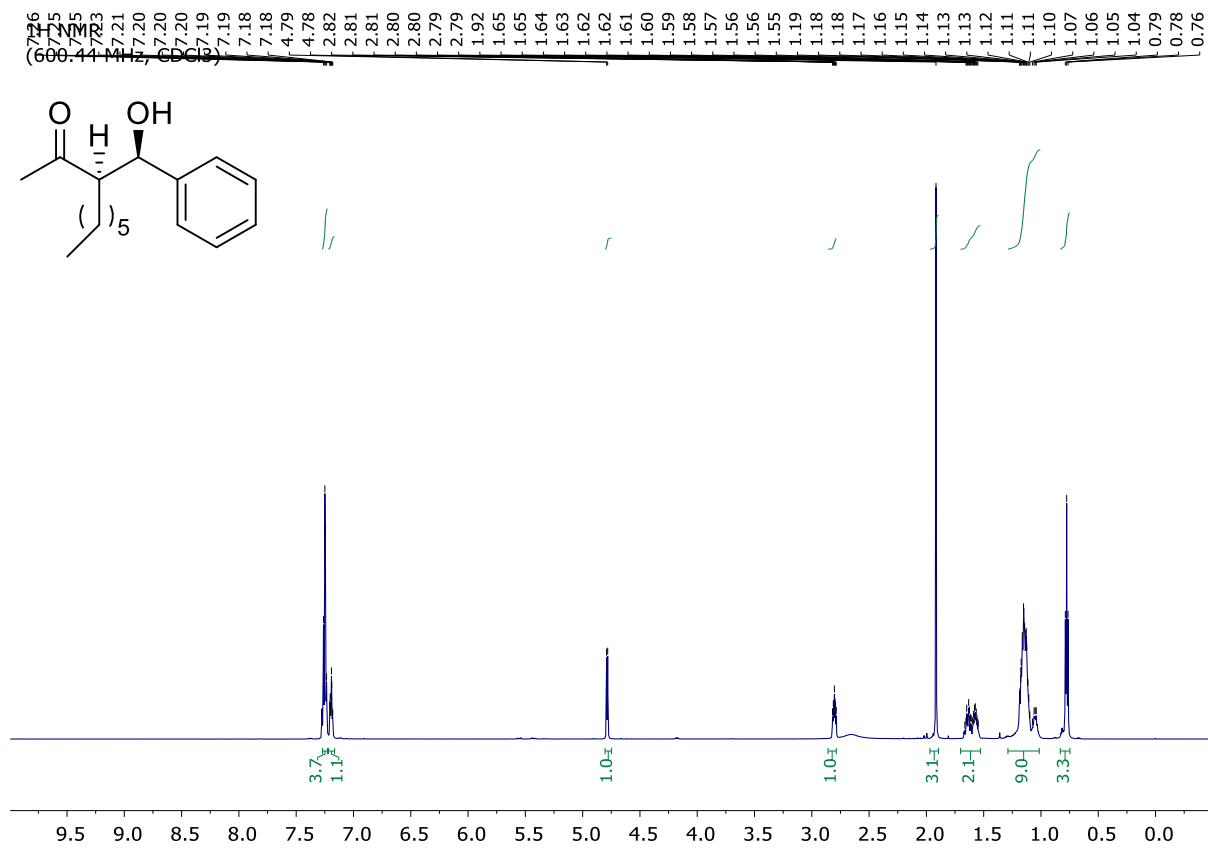
6-(hydroxy(phenyl)methyl)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-5-one (4e)



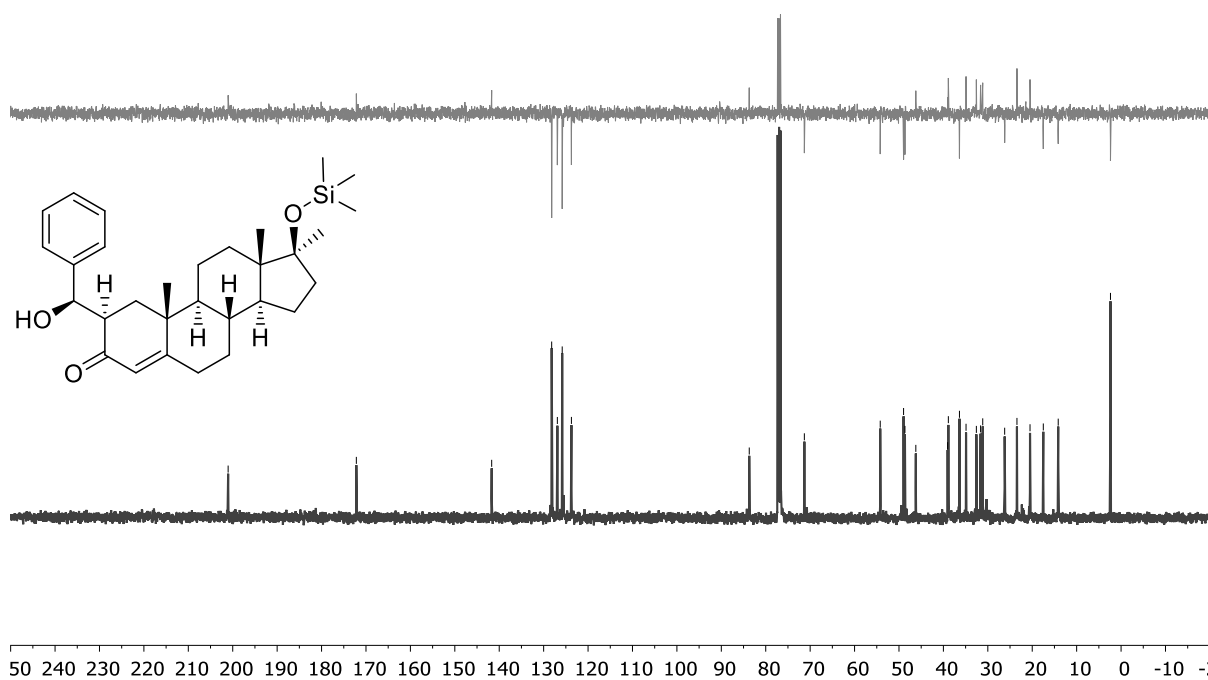
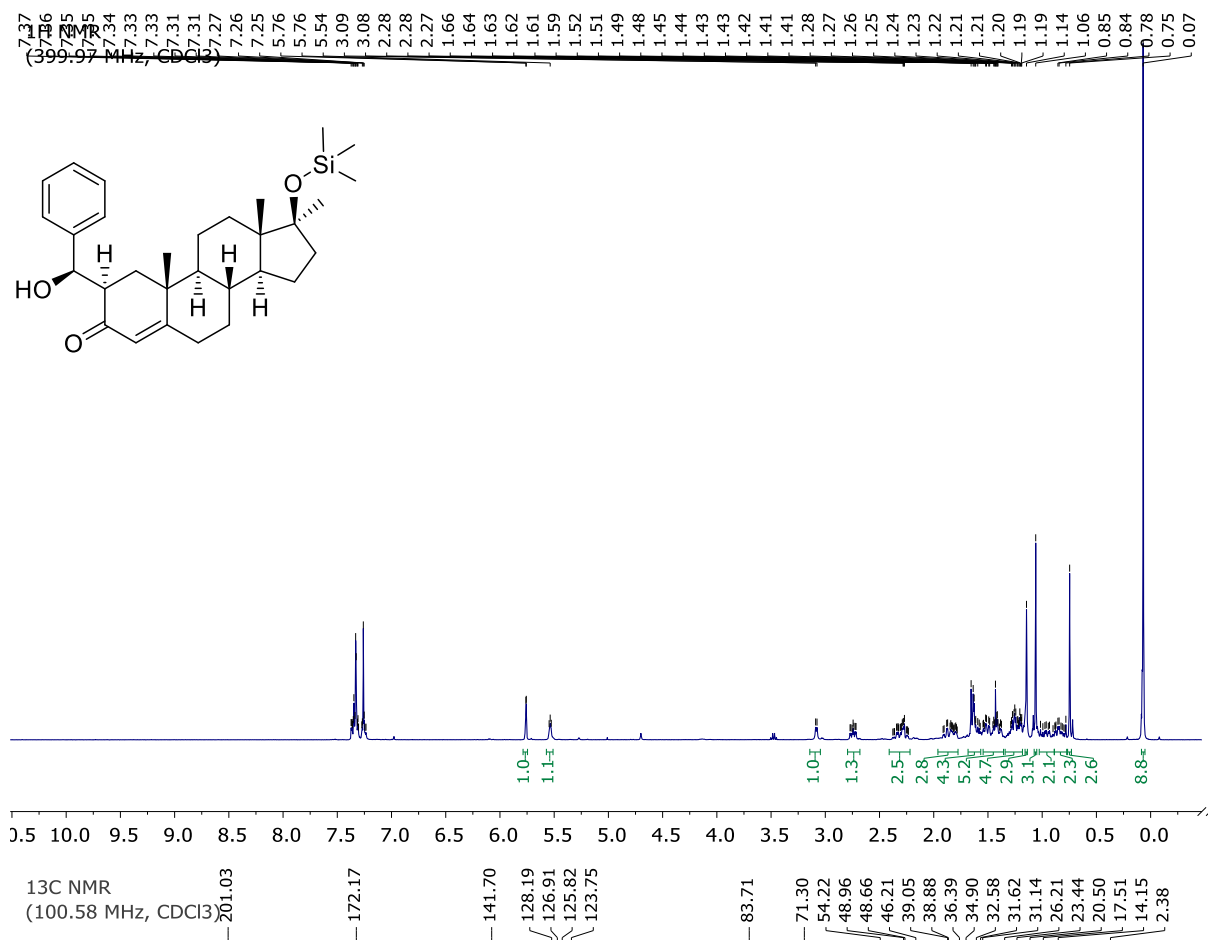
2-(hydroxy(phenyl)methyl)-2-methylcyclopentan-1-one (4f)



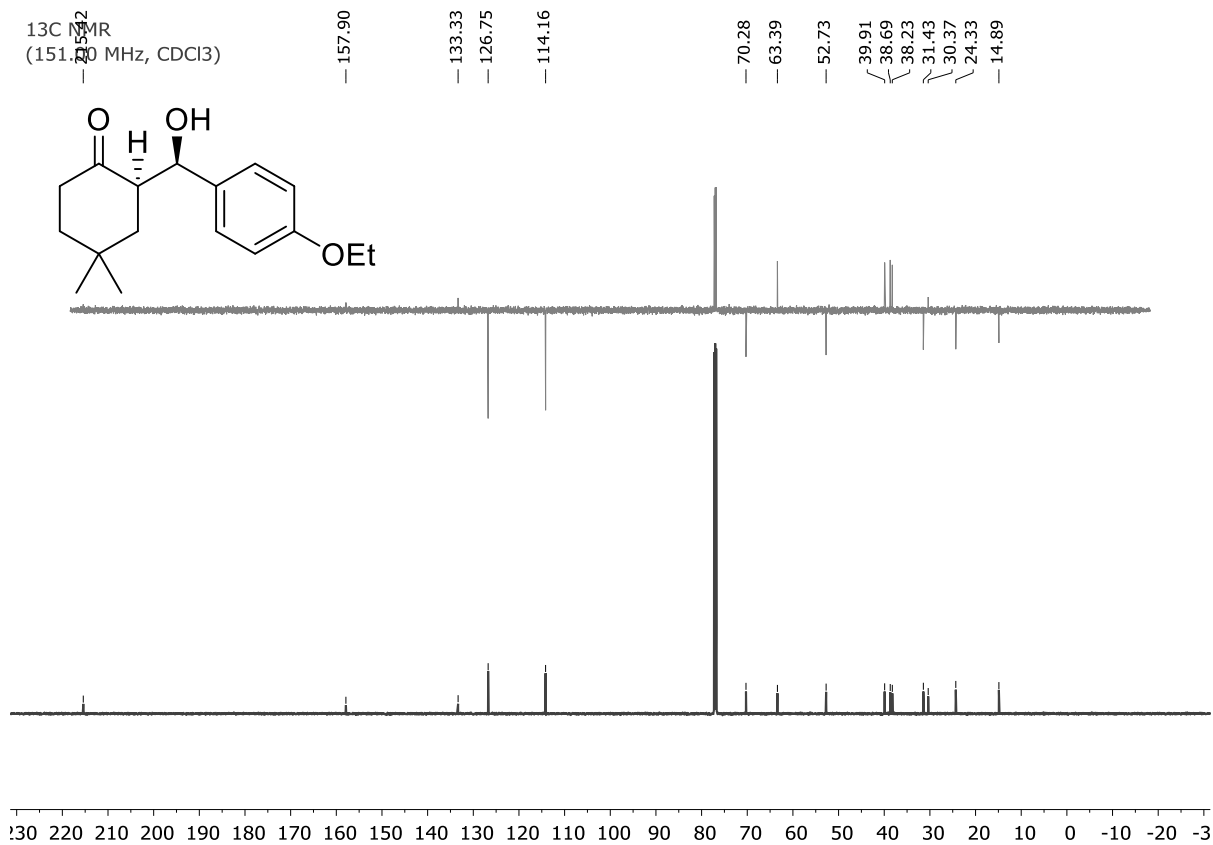
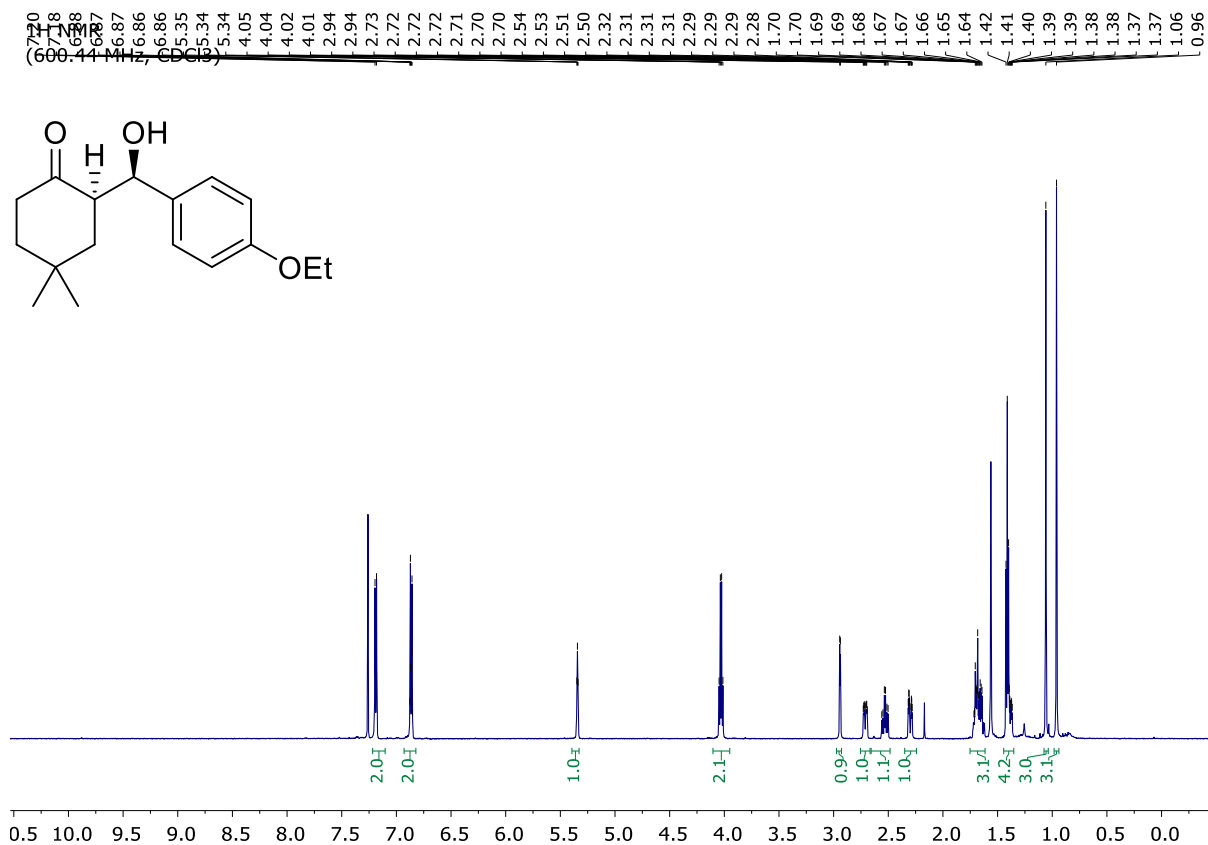
3-(hydroxy(phenyl)methyl)nonan-2-one (4g)



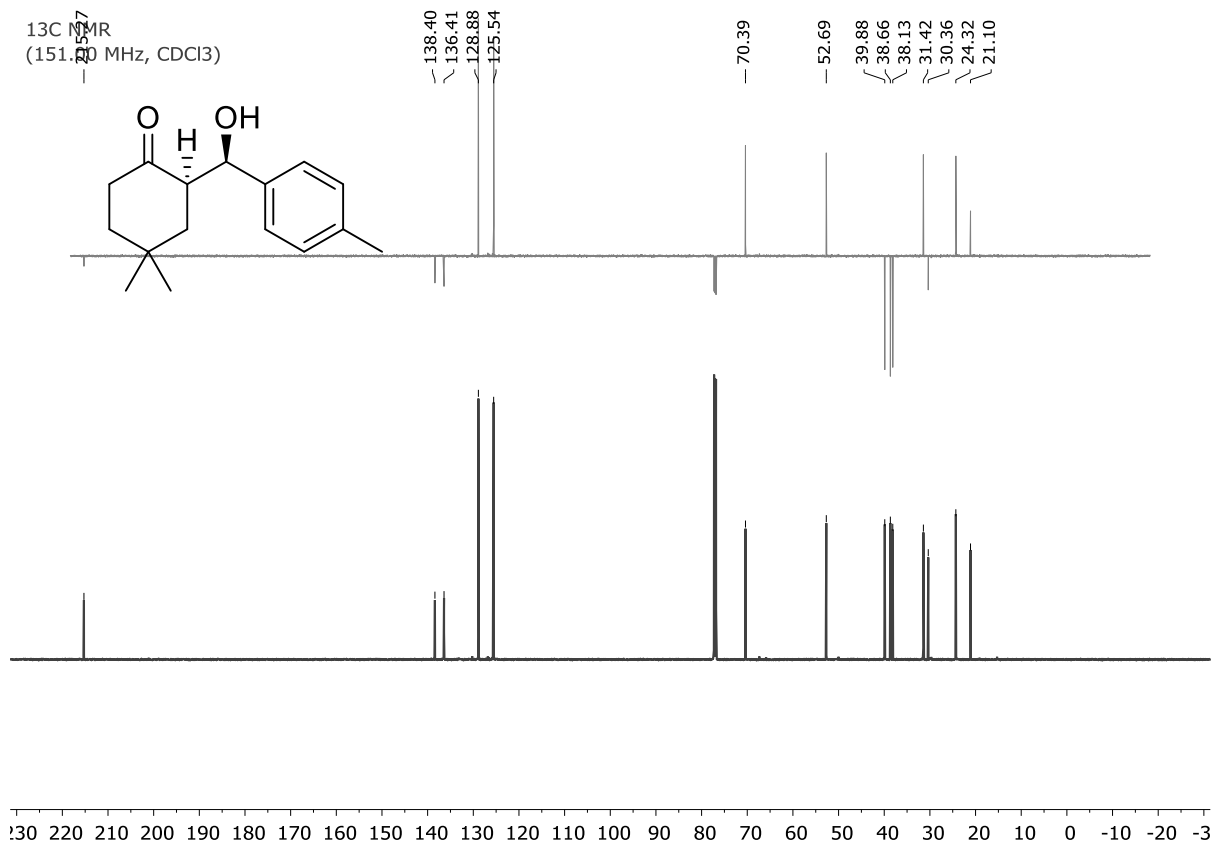
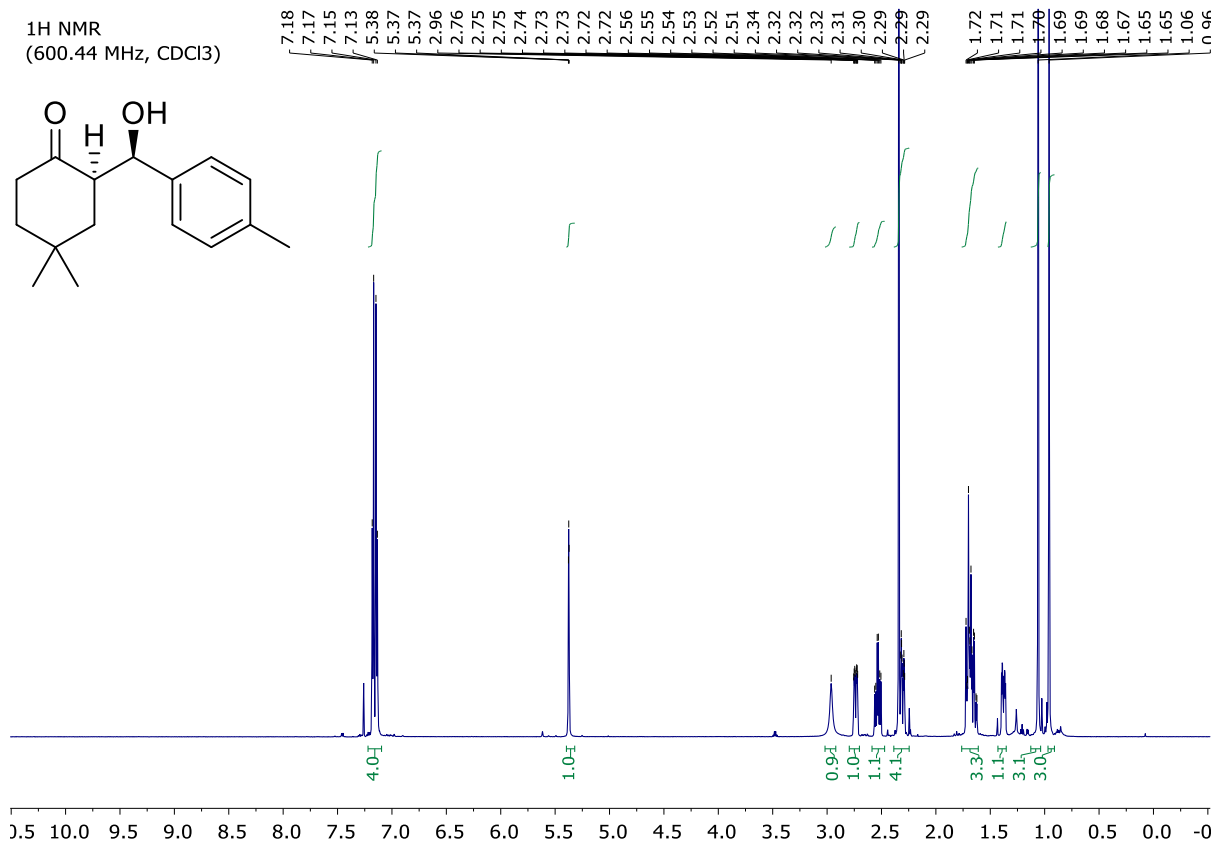
(2R,8R,9S,10R,13S,14S,17S)-2-(hydroxy(phenyl)methyl)-10,13,17-trimethyl-17-((trimethylsilyloxy)-1,2,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3H-cyclopenta[a]phenanthren-3-one (4h)



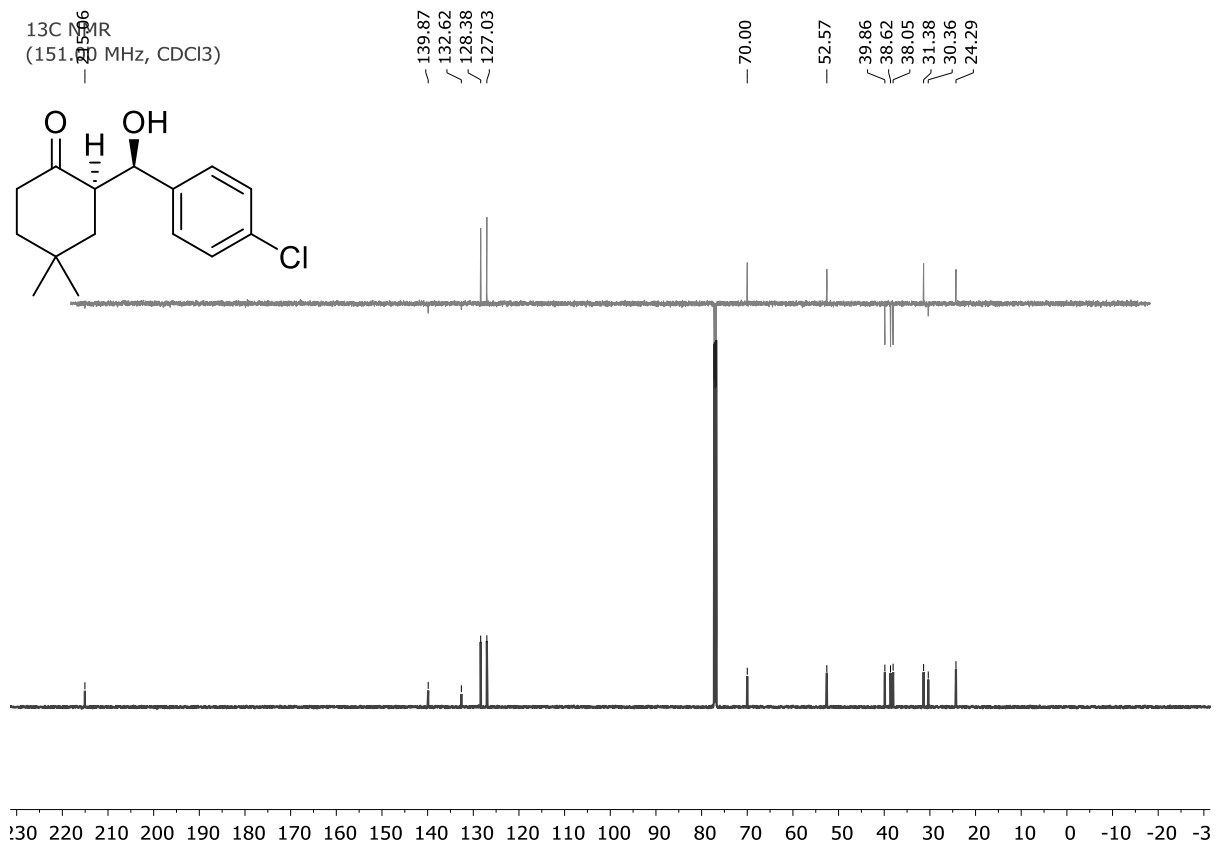
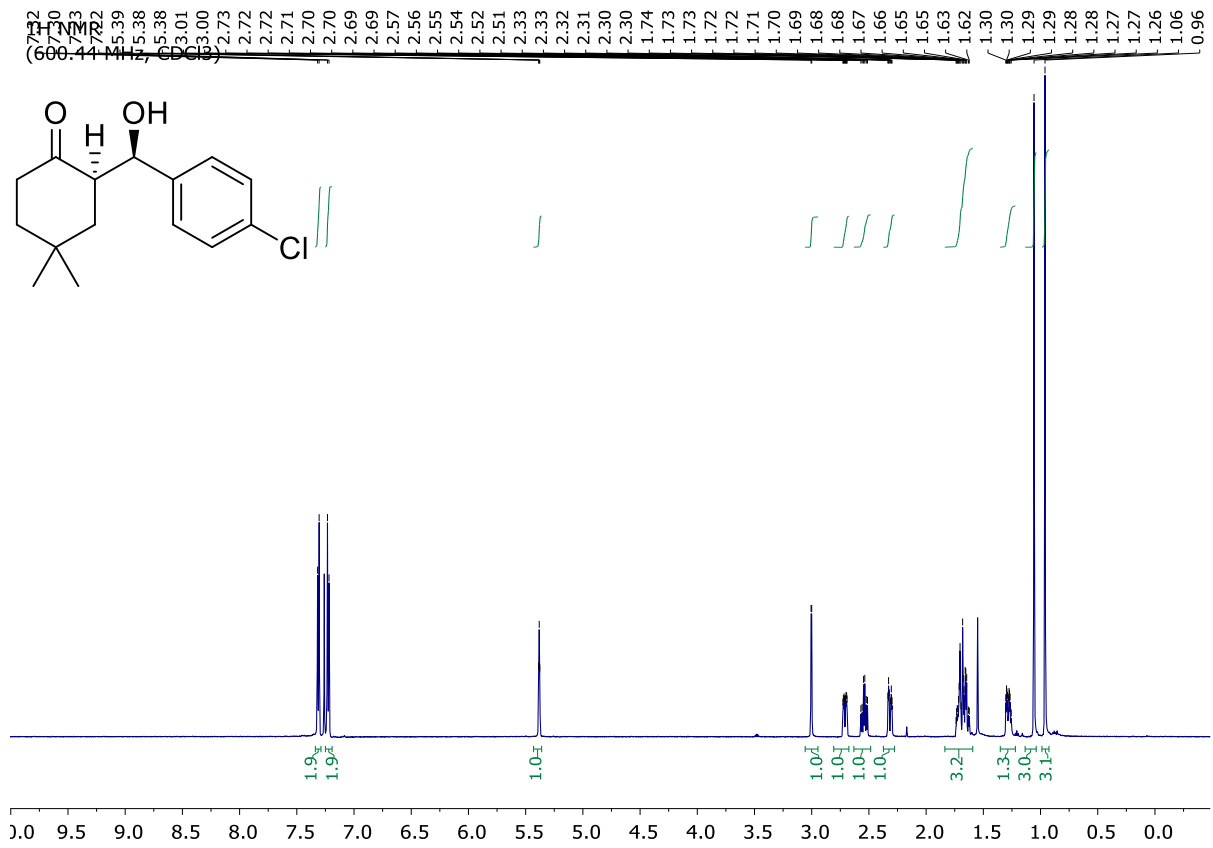
2-((4-ethoxyphenyl)(hydroxy)methyl)-4,4-dimethylcyclohexan-1-one (4i)



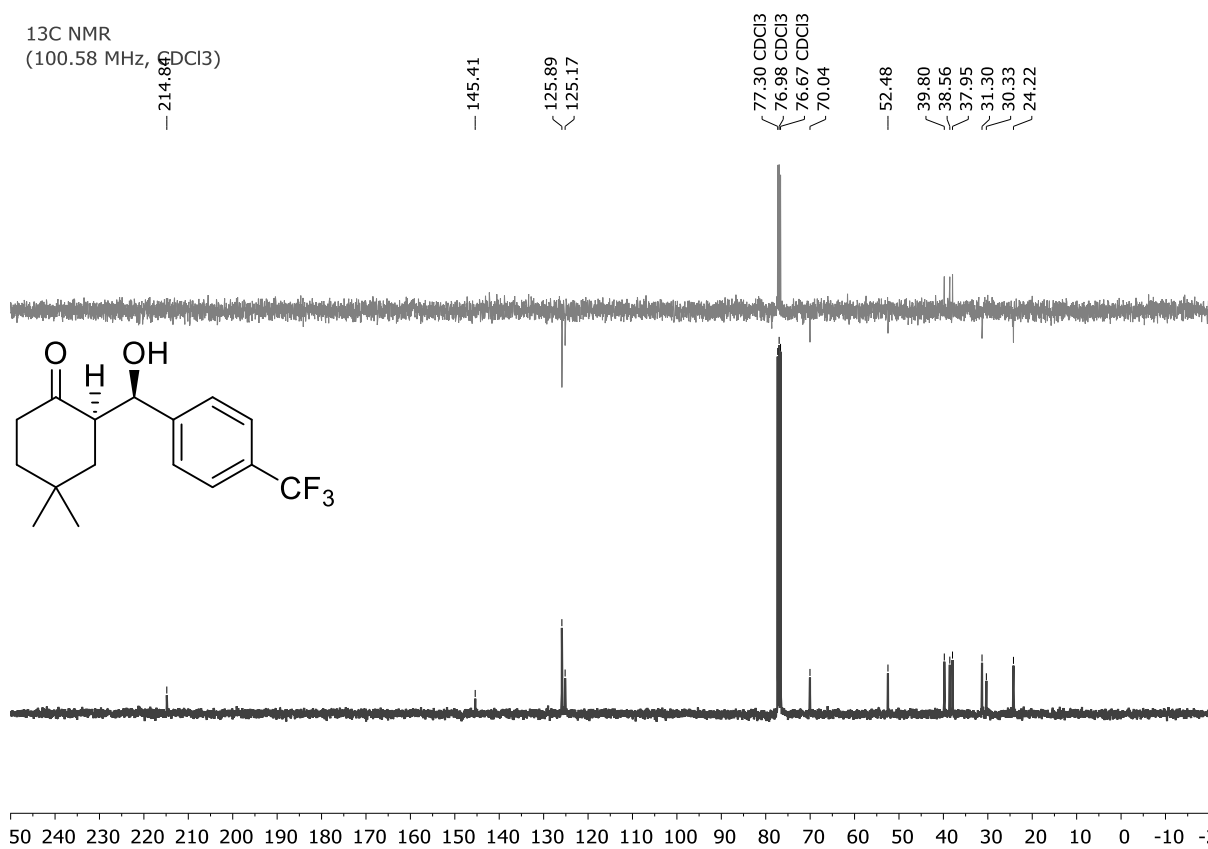
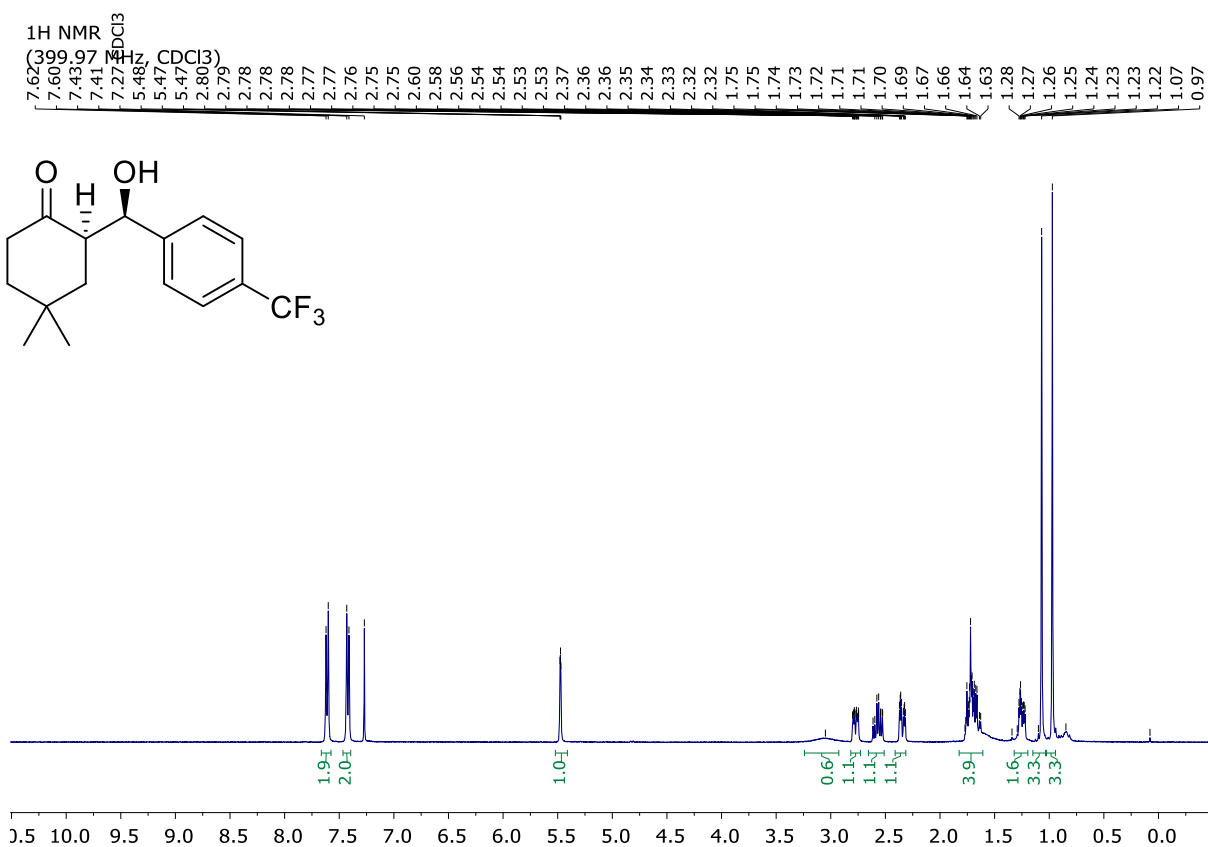
2-(hydroxy(p-tolyl)methyl)-4,4-dimethylcyclohexan-1-one (4j)



2-((4-chlorophenyl)(hydroxy)methyl)-4,4-dimethylcyclohexan-1-one (4k)

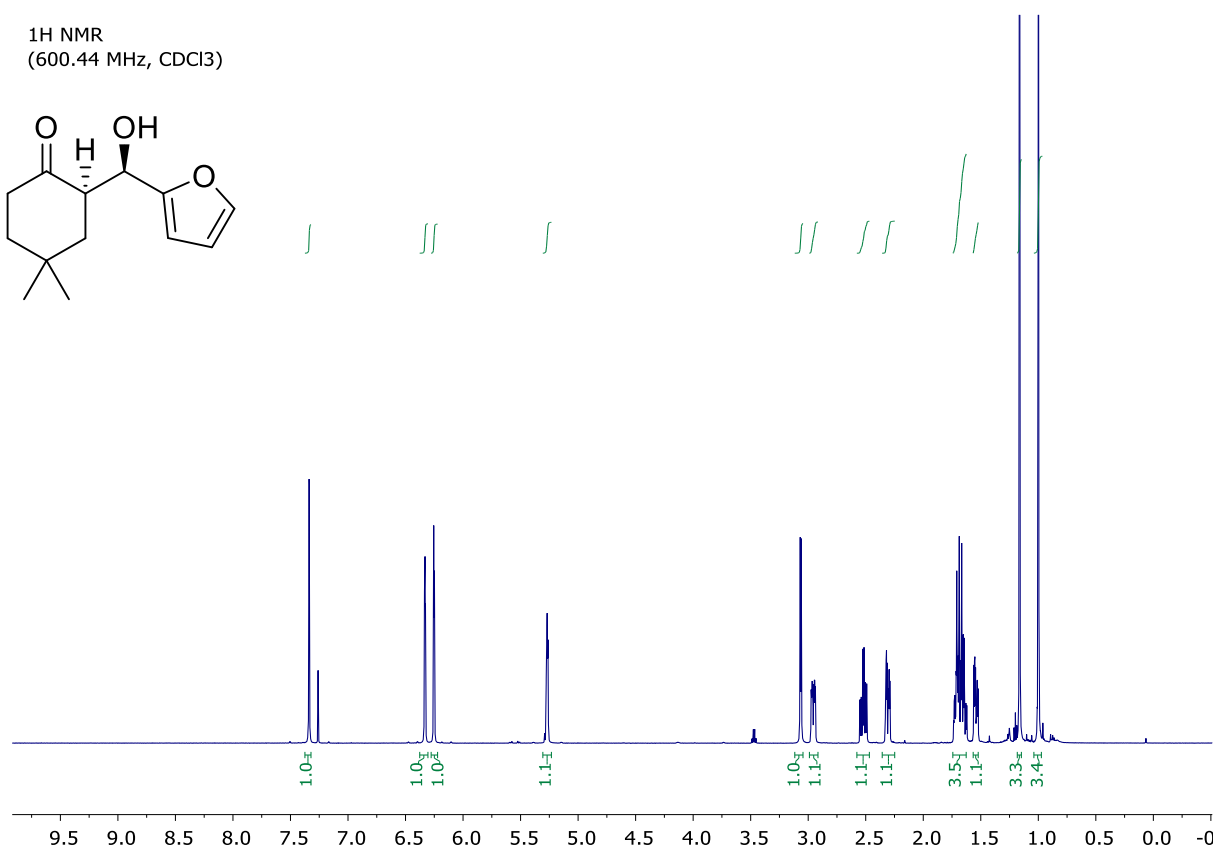
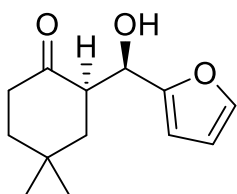


2-(4-(trifluoromethyl)phenyl)methyl-4,4-dimethylcyclohexan-1-one (4I)

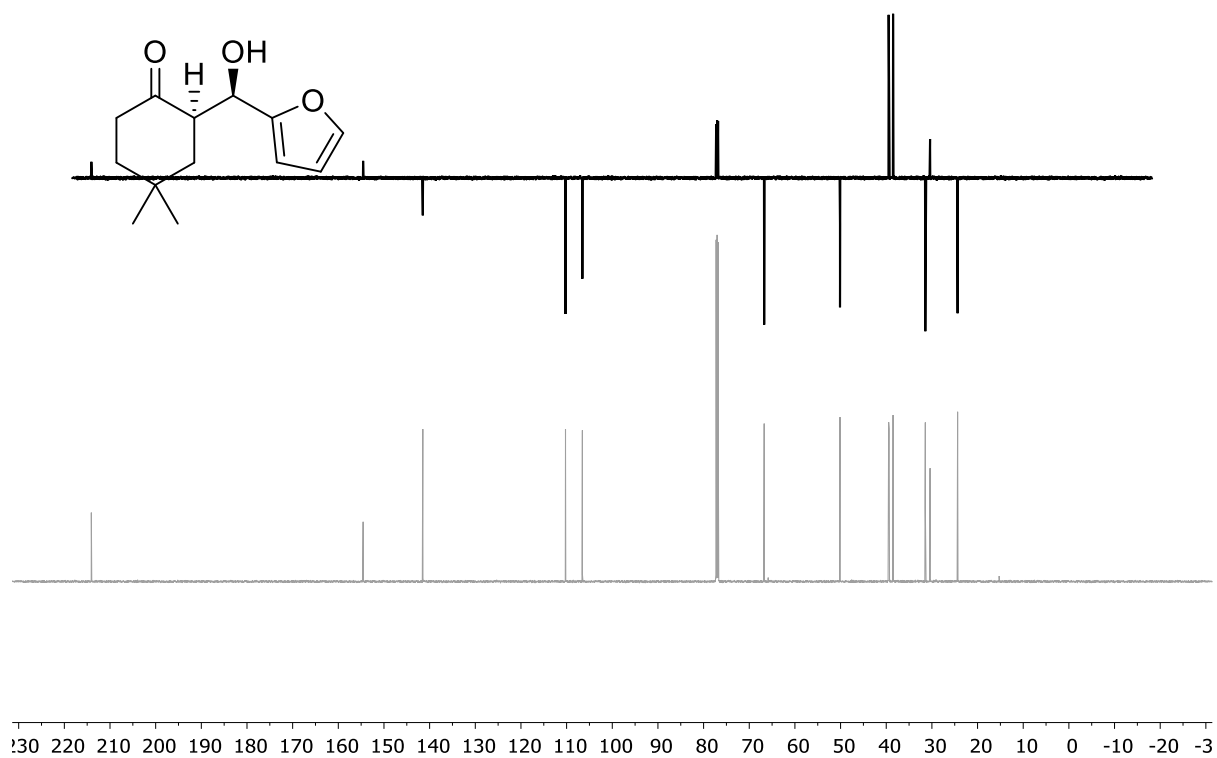
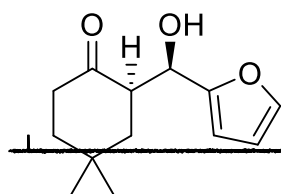


2-(furan-2-yl(hydroxy)methyl)-4,4-dimethylcyclohexan-1-one (4m)

¹H NMR
(600.44 MHz, CDCl₃)

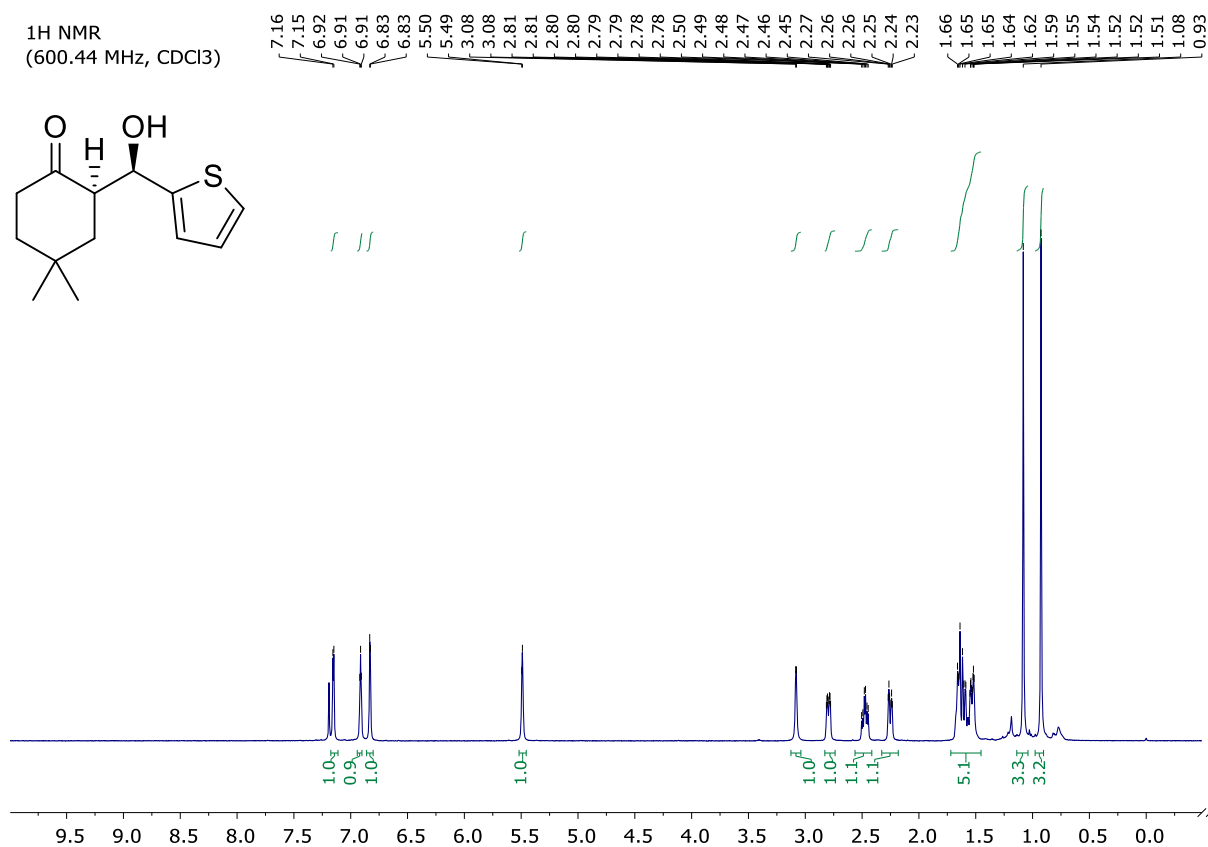


¹³C NMR
(151.00 MHz, CDCl₃)

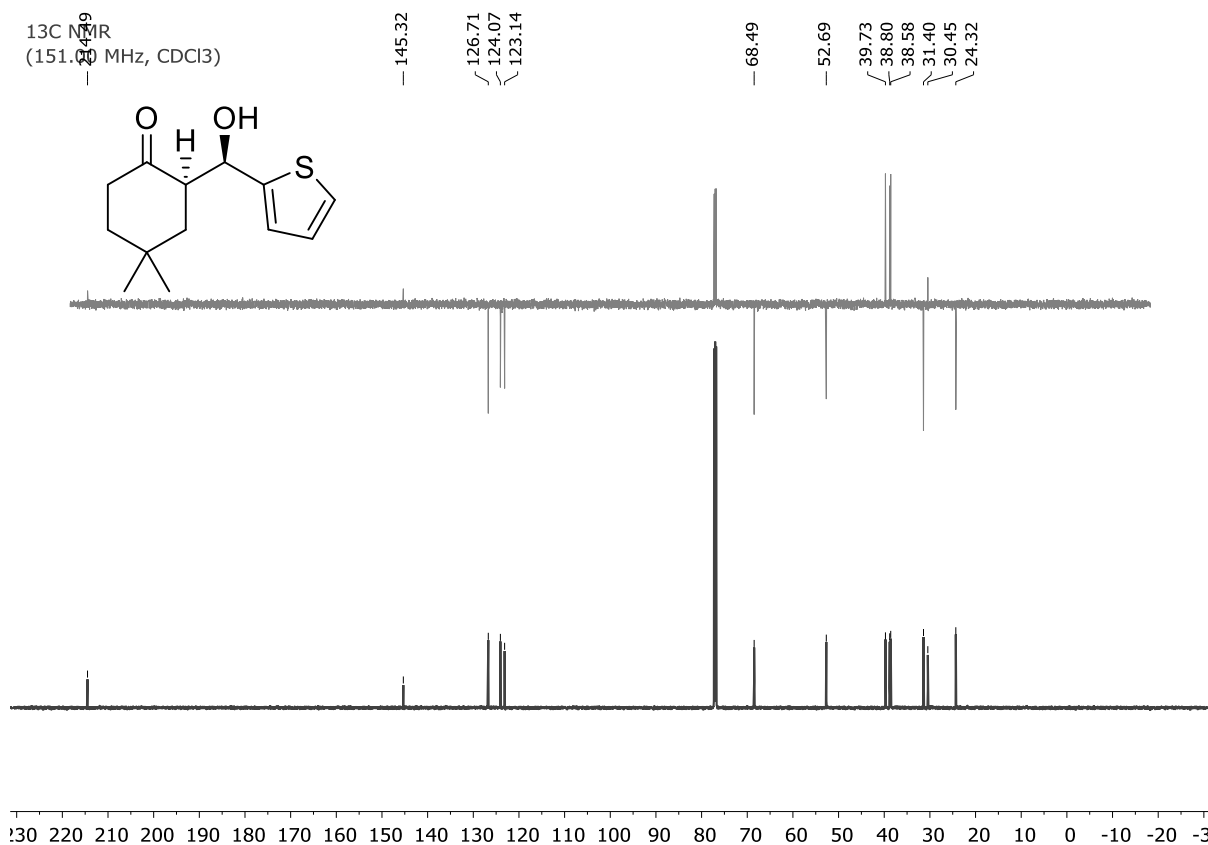


2-(hydroxy(thiophen-2-yl)methyl)-4,4-dimethylcyclohexan-1-one (4n)

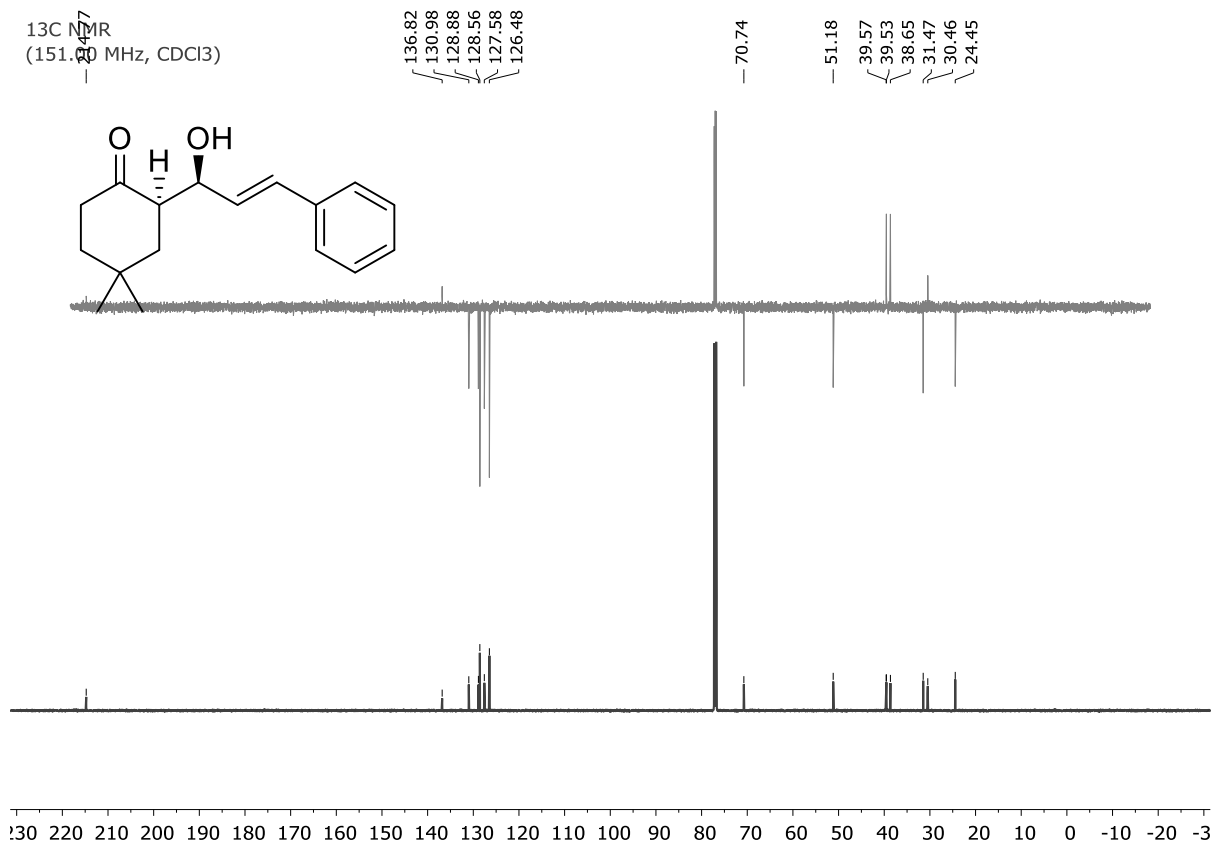
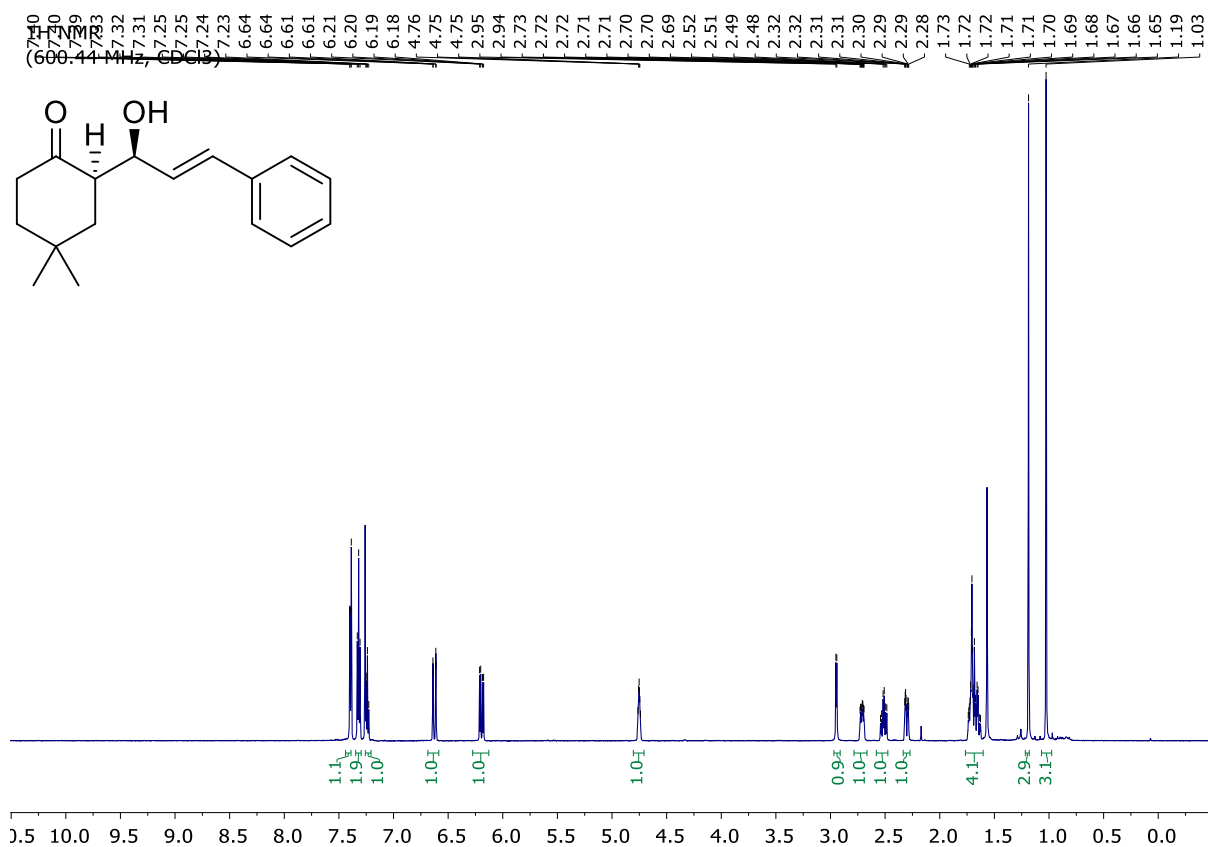
¹H NMR
(600.44 MHz, CDCl₃)



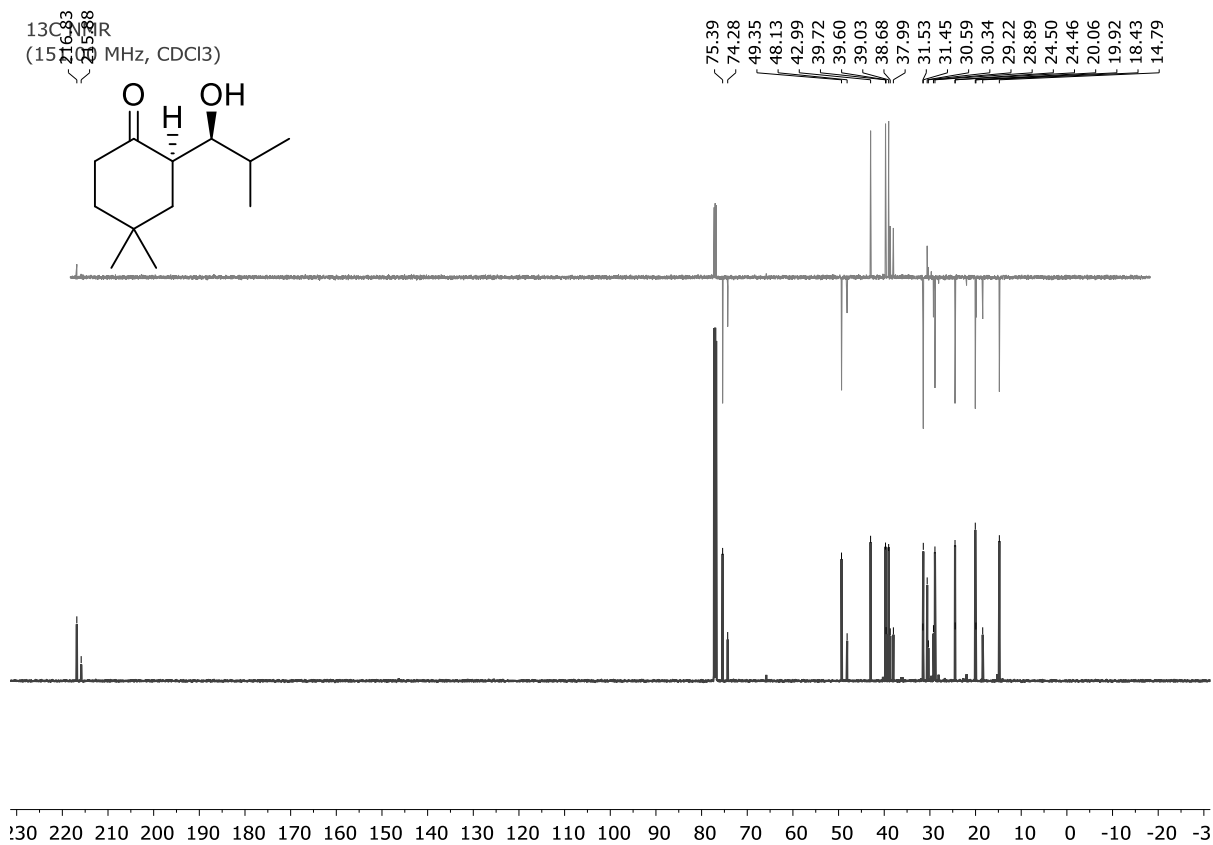
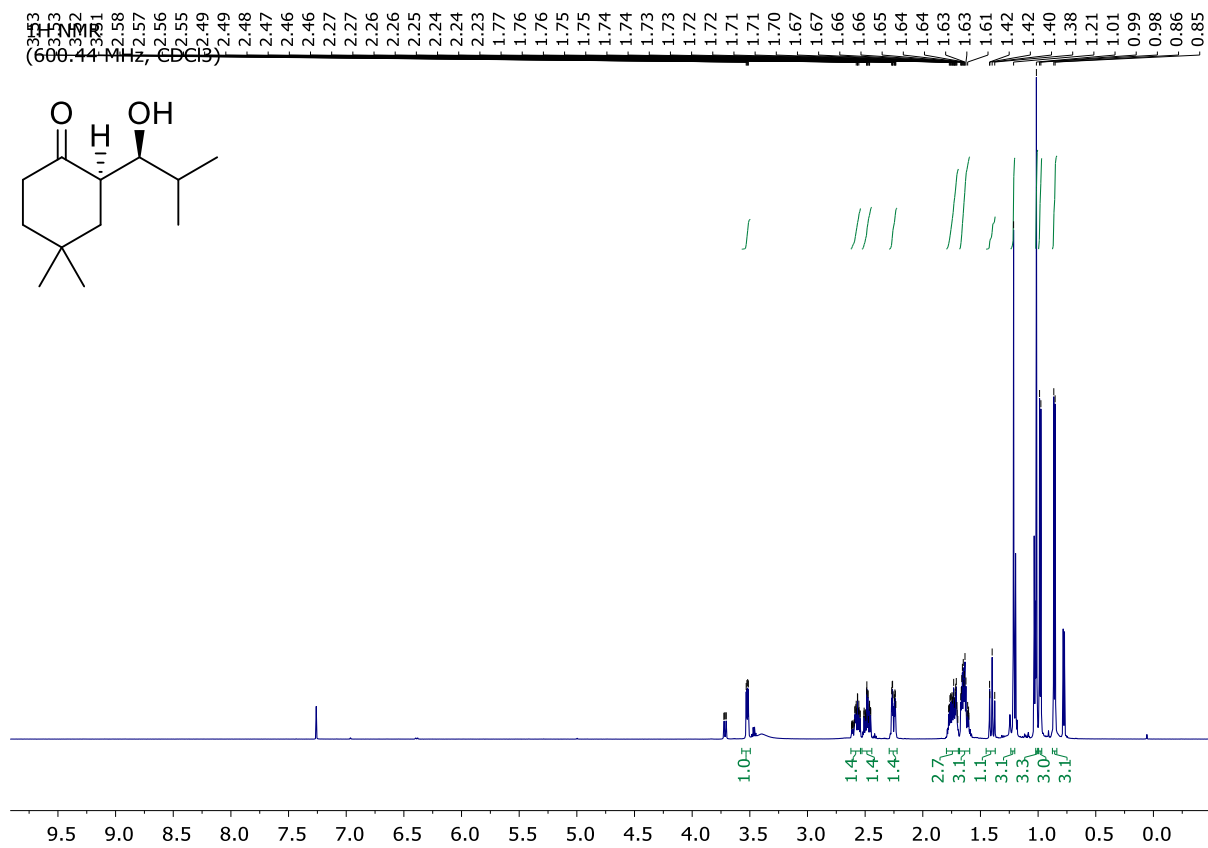
¹³C NMR
(151.80 MHz, CDCl₃)



2-(E-1-hydroxy-3-phenylallyl)-4,4-dimethylcyclohexan-1-one (4o)



2-(1-hydroxy-2-methylpropyl)-4,4-dimethylcyclohexan-1-one (4p)



8. References

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- (4) Yusubov, M. S.; Soldatova, N. S.; Postnikov, P. S.; Valiev, R. R.; Yoshimura, A.; Wirth, T.; Nemykin, V. N.; Zhdankin, V. V. 2-Iodoxybenzoic Acid Ditriflate: The Most Powerful Hypervalent Iodine(v) Oxidant. *Chem. Commun.* **2019**, *55* (54), 7760–7763. <https://doi.org/10.1039/C9CC04203B>.
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