Supplemental Data

Importance of Odorant Conformation to the Binding and Activation of a Representative Olfactory Receptor

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SUPPLEMENTAL EXPERIMENTAL PROCEDURES

Materials and General Methods

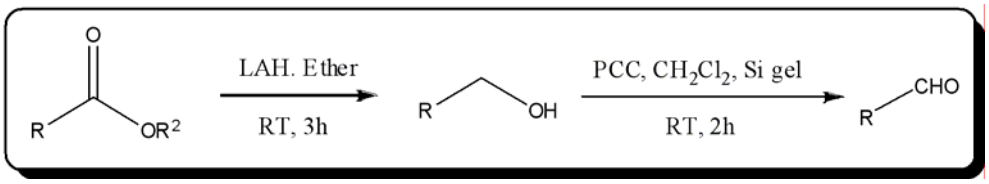
Commercial reagents and solvents were used without additional purification, unless otherwise noted. 3-cyclopentylpropanoic acid, cyclobutanemethanol, ethyl 2-cyclohexylacetate, 2-(2-bromoethyl)-1,3-dioxolane, 4-ethylcyclohexanone were purchased from Alfa Aesar. Cycloheptanecarboxylic acid was purchased from Frinton Labboratories, Inc. 7-octen-1-ol and 6-hepten-1-ol were purchased from TCI America. Ether and THF were dried and distilled from Na/benzophenone. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 plates. Column Chromatographic purifications were performed using 230-400 mesh silica gel from Alfa Aesar.

Spectral Characterization

^{1}H NMR spectra were obtained at 300 MHz. Chemical shifts are reported in parts per million (ppm) referenced to the appropriate solvent peak. The following abbreviations were used to describe peak patterns when appropriate: br = broad, s = singlet, d = doublet, t =triplet, q = quartet, m = multiplet, dd = doublet of doublet, dt = doublet of triplet.

Coupling constants, J, are reported in Hertz (Hz). ^{13}C NMR were recorded at 75 MHz. Infrared (IR) spectra were recorded using a Thermo Nicolet 6700 FT-IR Spectrometer. GC/MS analyses of **4** and **11,** and all other GC analyses, were performed on a Shimadzu GC/MS QP5000 with GC-17A Gas Chromatograph (capillary column: DB-1-30N-STD). Temperature programs for GC analysis: Program1: held at 50 °C for 1min, heated from 50 to 150 °C at 3 °C/min, and held at 150 °C for 4min; program 2: held at 60 °C for 1min, heated from 60 to 150 °C at 4 °C/min, and held at 150 °C for 4 min. Mass spectra for compounds **9**, **2a**, **11a**, **14** and **15** were recorded on a JOEL LCmate mass spectrometer at the Columbia University Chemistry Department Mass Spectrometry Facility.

Scheme S1. LAH Reduction and PCC Oxidation to Aldehyde



R	R^2	RCH_2OH(**a**)	RCHO
6-heptenyl	N/A	N/A	**1**
4-cyclopropylbutyl	N/A	**2a**	**2**
2-cyclopentylethyl	H	**4a**	**4**

cyclohexylmethyl	Et	**5a**	**5**
cycloheptyl	H	**6a**	**6**
(4-ethylcyclohexyl)methyl	Et	**11a**	**11**

General Procedure for Lithium Aluminum Hydride (LAH) Reduction (Dondoni and Perrone, 2000; Reetz et al., 1999)
To an ice-cold mixture of LAH (1.5 equiv for acids, 1.2 equiv for esters, 0.038 g/ mL) in dry ether under N_2, was added dropwise the acid or ester (1 equiv, 0.2g/ mL) in dry ether. The mixture was stirred at room temperature for 3 h then re-cooled to 0° C. The mixture was worked up by dropwise sequential addition of X ml H_2O, X ml 15% NaOH solution and 3X ml H_2O (X= grams of LAH used). After stirring briefly, the mixture was filtered through a celite pad and washed with ether. The solution was dried and concentrated under reduced pressure. The crude product can be purified by column chromatography with ether/hexane (3:7), but was typically used without further purification.

3-Cyclopentylpropanol (4a)
Now available from Aldrich**.** Prepared from 3-cyclopentylpropanoic acid. Yield: 80%. IR (thin film, NaBr plates), ν: 3331, 2949, 2867, 1452, 1057 cm^{-1}; ^1H NMR (300 MHz, CDCl3) δ 3.60 (t, J = 6.7, 2H), 1.86 – 1.63 (m, 4H), 1.63 – 1.39 (m, 6H), 1.39 – 1.18 (m, 2H), 1.15 – 0.90 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 63.4, 40.1, 32.9, 32.3, 32.2, 25.3; GC retention time: 15.16 min (program 1)

2-Cyclohexylethanol (5a) (Ohta et al., 2005)
Prepared from ethyl 2-cyclohexylacetate. Yield: 85%. IR (thin film, NaBr plates), ν: 3331, 2923, 2852, 1448, 1051 cm^{-1}; ^1H NMR (300 MHz, CDCl3) δ 3.65 (t, J = 6.5, 2H), 1.78 – 1.54 (m, 5H), 1.51 – 1.31 (m, 4H), 1.27 – 1.05 (m, 3H), 0.99 – 0.79 (m, 2H); ^{13}C NMR (75 MHz, CDCl3) δ 61.0, 40.5, 34.4, 33.5, 26.7, 26.4; GC retention time: 15.04 min (program 1)

Cycloheptylmethanol (6a)
Now available from Aldrich**.** Prepared from cycloheptanecarboxylic acid. Yield: 84%. IR (thin film, NaBr plates), ν: 3332, 2922, 2854, 1460, 1075, 1020 cm^{-1}; ^1H NMR (300 MHz, CDCl3) δ 3.39 (d, J = 6.5, 2H), 1.81 – 1.28 (m, 12H), 1.15 (dd, J = 11.2, 21.0, 2H); ^{13}C NMR (75 MHz, CDCl3) δ 68.8, 42.2, 30.9, 28.7, 26.7; GC retention time: 12.13 min (program 2)

General Procedure for Pyridinium Chlorochromate Oxidation (Srikrishna et al., 2007; Yoshida et al., 2007)
To a stirred suspension of PCC (1.5 equiv,) and silica gel (1 g/ g of PCC) in CH_2Cl_2 (10 mL/ g of PCC) was added a solution of the alcohol (1 equiv, 0.083 g/ mL) in CH_2Cl_2. The mixture was stirred at room temperature for 2 h and then filtered through a silica gel pad and followed by fresh solvent. The solvent was evaporated and the crude product was purified by column chromatography with ether/hexane (1:19) to give the aldehyde product.

^1H NMRs of All Aldehydes Are Shown at the End of the Supplemental Experimental Procedures

7-Octenal (1) (Hon et al., 2007)
Prepared from 7-octen-1-ol. Yield: 61%. IR (thin film, NaBr plates), ν: 3077, 2932, 2858, 2719, 1728, 1641, 996, 911 cm^{-1}; ^1H NMR (300 MHz, CDCl3) δ 9.76 (s, 1H), 5.78 (dt, J = 6.9, 16.2, 1H), 4.81-5.09 (m, 2H), 2.42 (t, J = 7.3, 2H), 2.17 – 1.86 (m, 2H), 1.74 – 1.50 (m, 2H), 1.10-1.49 (m, 4H); ^{13}C NMR (75 MHz, CDCl3) δ 202.9, 138.8, 114.7, 44.0, 33.7, 28.7, 22.1; GC retention time: 12.75 min (program 2)

5-Cyclopropylpentanal (2)
Prepared from **2a** (see below)**.** GC/MS showed that the final product contained 4% heptanal, which could not be removed by column chromatography. The source appears to be the Simmons-Smith reaction sequence (see below). This relatively small amount has no measurable effect in the assays, since the highest amount of **2** used, 30 μM, contains at most 1.2 μM heptanal, a concentration that is not detectable in the activation assay (Fig. 3). Yield: 50%. IR (thin film, NaBr plates), ν: 3077, 3001, 2928, 2856, 2718, 1728, 1481, 1015, 822 cm^{-1}; ^{1}H NMR (300 MHz, CDCl3) δ 9.73 (s, 1H), 2.39 (t, *J* = 7.3, 2H), 1.74 – 1.51 (m, 2H), 1.48 – 1.31 (m, 2H), 1.17 (dd, *J* = 7.1, 14.5, 2H), 0.70 – 0.50 (m, 1H), 0.35 (q, *J* = 4.8, 2H), -0.05 (q, *J* = 4.8, 2H); ^{13}C NMR (75 MHz, CDCl3) δ 203.1, 44.1, 34.6, 29.4, 22.1, 10.8, 4.5; GC retention time: product: 11.60 min, (Contaminating heptanal: 7.19 min (program1)).

3-Cyclopentylpropanal (4)
Prepared from **4a**. Yield: 50%. IR (thin film, NaBr plates), ν: 2950, 2867, 2717, 1727, 1452 cm^{-1}; ^{1}H NMR (300 MHz, CDCl3) δ 9.76 (t, *J* = 1.7, 1H), 2.43 (td, *J* = 1.7, 7.8, 2H), 1.85 – 1.37 (m, 9H), 1.08 (br, 2H); ^{13}C NMR (75 MHz, CDCl3) δ 203.2, 43.5, 39.8, 32.7, 28.3, 25.3; GC retention time: 12.03 min (program 1); LRMS (EI): 126(M^{+}).

2-Cyclohexylacetaldehyde (5) (Roberts et al., 1990; Sheng et al., 2006) Prepared from **5a**. Yield: 57%. IR (thin film, NaBr plates), ν: 2934, 2852, 2713, 1728, 1449, 1020, 899 cm^{-1}; ^{1}H NMR (300 MHz, CDCl3) δ 9.74 (s, 1H), 2.27 (d, *J* = 6.7, 2H), 1.98 – 1.54 (m, 6H), 1.39 – 0.81 (m, 5H); ^{13}C NMR (75 MHz, CDCl3) δ 203.2, 51.6, 33.4, 32.8, 26.2; GC retention time: 13.99 min (program 2)

Cycloheptanecarbaldehyde (6) (Vincek et al., 1981)
Prepared from **6a.** Yield: 50% IR (thin film, NaBr plates), ν: 2926, 2856, 2707, 1728, 1460, 1182, 888 cm^{-1}; ^{1}H NMR (300 MHz, CDCl3) δ 9.63 (s, 1H), 2.44 – 2.30 (br, 1H), 2.02 – 1.85 (m, 2H), 1.81 – 1.35 (m, 10H); ^{13}C NMR (75 MHz, CDCl3) δ 204.9, 52.0, 28.7, 27.4, 26.4; GC retention time: product: 13.22 min. (The product contained ~2 % of an unknown contaminant by NMR (see spectrum below) and GC). GC Retention time: 14.06 min (program 1).

Sequence to Produce Compound 3 (see Fig. 1B for Synthetic Scheme)
2-(1,3-dioxolan-2-yl)ethyl)triphenylphosphonium bromide (8) was prepared by refluxing 2-(2-bromoethyl)-1,3-dioxolane (5 g, 27.6 mmol) and triphenylphosphine (7.24 g, 27.6 mmol) in 25 mL acetonitrile for 24 h. The mixture was then cooled to room temperature. Dry ether was added and the starting material in the ethereal solution was removed by decantation. This procedure was repeated 3 times and the resulting phosphonium salt was dried under vacuum to give 11g of 2-(1,3-dioxolan-2-yl)ethyl)triphenylphosphonium bromide. Used without further purification.

2-(3-Cyclobutylallyl)-1,3-dioxolane (9) (Dirat et al., 1998; Sakata et al., 1989). 1.6 M n-BuLi solution in hexane (Alpha Aesar) (11.6 mL, 18.5 mmol) was added dropwise to a stirred suspension of **8** (8.2 g, 18.5 mmol) in dry THF (200 mL) at –75 °C under N_2. The orange solution was stirred for 1 h then **7** (see next entry) (1.41 g, ~16.8 mmol) in dry THF (150 mL) was added dropwise. The mixture was then allowed to warm to room temperature and continued to stir overnight (12 h). The reaction was quenched by adding saturated NaCl solution and the triphenylphosphine oxide was removed by filtration. The aqueous phase was extracted with ether and combined organic phase was washed with brine and dried ($MgSO_4$). Evaporation of the solvent and purification by column chromatography using ether/hexane (1:19) furnished the compound (1.5 g, 53%). IR (thin film, NaBr plates), ν: 2960, 2880, 1397, 1136, 1036, 944, 842;

^{1}H NMR (300 MHz, CDCl3) δ 5.65 (ddt, *J* = 1.6, 8.7, 10.3, 1H), 5.27 (dtd, *J* = 1.3, 7.3, 10.8, 1H), 4.82 (t, *J* = 4.8, 1H), 4.11 – 3.60 (m, 4H), 3.30-3.02 (m, 1H), 2.37 (ddd, *J* = 3.9, 6.3, 11.1, 2H), 2.21-1.99 (m, 2H), 1.95 – 1.54 (m, 4H); ^{13}C NMR (75 MHz, CDCl3) δ 138.8, 121.0, 104.2, 65.1, 34.0, 32.6, 29.8, 19.1; GC retention times: 16.36 min (major isomer) and 16.42 (minor isomer) (program 2); Cis/trans ratio 8:1; LRMS (APCI+): 169 $(M+H)^+$. (APCI, atmospheric pressure chemical ionization).

Cyclobutanecarbaldehyde (7) Prepared by PCC oxidation of cyclobutylmethanol. Most methylene chloride solvent was removed from the filtered crude product by simple distillation followed by adding excess ether and removing the ether also by simple distillation. Repeated ether treatment one time. Only a trace of methylene chloride (by ^{1}H-NMR) was left after this treatment. Used without further purification.

2-(3-Cyclobutylpropyl)-1,3-dioxolane (15). A mixture of **9** (1.5 g, 8.93 mmol) and palladium on carbon (Acros, 10% Pd on carbon, 50% wet with water, 0.15 g) in ethyl acetate (60 mL) was stirred under an H_2 balloon for 2 h at room temperature. The mixture was then filtered. Evaporation of the solvent furnished the product (1.4 g, 92%) which was used in the next step without further purification. IR (thin film, NaBr plates), ν: 2948, 2863, 1410, 1142, 1050, 944; ^{1}H NMR (300 MHz, CDCl3) δ 4.81 (t, *J* = 4.8, 1H), 4.04 – 3.75 (m, 4H), 2.34 – 2.10 (m, 1H), 2.09-1.91 (m, 2H), 1.90 – 1.67 (m, 2H), 1.66 – 1.46 (m, 4H), 1.44 – 1.19 (m, 4H). ^{13}C NMR (75 MHz, CDCl3) δ 104.9, 65.0, 37.1, 36.2, 34.1, 28.5, 21.9, 18.6; GC retention time: 16.74 min (program 2); LRMS (APCI+): 171 $(M+H)^+$, 169 $(M-H)^+$.

4-Cyclobutylbutanal (3). A mixture of **15** (1g, 5.88 mmol) in 60mL 2 N HCl and 60 mL THF was refluxed with stirring for 3 h. The mixture was cooled to room temperature and extracted with ether. The combined organic layer was extracted with saturated $NaHCO_3$ solution, brine and dried ($MgSO_4$). Evaporation of the solvent and purification of the crude by column chromatography using CH_2Cl_2/pentane (1:4) furnished the aldehyde (0.25 g, 34%). IR (thin film, NaBr plates), ν: 2933, 2860, 2717, 1727; ^{1}H NMR (300 MHz, CDCl3) δ 9.75 (s, 1H), 2.39 (t, *J* = 7.2, 2H), 2.32 -2.16 (m, 1H), 2.12 – 1.94 (m, 2H), 1.91-1.71 (m, 2H), 1.68 – 1.25 (m, 6H). ^{13}C NMR (75 MHz, CDCl3) δ 203.1, 44.0, 36.5, 35.9, 28.4, 19.9, 18.6; GC retention time: 11.72 min (program 1).

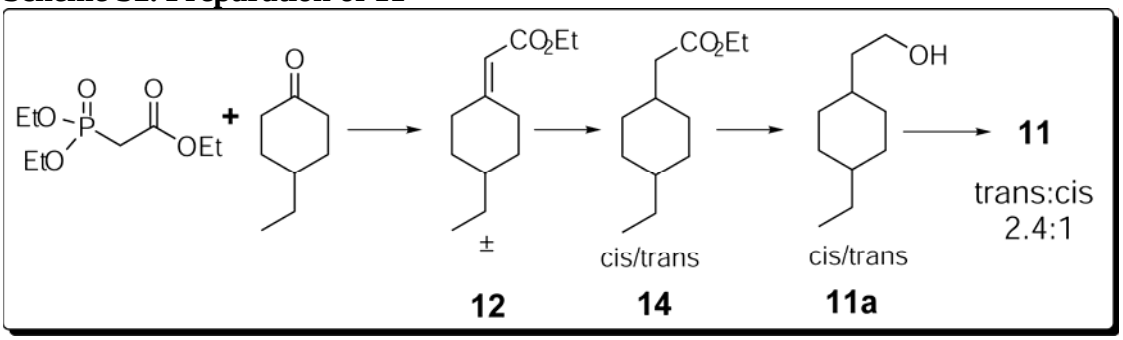
5-Cyclopropylpentanol (2a) (Smith and Simmons, 1961) 6-hepten-1-ol (2 g, 17.5 mmol), diiodomethane (18.76 g, 70.0 mmol) in 8 mL dry ether were added to a mixture of Zinc-Copper couple (made according to (Smith and Simmons, 1961) (6.84 g) and 0.44 g I_2 in 8 mL dry ether at room temperature. After 20 min, an exothermic reaction occurred and the mixture started to reflux. After 15 min the exothermic reaction subsided, the reaction was gently heated to keep refluxing for another 30 min. The mixture was then transferred to a sealed heavy walled glass tube, flushed with N_2 and sealed. (CAUTION: It is critical to wait for the exothermic reaction to subside before transferring the mixture to the sealed tube, and then to keep the oil bath temperature below 70 °C. Otherwise, the glass tube may explode.) The reaction was stirred at 55 °C for 18 h. NMR showed that 70% of the olefin was converted to the cyclopropyl group. The mixture was diluted with $CHCl_3$, filtered through celite and washed with saturated NH_4Cl solution. The aqueous solution was extracted with $CHCl_3$. The combined organic layers were dried and concentrated under vacuum to give 3.6 g of a crude product which contained ether and acetal byproducts (Takakis and Rhodes, 1978).

The unreacted 6-hepten-1-ol could not be separated by column chromatography. We therefore used hydroboration to convert it into a more polar compound that could be separated: To a solution of the crude product (3.6 g in 15 mL dry THF) was added 1 M BH_3 in THF (2.98 mL, 2.89 mmol) dropwise. After 10 min, a 50% Na_2CO_3 solution (1.74 mL) was added, followed

by 30% H_2O_2 (1.31 mL). The mixture was stirred for 2 h. 5 mL H_2O was added and the layers were separated. The aqueous layer was washed with ether. The combined organic layers were washed with brine and dried ($MgSO_4$). The solvent was evaporated, and the residue (3 g) was used directly in the next step. ^{1}H-NMR showed that all the olefin had been consumed.

To convert the acetal side products into the alcohol prior to oxidation, the crude product was refluxed in 100 mL 2 N HCl and 100 mL THF for 4 h. The mixture was cooled and extracted with ether. The combined organic layer was washed with saturated $NaHCO_3$ solution, saturated NaCl solution and dried ($MgSO_4$). Evaporation of the solvent and purification of the crude by column chromatography using CH_2Cl_2 furnished the alcohol **2a** (1 g, 45%). GC/MS showed that the product contains 4 % heptanol as a by-product. IR (thin film, NaBr plates), ν: 3332, 3076, 3000, 2928, 2855, 1462, 1056, 1014; ^{1}H NMR (300 MHz, CDCl3) δ 3.59 (t, *J* = 6.6, 2H), 1.86 (s, 1H), 1.53 (dt, *J* = 6.7, 13.7, 2H), 1.45 – 1.23 (m, 4H), 1.16 (dd, *J* = 6.9, 13.8, 2H), 0.51-0.70 (m, 1H), 0.35 (ddd, *J* = 3.9, 5.6, 8.0, 2H), 0.02 – -0.16 (m, 1H). ^{13}C NMR (75 MHz, CDCl3) δ 63.1, 34.9, 33.0, 29.6, 25.8, 11.0, 4.5; GC retention time: product: 14.72 min, heptanol impurity: 9.75 min (program 1); LRMS (APCI+): 129 $(M+H)^+$. See above for PCC oxidation to aldehyde.

Scheme S2. Preparation of 11



Ethyl 2-(4-ethylcyclohexylidene)acetate (12). Ethyl 2-(diethoxyphosphoryl)acetate (8.88 g, 39.6 mmol) in 15 mL dry THF was added dropwise to NaH in 50 mL THF. After the addition, the reaction mixture was stirred for 1 h at room temperature. 4-ethylcyclohexanone (5 g, 39.6 mmol) in 10 mL dry THF was added at a rate that the temperature of the mixture was kept below 30 °C. The solution was then stirred for 15 min during which time a viscous semi-solid appeared. The mixture was taken up in a large excess of water and the aqueous solution was extracted with ether. The ether layer was dried and concentrated. The crude product was purified by column chromatography using ether/hexane (1:19) to give racemic **12** (6.84 g, 88%). IR (thin film, NaBr plates), ν: 2933, 2855, 1716, 1650, 1186, 1150; ^{1}H NMR (300 MHz, CDCl3) δ 5.58 (s, 1H), 4.12 (q, *J* = 7.1, 2H), 3.73 (d, *J* = 14.2, 1H), 2.34 – 2.03 (m, 2H), 2.01 – 1.79 (m, 3H), 1.46 – 1.31 (m, 1H), 1.30 – 1.14 (m, 5H), 1.12 – 0.95 (m, 2H), 0.87 (t, *J* = 7.4, 3H); NMR (75 MHz, CDCl3) δ 167.0, 163.8, 113.1, 59.6, 39.1, 37.5, 34.3, 33.6, 29.1, 14.5, 11.8; GC retention time: 29.22 min (program 1) (Wu et al., 2006).

Ethyl (4-ethylcyclohexyl)acetate (14). Racemic **12** (5.3 g, 27 mmol) was hydrogenated with the procedure described above to give ethyl 2-(4-ethylcyclohexyl)acetate (5.1 g, 95%, mixture of cis and trans isomers). IR (thin film, NaBr plates), ν: 2961, 2920, 2852, 1736, 1174; ^{1}H NMR (300 MHz, CDCl3) δ 4.10 (q, *J* = 7.1, 2H), 2.33 – 1.93 (m, 2H), 1.82 – 0.60 (m, 18H); ^{13}C NMR (75 MHz, CDCl3) δ 173.6, 173.4, 60.2, 42.4, 39.3, 37.2, 35.3, 33.1, 32.6, 30.0, 28.9, 28.4, 14.4, 12.0, 11.6; (The ^{13}C NMR of compounds **14**, **11a** and **11** show more than the expected number of resonances due to the presence of cis and trans isomers. The ratio of the two isomers was determined to be ~2.4:1 by GC/MS (See entry for compound **11** for assignment of major and

minor isomers). GC retention time: 26.78 min and 27.15 min in 2.4:1 ratio (program 1). LRMS (APCI+): 199 $(M+H)^+$.

2-(4-Ethylcyclohexyl)ethanol (11a). Prepared by LAH reduction of compound 14 (see General procedure above). The product is a mixture of cis and trans isomers. The ^{1}H NMR of the product shows two partial overlapping triplets at δ 3.78-3.57 in about 2:1 ratio (-CH_2OH). Yield: 93%. IR (thin film, NaBr plates), ν: 3331, 2960, 2920, 2852, 1448, 1047; ^{1}H NMR (300 MHz, CDCl3) δ 3.78 – 3.57 (m, 2H), 1.85 – 0.67 (m, 18H); ^{13}C NMR (75 MHz, CDCl3) δ 61.4, 61.0, 40.5, 39.6, 34.6, 33.4, 32.9, 31.9, 30.2, 29.1, 28.6, 12.0, 11.7; GC retention times: 22.08 and 22.63 min (program 1, broad trailing peaks); LRMS (EI): 156 (M^+)

2-(4-Ethylcyclohexyl)acetaldehyde (11). Prepared from **11a** by the General PCC oxidation procedure described above. The product is a mixture of cis and trans isomers in 2.4:1 ratio based on GC/MS. Based on the closest literature precedent (Munro, 2000), we tentatively assign the trans isomer to be the major product. IR (thin film, NaBr plates), ν: 2980, 2920, 2852, 2712, 1727, 1448; ^{1}H NMR (300 MHz, CDCl3) δ 9.73 (s, 1H), 2.45 – 2.02 (m, 2H), 1.92 – 0.60 (m, 15H); ^{13}C NMR (75 MHz, CDCl3) δ 203.3, 51.5, 39.2, 33.3, 33.1, 32.7, 30.0, 29.1, 28.3, 11.6; GC retention time: 18.74 min (trans) and 19.28 min (cis) in 2.4:1 ratio (program 1); LRMS (EI): 154(M^+)

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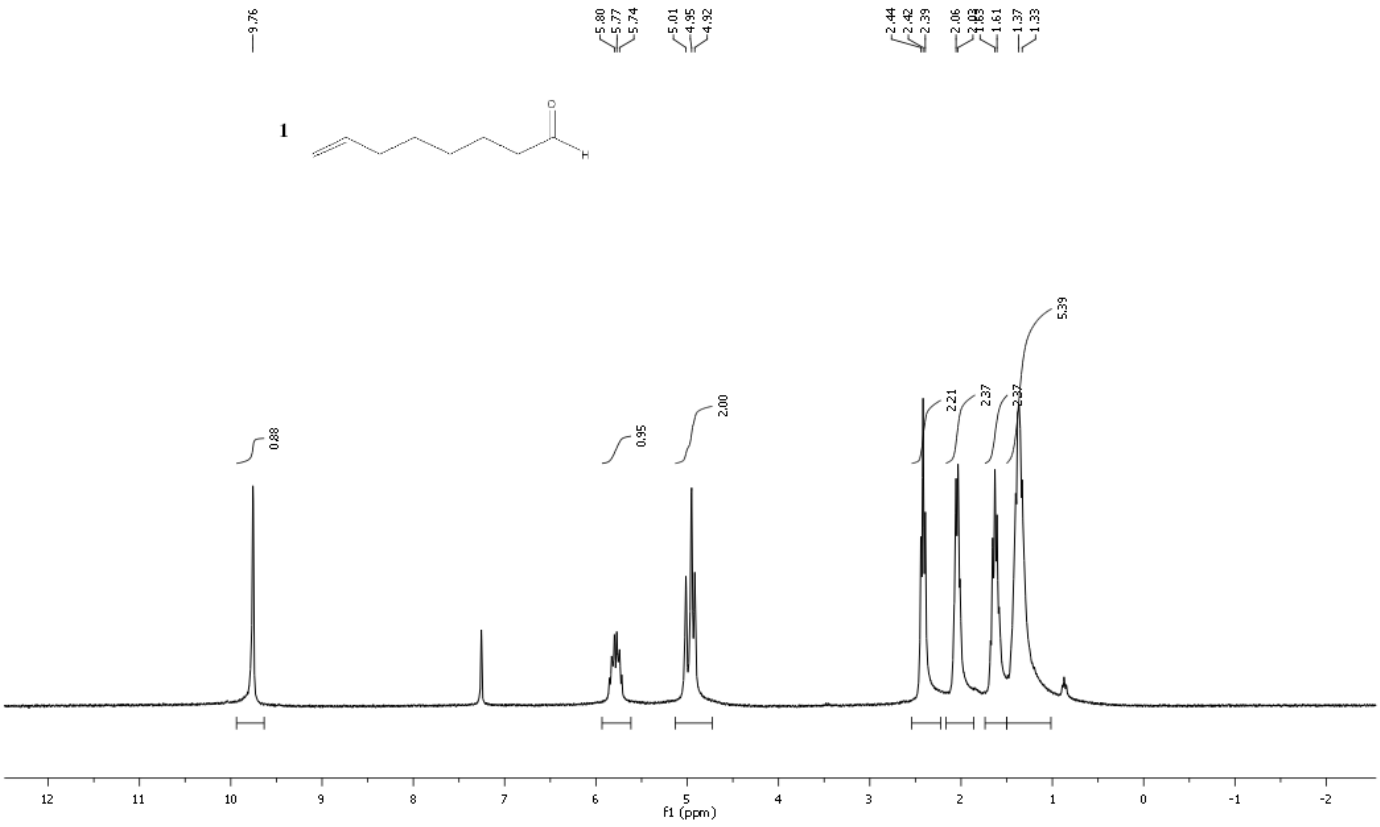
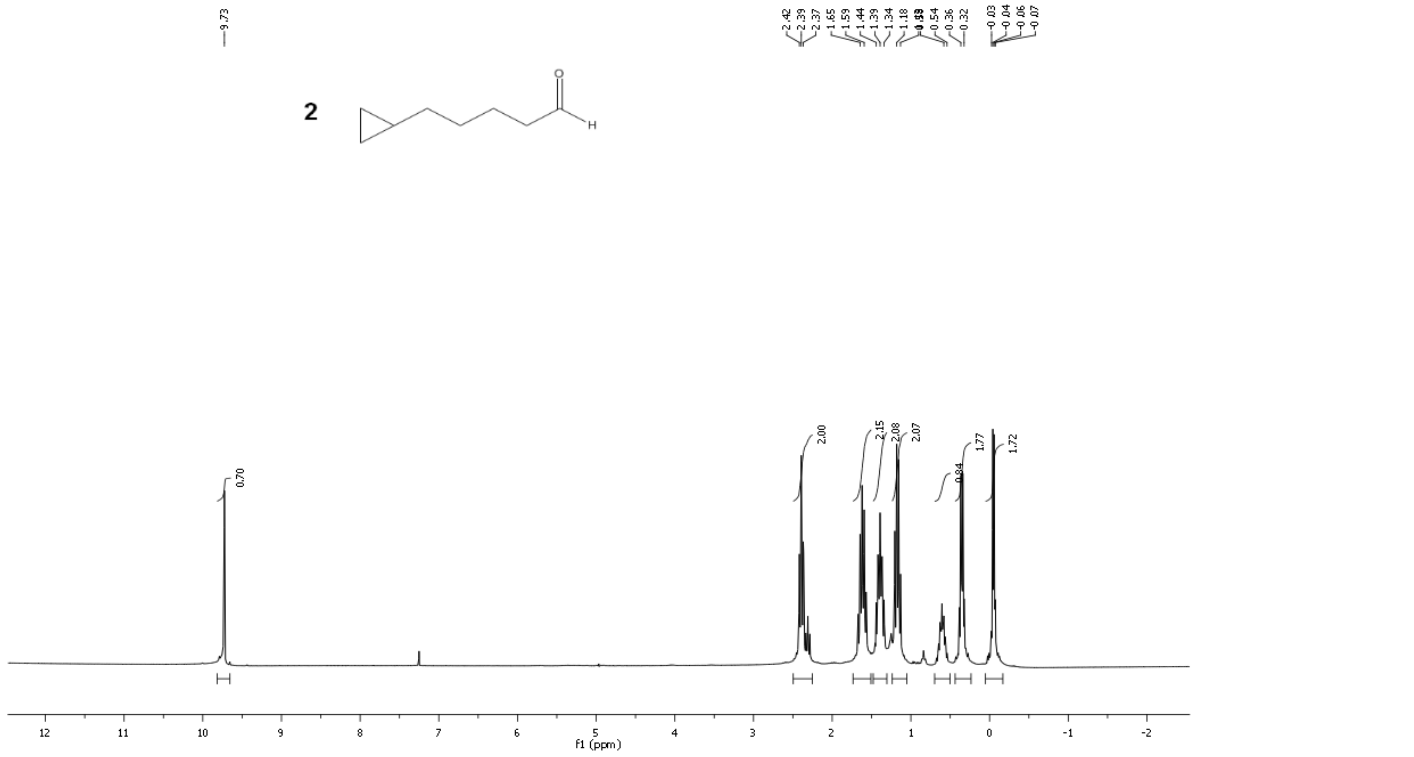
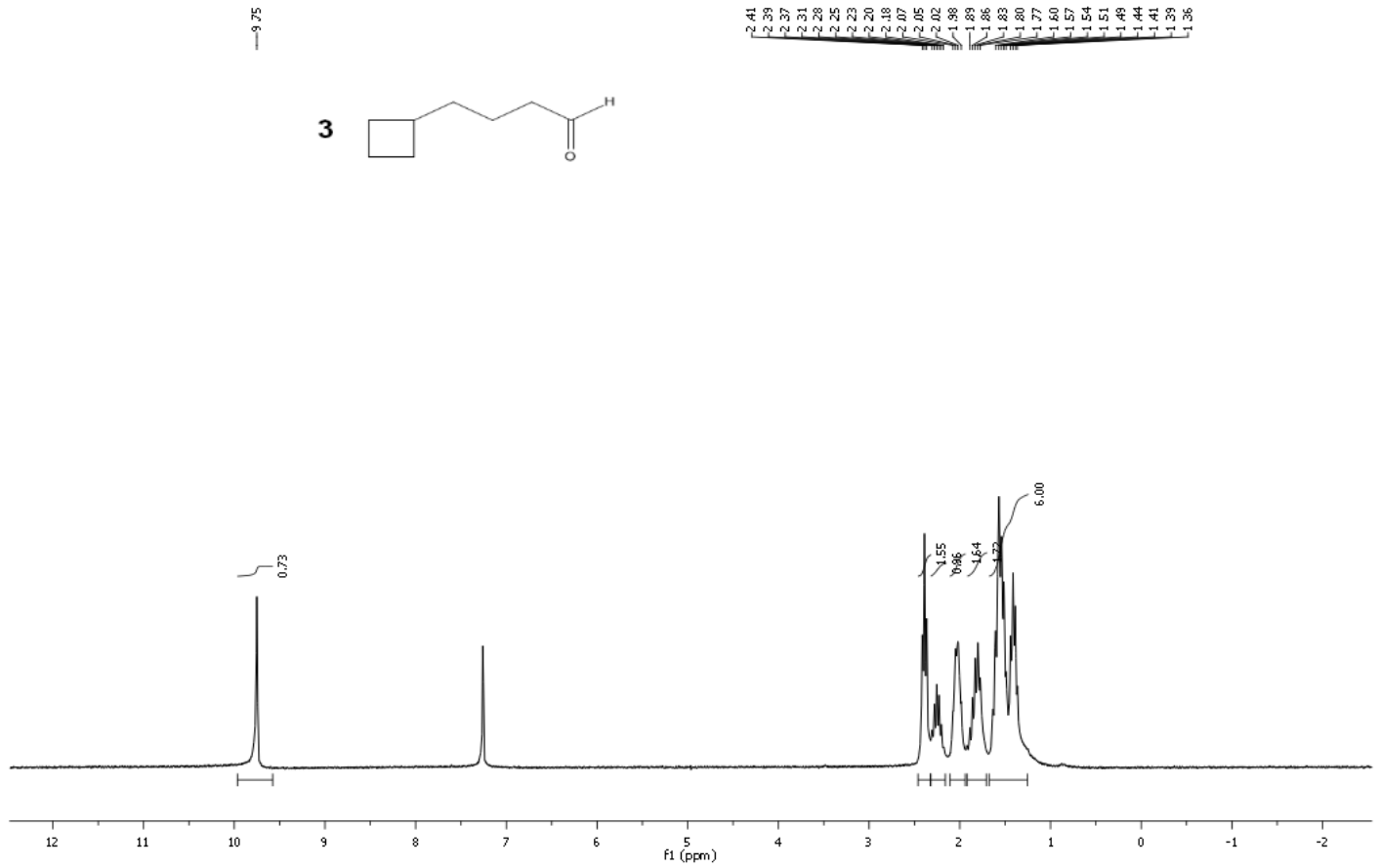
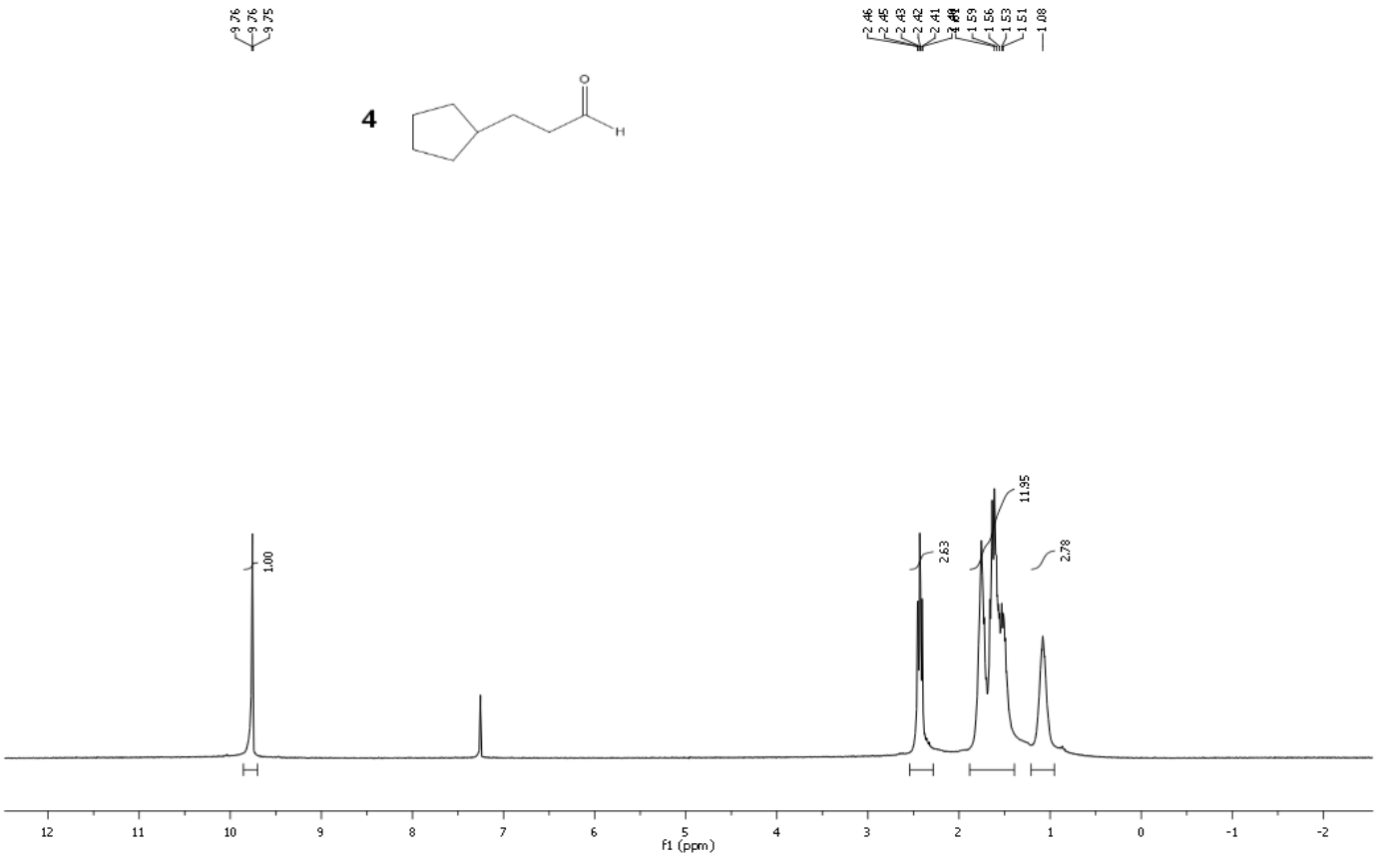
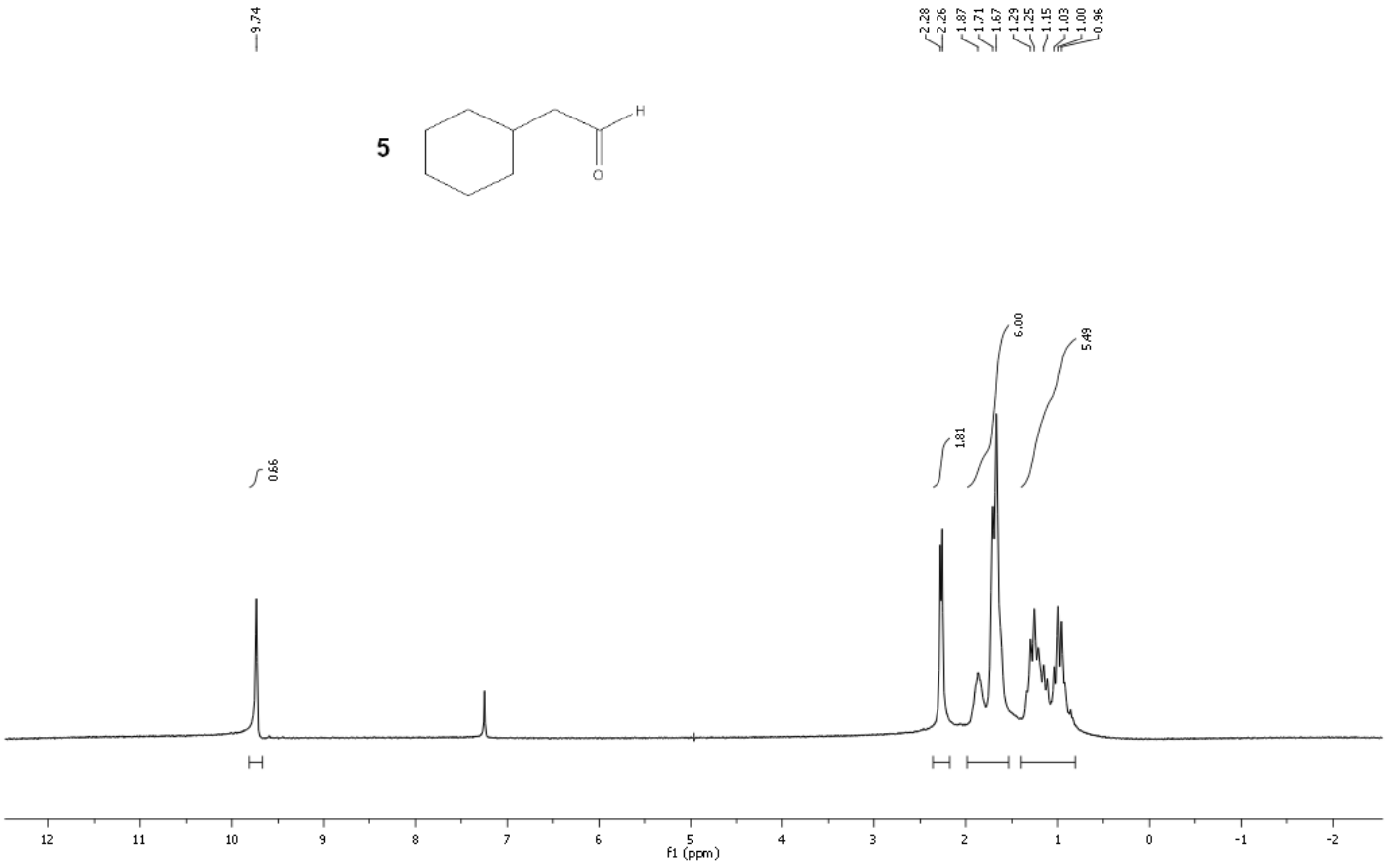
NMR Spectra of Final Aldehydes Used for Testing

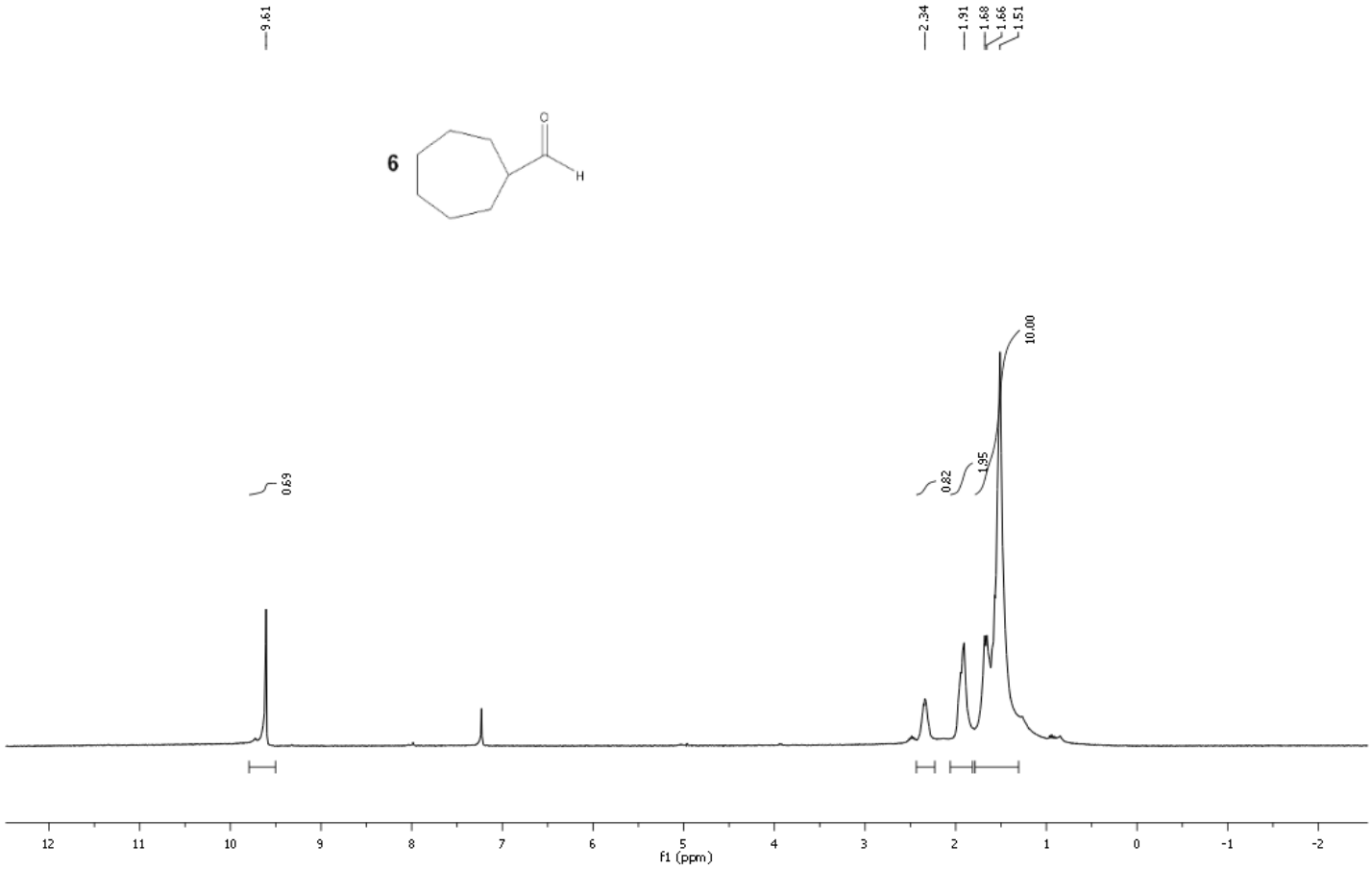


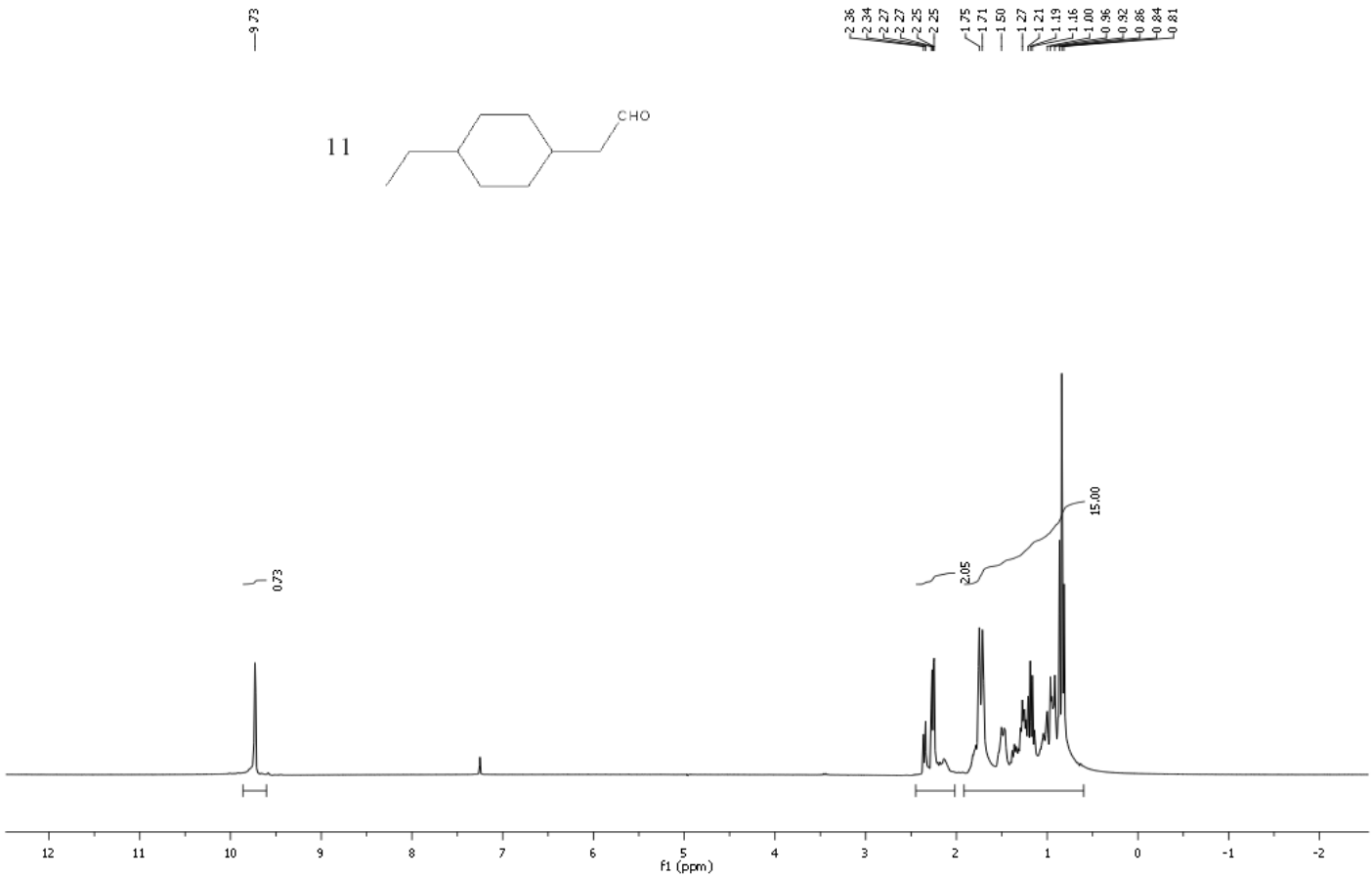

9.73
2.42
2.39
2.37
1.65
1.59
1.44
1.39
1.34
1.18
0.54
0.36
0.32
0.03
0.04
0.06
0.07
2
O
H
0.70
2.00
2.15
2.08
2.07
0.94
1.77
1.72
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


9.75
2.41
2.39
2.37
2.31
2.28
2.25
2.23
2.20
2.18
2.07
2.05
2.02
1.98
1.89
1.86
1.83
1.80
1.77
1.60
1.57
1.54
1.51
1.49
1.44
1.41
1.39
1.36
3
H
O
0.73
1.55
0.96
1.64
1.32
6.00
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


9.76
9.76
9.75
2.46
2.45
2.43
2.42
2.41
1.59
1.56
1.53
1.51
1.08
4
O
H
1.00
2.63
11.95
2.78
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


9.74
2.28
2.26
1.87
1.71
1.67
1.29
1.25
1.15
1.03
1.00
0.96
5
H
O
0.66
1.81
6.00
5.49
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


9.61
2.34
1.91
1.68
1.66
1.51
6
O
H
10.00
0.69
0.82
1.95
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


9.73
2.36
2.34
2.27
2.27
2.25
2.25
1.75
1.71
1.50
1.27
1.21
1.19
1.16
1.00
0.96
0.92
0.86
0.84
0.81
11
CHO
15.00
2.05
0.73
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)