

Supporting Information for

CeO₂-Supported Pd(II)-on-Au Nanoparticle Catalyst for Aerobic Selective α,β -Desaturation of Carbonyl Compounds Applicable to Cyclohexanones

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Experimental Section

Instruments and Regents

Gas Chromatography (GC) analyses were performed on Shimadzu GC2014 equipped with a flame ionization detector (FID) and capillary columns (TC-5) using Shimadzu C-R8A Chromatopac Data Processor for area calculations. GC mass spectroscopy (GC-MS) spectra were recorded on Shimadzu GCMSQP2010 equipped with an InertCap5 capillary column at an ionization voltage of 70 eV. Liquid-state NMR spectra were recorded on JEOL JNM-ECA-500. ¹H and ¹³C NMR spectra were measured at 500.2 and 125.8 MHz, respectively, using tetramethylsilane (TMS) as an internal standard ($\delta = 0$ ppm). ICP-AES analyses were performed on Shimadzu ICPS-8100. Transmission electron microscopy (TEM) observations were performed on JEOL JEM-2000EX. Scanning transmission electron microscopy (STEM) observations were performed on a JEOL JEM-ARM200F. The XPS spectra were measured on a JEOL JPS-9000 using Mg K α radiation ($h\nu = 1253.6$ eV, 8 kV, 10 mA). The binding energies were calibrated by using the C 1s signal at 284.6 eV. XRD patterns were recorded using a Rigaku SmartLab instrument under Cu K α radiation (45 kV, 200 mA). BET surface areas were measured on micromeritics ASAP 2010 and calculated from the N₂ adsorption isotherm with the BET equation. Elemental analyses for C, H, and N were performed on Elementar vario MICRO cube. Elemental analysis for Cl was performed on Thermo Fisher Scientific ICS-1600. Pd K-edge X-ray absorption spectroscopy (XAS) was carried out using the transmission method at the BL11S2beamline of the Aichi Synchrotron Radiation Center (Proposal No. 201902024) or BL14B2beamline of SPring-8 (Proposal No. 2019B1820). The Pd K-edge spectra were analyzed by Athena. Column chromatography on silica gel was performed by using Biotage Isolera. CeO₂ (BET surface area: 92

$\text{m}^2 \text{g}^{-1}$ after calcination at $550\text{ }^\circ\text{C}$ for 3 h, JRC-CEO-5, Daiichi Kigenso Kagaku Kogyo), Al_2O_3 (BET surface area: $160\text{ m}^2 \text{g}^{-1}$ after calcination at $550\text{ }^\circ\text{C}$ for 3 h, KHS-24, Sumitomo Chemical), TiO_2 (BET surface area: $316\text{ m}^2 \text{g}^{-1}$, ST-01, Ishihara Sangyo Kaisya), $\text{Mg}_6\text{Al}_2(\text{OH})_{16}\text{CO}_3\cdot 4\text{H}_2\text{O}$ (LDH, BET surface area: $51\text{ m}^2 \text{g}^{-1}$, Tomita Pharmaceutical Co., Ltd.), were commercially available. Solvents, substrates, and metal sources were obtained from TCI, Aldrich, Kanto Chemical, FUJIFILM Wako Pure Chemical, Nacalai Tesque, Kojima Chemicals, or Combi-Blocks (reagent grade). Some substrates were purified by kugelrohr distillation just before the use for reactions.

Preparation of Catalysts

Pd/Au/CeO_2 ($\text{Pd/Au} = 1/5$) was typically prepared as follows. CeO_2 (2 g) was added to an aqueous solution (60 mL) of HAuCl_4 (6.25 mM) and K_2PdCl_4 (0.83 mM) which was generated *in situ* from a mixture of PdCl_2 (0.05 mmol) and KCl (0.1 mmol), and the slurry was stirred for 15 min, followed by the dropping of aqueous NaOH (1 M) up to $\text{pH} = 10$. After stirring for 24 h, the resulting mixture was filtered, washed with deionized water (1 L), and dried *in vacuo*, affording a supported Au–Pd hydroxide precursor. The Au–Pd hydroxide precursor was dispersed in 50 mL water and reduced with NaBH_4 (70 mg). The resulting slurry was then stirred vigorously at room temperature for 2 h in open air conditions. The solid was then filtered off, washed with water (1 L), and dried *in vacuo* overnight, giving Pd/Au/CeO_2 as a dark-gray powder (Au content: 2.1 wt%, Pd content: 0.21 wt%). Pd/Au/CeO_2 catalysts with different Au/Pd ratios were prepared with different concentration of HAuCl_4 and K_2PdCl_4 .

$\text{Pd(OH)}_x/\text{CeO}_2$ was prepared as follows. CeO_2 (2 g) was added to an aqueous solution (60 mL) of K_2PdCl_4 which was generated *in situ* from a mixture of PdCl_2 and KCl , and the slurry was stirred for 15 min, followed by the dropping of aqueous NaOH (1 M) up to $\text{pH} = 10$. After stirring for 24 h, the resulting mixture was filtered, washed with deionized water (1 L), and dried *in vacuo*, affording $\text{Pd(OH)}_x/\text{CeO}_2$. Pd/CeO_2 , reduced $\text{Pd(OH)}_x/\text{CeO}_2$ using NaBH_4 , was prepared as follows. $\text{Pd(OH)}_x/\text{CeO}_2$ was dispersed in 50 mL water and NaBH_4 (70 mg) was added in the slurry. The resulting slurry was then stirred vigorously at room temperature for 2 h. The solid was then filtered off, washed with water (1 L), and dried *in vacuo* overnight, giving Pd/CeO_2 as a brown powder. By changing K_2PdCl_4 to HAuCl_4 , Au/CeO_2 was prepared by the same method as Pd/CeO_2 .

Catalytic Reaction

The catalytic reaction was typically carried out according to the following procedure. Into a Pyrex test tube (volume: approximately 20 mL) were successively added Pd/Au/CeO_2 (200 mg, Au: 4.3 mol%, Pd: 0.8 mol%), biphenyl (0.1 mmol, internal standard), cyclohexanone (**1a**, 0.5 mmol), dimethylacetamide (2 mL), and a Teflon-coated magnetic stir bar; the mixture was then stirred at $70\text{ }^\circ\text{C}$ under an open air atmosphere without closing the cap. The yields of products were determined by GC

analysis using biphenyl as an internal standard. The products were identified by the GC-MS, NMR, and/or elemental analysis.

Isolation of Products

After the reaction was finished, the catalyst was filtered off and the filtrate was added to CH₂Cl₂ (20 mL). Next, to remove DMA, the solution was washed with H₂O (5 mL) and then evaporated to remove solvents. The crude product was subjected to silica-gel column chromatography using hexane and ethyl acetate (9:1) as the eluent, giving the pure product. Regarding the yields of isolated products, separations of substrates and α,β -desaturated products were very difficult by silica-gel column chromatography, giving substantially low isolated yields in comparison with the corresponding GC yields.

Catalyst Reuse

The reuse of catalyst was carried out as follows. After the reaction, Pd/Au/CeO₂ was filtered off and washed with acetone (100 mL). The used Pd/Au/CeO₂ was calcinated at 300 °C for 2 h under an air atmosphere. The calcinated Pd/Au/CeO₂ (200 mg) was dispersed in 5 mL water reduced with NaBH₄ (7 mg). The resulting slurry was then stirred vigorously at room temperature for 2 h. The solid was then filtered off, washed with water (100 mL), and dried *in vacuo* overnight, giving the regenerated catalyst as a dark-gray powder.

Hot Filtration

Hot filtration test was carried out as follows. Into a Pyrex test tube (volume: approximately 20 mL) were successively added Pd/Au/CeO₂ (100 mg, Au: 2.1 mol%, Pd: 0.4 mol%), biphenyl (0.1 mmol, internal standard), cyclohexanone (**1a**, 0.5 mmol), dimethylacetamide (2 mL), and a Teflon-coated magnetic stir bar; the mixture was then stirred at 70 °C under an open air atmosphere without closing the cap. Thirty minutes after the reaction had started, the catalyst was quickly filtered off from the solution before the solution cooled. Then, the filtrate was continued to be reacted at 70 °C for further 3.5 h.

O₂ Pressure Dependence on Production Rates

Experiments of O₂ pressure dependence on production rates of cyclohexenone were carried out as follows. Into a schlenk flask, an internal standard, a substrate, the catalyst and DMA solvent were added. After the flask was degassed by freeze-pump-thaw cycling, the reaction started under an atmosphere of O₂/N₂ mixed gas balloon with controlled O₂ partial pressures of them using flow meters (for 0.2 atm of O₂, an open air was used in a test tube). The solutions sampled every 5 min for 30 min were analyzed by GC. The conversion as of 30 min was less than 10%. Thus, the concentration change

of substrates can be considered little. The error range was estimated from uncertainty of C-R8A Chromatopac Data Processor and flow meters to make O₂/N₂ mixed gas balloons.

Kinetic Isotope Effects (KIE)

KIE experiments were carried out by comparison of independent initial reaction rates. After a test tube was warmed to 70 °C with the catalyst, DMA solvent, and an internal standard, a substrate (cyclohexanone, cyclohexanone- α -*d*₄, or cyclohexanone-*d*₁₀) was added to start the reaction (0 min). The solutions sampled every 5 min for 30 min were analyzed by GC. The substrate conversion as of 30 min was less than 10%. Thus, the concentration change of substrates can be considered little during the reaction. The error range was estimated from uncertainty of C-R8A Chromatopac Data Processor.

Preparation of 3-Phenylcyclohexanone

3-Phenylcyclohexanone was synthesized by the same method as our previous report.^{S1} In a 50 mL Schlenk tube, [Rh(cod)Cl]₂ (0.05 mmol), 2-cyclohexen-1-one (10 mmol), phenylboronic acid (10 mmol), Na₂CO₃ (20 mmol), H₂O (10 mL) and a Teflon-coated magnetic stir bar were successively placed and the reaction mixture was stirred for 1 h at 80 °C. After the reaction, the solids were filtered off and the filtrate was washed with CH₂Cl₂ (10 mL) three times. The solvents were removed by rotavap and the crude product was subjected to column chromatography on silica gel (using hexane/EtOAc = 85/15, *R*_f = 0.38 as the eluent), giving the pure product (isolated as light yellow oil in 69% yield). ¹H NMR (500 MHz, CDCl₃, TMS): δ 7.34–7.17 (m, 5H), 3.03–2.96 (m, 1H), 2.62–2.32 (m, 4H), 2.17–2.03 (m, 2H), 1.89–1.71 (m, 2H). MS (70 eV, ED): *m/z* (%): 175 (11), 174 (86) [*M*⁺], 146 (6), 145 (6), 132 (12), 131 (79), 130 (8), 129 (6), 128(5), 118 (31), 117 (100), 116 (8), 115 (25), 105 (19), 104 (77), 103 (34), 102 (6), 92 (7), 91 (39), 83(18), 82 (7), 78 (27), 77 (24), 70 (14), 65 (10), 63 (6), 55 (9), 52 (6), 51 (17) 50 (6).

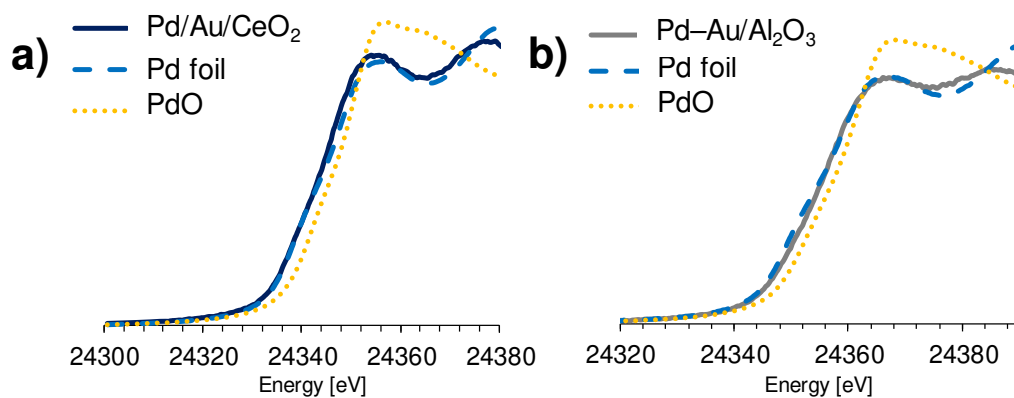


Figure S1. XANES spectra around Pd-K edge of a) Pd/Au/CeO₂ prepared under an Ar atmosphere and b) Pd-Au/Al₂O₃. Pd foil (blue) and Pd oxide (orange) are shown as the references.

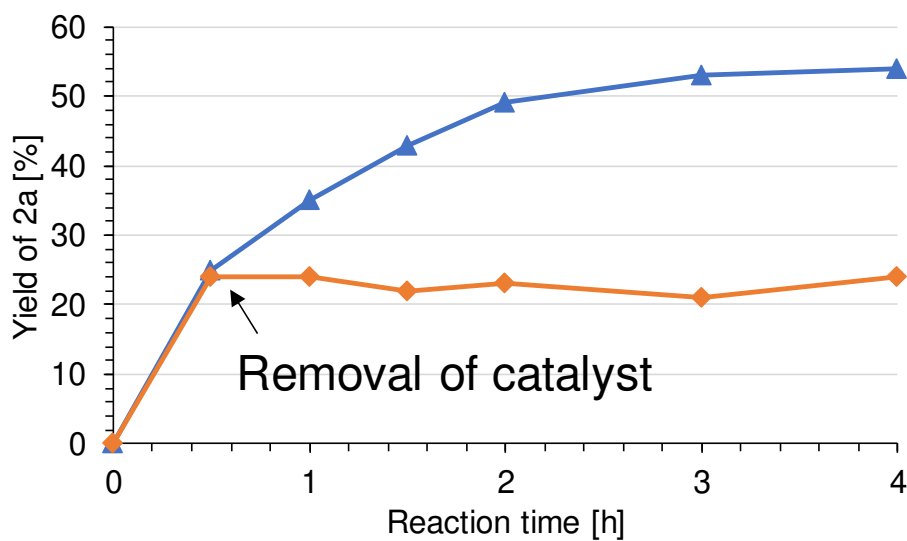
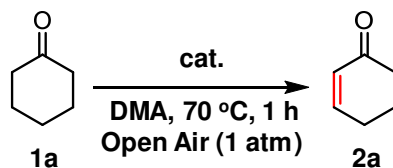
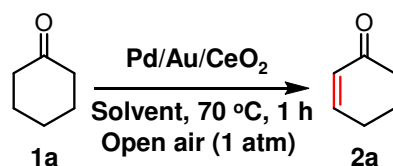


Figure S2. Leaching test. Reaction conditions: cyclohexanone (0.5 mmol), dimethylacetamide (2 mL), open air (1 atm), Pd/Au/CeO₂ (100 mg, Au: 2.1 mol%, Pd: 0.4 mol%), 70 °C. Yields were determined by GC analysis using biphenyl as an internal standard.

Table S1. Effect of Molar Ratio of Pd/Au/CeO₂^a

Entry	Catalyst	Amount (mol%)		Yield (%)	
		Au	Pd	2a	3a
1	Pd/Au/CeO ₂	3.0	0.6	74	<1
2	Pd/Au/CeO ₂	1.4	0.6	56	<1
3	Pd/Au/CeO ₂	0.5	0.5	54	<1
4	Pd/Au/CeO ₂	0.07	0.6	9	<1

^aReaction conditions: Catalyst (140 mg), **1a** (0.5 mmol), DMA (2 mL), open air (1 atm), 70 °C, 1 h. Yields were determined by GC analysis using biphenyl as the internal standard.

Table S2. Effect of Solvents^a

Entry	Solvent	Yield (%)	
		2a	3a
1	<i>N,N</i> -Dimethylacetamide	74	<1
2	Cyclopentylmethylether	56	<1
3	Toluene	51	<1
4	Dioxane	43	<1
5	Butyl Acetate	37	<1
6	Heptane	32	<1
7	Dimethylformamide	32	<1
8	Mesitylene	31	<1
9	<i>N</i> -methyl pyrrolidone	16	<1
10	Dimethyl Sulfoxide	<1	<1

^aReaction conditions: **1a** (0.5 mmol), solvent (2 mL), open air (1 atm), Pd/Au/CeO₂ (140 mg, Au: 3.0 mol%, Pd: 0.6 mol%), 70 °C, 1 h. Yields were determined by GC analysis using biphenyl as an internal standard.

Table S3. Optimization of the Reaction Conditions of the Aerobic Dehydrogenation of 1-Octanal (1b) to 2-Octenal (2b)^a

$\text{C}_5\text{H}_{11}\text{CH}_2\text{CH}_2\text{CHO}$ (1w) $\xrightarrow[\text{DMA, 50 }^\circ\text{C, Open air (1 atm)}]{\text{catalyst}}$ $\text{C}_5\text{H}_{11}\text{CH}=\text{CHCHO}$ (2w) + $\text{C}_5\text{H}_{11}\text{CH}_2\text{CH}_2\text{COOH}$ (3w)

Entry	Catalyst	Yield [%]	
		2w	3w
1	Au/Al ₂ O ₃	<1	15
2	Pd/Al ₂ O ₃	<1	23
3 ^b	Pd–Au/Al ₂ O ₃	60	12
4	Au/Al ₂ O ₃ + Pd/Al ₂ O ₃	9	15
5	Al ₂ O ₃	<1	<1
6	None	<1	71

^aReaction conditions: Catalyst (100 mg, total metal: 4 mol%), **1w** (0.5 mmol), DMA (2 mL), open air (1 atm), 50 °C, 24 h. Yields were determined by GC analysis using biphenyl as the internal standard.

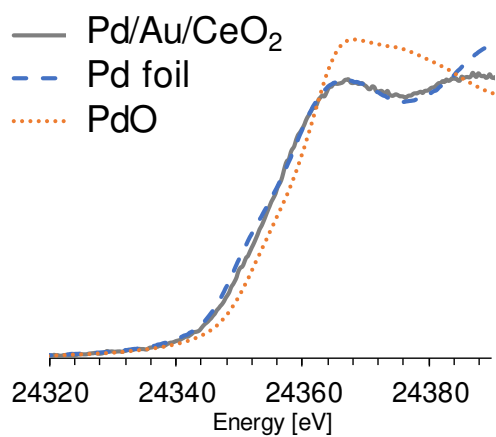


Figure S3. XANES spectra around Pd-K edge of the used catalyst. Pd foil (blue) and Pd oxide (orange) are shown as the references.

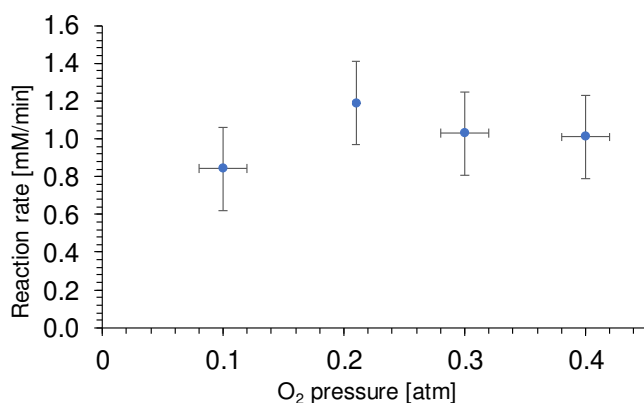


Figure S4. The initial rates of dehydrogenation of cyclohexanone by Pd/Au/CeO₂ under various O₂ pressures. Reaction conditions: Pd/Au/CeO₂ (50 mg; Pd: 0.2 mol%, Au: 1.1 mol%), **1a** (0.5 mmol), DMA (2 mL), 70 °C. Yields were determined by GC using biphenyl as the internal standard.

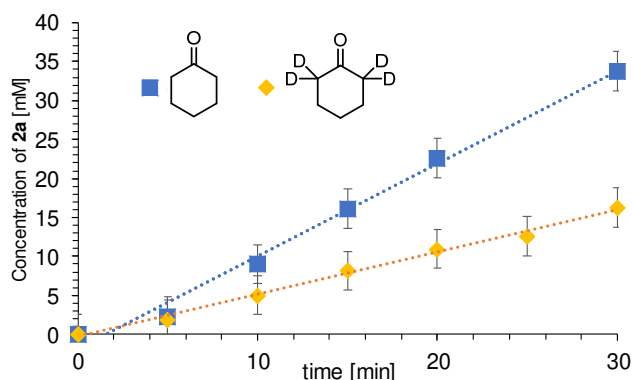


Figure S5. The reaction profile of dehydrogenation of cyclohexanone (blue profile) and cyclohexanone-d₄ (α -deuterated cyclohexanone, orange profile). Reaction conditions: Pd/Au/CeO₂ (50 mg; Pd: 0.2 mol%, Au: 1.1 mol%), substrate (0.5 mmol), DMA (2 mL), open air (1 atm), 70 °C. Yields were determined by GC using biphenyl as the internal standard.

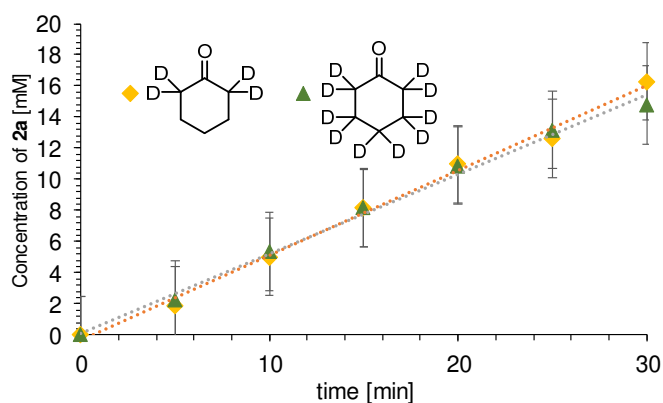
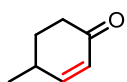


Figure S6. The reaction profile of dehydrogenation of cyclohexanone-d₄ (orange profile) and cyclohexanone-d₁₀ (completely deuterated cyclohexanone, green profile). Reaction conditions: Pd/Au/CeO₂ (50 mg; Pd: 0.2 mol%, Au: 1.1 mol%), substrate (0.5 mmol), DMA (2 mL), open air (1 atm), 70 °C. Yields were determined by GC using biphenyl as the internal standard.

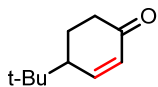
Spectral Data of Products



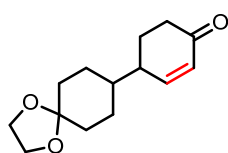
2-Cyclohexen-1-one (CAS No. 930-68-7), Table 2, entry 1, 80% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 8.3 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.46 (calculated by calibration curve using a commercial substance). MS (EI): *m/z* (%): 96 (37) [*M*⁺], 69 (5), 68 (100), 67 (5), 55 (6), 53 (5). Spectral data matched the data obtained from Wiley Subscription Services, Inc.



4-Methyl-2-cyclohexen-1-one (CAS No. 5515-76-4), Table 2, entry 2, 79% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 10.5 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.49 (estimated by the effective carbon number concept^{S2}). MS (EI): *m/z* (%): 110 (54) [*M*⁺], 82 (100), 81 (25), 68 (56), 67 (30), 55 (21), 54 (50), 53 (20).^{S3}

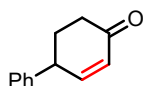


4-(tert-Butyl)-2-cyclohexen-1-one (CAS No. 937-07-5), Table 2, entry 3, 74% GC yield. 32% isolated yield (24.5 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 17.7 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.74 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 7.02 (dd, *J* = 10.5 and 2.0 Hz, 1H), 6.04 (d, *J* = 10.5 Hz, 1H), 2.56–2.49 (m, 1H), 2.39–2.30 (m, 1H), 2.23–2.18 (m, 1H), 2.14–2.07 (m, 1H), 1.80–1.72 (m, 1H), 0.98 (s, 9H); ¹³C NMR (125 MHz, CDCl₃): δ 24.56, 27.56, 33.11, 38.04, 47.02, 130.16, 153.22, 200.34. MS (EI): *m/z* (%): 96 (100), 95 (29), 67 (15), 57 (97).^{S4}



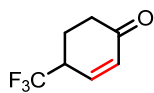
4-(1,4-Dioxaspiro[4.5]decan-8-yl)cyclohex-2-en-1-one, Table 2, entry 4, >99% GC yield, 49% isolated yield (58.4 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 26.6 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.91 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 6.96–6.91 (m, 1H), 6.04–5.98 (m, 1H), 3.98–3.91 (m, 4H), 2.55–2.48 (m, 1H), 2.40–2.31 (m, 2H), 2.07–1.99 (m, 1H), 1.88–1.72 (m, 4H), 1.70–1.64 (m, 1H), 1.60–1.36 (m, 5H); ¹³C NMR

(125 MHz, CDCl₃): δ 25.87, 27.13, 27.33, 34.85, 37.56, 40.55, 41.14, 64.43, 108.68, 129.79, 154.24, 200.16. MS (EI): m/z (%): 236 (12) [M^+], 100 (15), 86 (33), 55 (18). Anal. Calc. for C₁₄H₂₀O₃·0.3H₂O: C, 69.57; H, 8.59. Found: C, 69.67; H, 8.57.



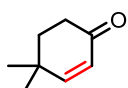
4-Phenyl-2-cyclohexen-1-one (CAS No. 51171-72-3), Table 2, entry 5, 57% GC yield.

19% isolated yield (17 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 22.6 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.91 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 7.39–7.34 (m, 2H), 7.31–7.25 (m, 1H), 7.25–7.20 (m, 2H), 7.02–6.97 (m, 1H), 6.19–6.14 (m, 1H), 3.76–3.71 (m, 1H), 2.59–2.44 (m, 2H), 2.40–2.33 (m, 1H), 2.10–2.01 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 32.70, 37.19, 42.85, 127.32, 127.78, 129.09, 130.21, 143.03, 153.17, 199.56. MS (EI): m/z (%): 174 (12), 172 (65) [M^+], 144 (26), 131 (13), 130 (100), 129 (53), 128 (16), 117 (18), 116 (53), 115 (90), 104 (20), 91 (22), 89 (13), 77 (11), 63 (12), 58 (17), 57 (11), 51 (14).^{S5}



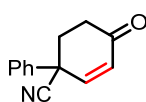
4-(Trifluoromethyl)-2-cyclohexen-1-one (CAS No. 81206-69-1), Table 2, entry 6,

10% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 7.4 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.49 (estimated by the effective carbon number concept^{S2}). MS (EI): m/z (%): 164 (41) [M^+], 136 (100), 108 (55), 87 (35), 68 (81).

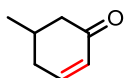


4,4-Dimethyl-2-cyclohexen-1-one (CAS No. 1073-13-8), Table 2, entry 7, 94% GC

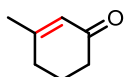
yield, 49% isolated yield (29.8 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 11.7 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.58 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 6.66 (d, J = 10.0 Hz, 1H), 5.84 (d, J = 10.0 Hz, 1H), 6.44–6.41 (m, 1H), 2.48–2.42 (m, 2H), 1.90–1.84 (m, 2H), 1.17 (s, 6H); ¹³C NMR (125 MHz, CDCl₃): δ 27.92, 33.04, 34.61, 36.31, 127.07, 160.07, 199.84. MS (EI): m/z (%): 124 (49) [M^+], 109 (10), 96 (86), 95 (16), 82 (100), 81 (92), 79 (22), 68 (33), 67 (62), 55 (13), 53 (36), 51 (12).^{S6}



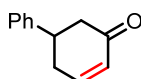
4-Cyano-4-phenyl-2-cyclohexen-1-one (CAS No. 106920-49-4), Table 2, entry 8, 58% GC yield. 28% isolated yield (27.5 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 24.2 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.93 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 7.49–7.39 (m, 5H), 7.31–7.25 (m, 1H), 7.25–7.20 (m, 2H), 6.92–6.87 (m, 1H), 6.36–6.32 (m, 1H), 2.85–2.77 (m, 1H), 2.70–2.64 (m, 1H), 2.60–2.53 (m, 1H), 2.44–2.36 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 34.99, 37.98, 43.05, 119.40, 126.25, 129.14, 129.69, 132.05, 137.78, 145.24, 196.26.^{S7} MS (EI): *m/z* (%): 197 (48) [*M*⁺], 170 (13), 169 (100), 141 (65), 140 (41), 115 (20), 114 (25), 113 (11), 77 (11), 77 (11), 70 (14), 68 (55), 63 (12), 51 (18).



5-Methyl-2-cyclohexen-1-one (CAS No. 7214-50-8), Table 2, entry 9, 43% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 12.9 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.49 (estimated by the effective carbon number concept^{S2}). MS (EI): *m/z* (%): 110 (22) [*M*⁺], 68 (100).^{S3}

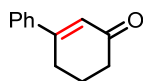


3-Methyl-2-cyclohexen-1-one (CAS No. 1193-18-6), Table 2, entry 9, 14% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 10.3 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.49 (estimated by the effective carbon number concept^{S2}). MS (EI): *m/z* (%): 110 (36) [*M*⁺], 82 (100), 54 (33).^{S3}

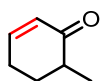


5-Phenyl-2-cyclohexen-1-one (CAS No. 35376-41-1), Table 2, entry 10, 39% GC yield, 29% isolated yield (25.1 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 22.8 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.91 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 7.38–7.32 (m, 2H), 7.28–7.23 (m, 3H), 7.08–7.03 (m, 1H), 6.16–6.11 (m, 1H), 3.39–3.31 (m, 1H), 2.75–2.62 (m, 3H), 2.58–2.50 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 33.91, 41.18, 45.09, 126.91, 127.21, 128.99, 130.00, 143.41, 149.68, 199.38.^{S8}

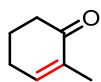
MS (EI): m/z (%): 172 (43) [M^+], 130 (15), 128 (10), 104 (92), 103 (16), 78 (18), 77 (15), 68 (100), 51 (10).



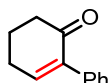
1-Phenyl-1-cyclohexen-3-one (CAS No. 10345-87-6), Table 2, entry 10, 42% GC yield, 27% isolated yield (24.0 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column temp., 280 $^{\circ}$ C, progress rate, 1 $^{\circ}$ C \cdot min $^{-1}$ (10 min), 10 $^{\circ}$ C \cdot min $^{-1}$ (12 min), 20 $^{\circ}$ C \cdot min $^{-1}$ (4 min), injection temp., 280 $^{\circ}$ C; detection temp., 300 $^{\circ}$ C; retention time, 23.9 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.91 (estimated by the effective carbon number concept^{S2}). 1H NMR (500 MHz, $CDCl_3$): δ 7.57–7.51 (m, 2H), 7.44–7.38 (m, 3H), 6.44–6.41 (m, 1H), 2.82–2.75 (m, 2H), 2.52–2.45 (m, 2H), 2.20–2.12 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 23.02, 28.32, 37.47, 125.63, 126.29, 128.97, 130.20, 139.00, 160.09, 200.19. MS (EI): m/z (%): 172 (49) [M^+], 145 (12), 144 (100), 129 (11), 128 (13), 116 (56), 115 (70).^{S9}



6-Methyl-2-cyclohexen-1-one (CAS No. 6610-21-5), Table 2, entry 11, 14% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column temp., 280 $^{\circ}$ C, progress rate, 1 $^{\circ}$ C \cdot min $^{-1}$ (10 min), 10 $^{\circ}$ C \cdot min $^{-1}$ (12 min), 20 $^{\circ}$ C \cdot min $^{-1}$ (4 min), injection temp., 280 $^{\circ}$ C; detection temp., 300 $^{\circ}$ C; retention time, 10.1 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.49 (estimated by the effective carbon number concept^{S2}). MS (EI): m/z (%): 110 (21) [M^+], 68 (100).^{S10}

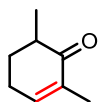


2-Methyl-2-cyclohexen-1-one (CAS No. 1121-18-2), Table 2, entry 11, 13% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column temp., 280 $^{\circ}$ C, progress rate, 1 $^{\circ}$ C \cdot min $^{-1}$ (10 min), 10 $^{\circ}$ C \cdot min $^{-1}$ (12 min), 20 $^{\circ}$ C \cdot min $^{-1}$ (4 min), injection temp., 280 $^{\circ}$ C; detection temp., 300 $^{\circ}$ C; retention time, 10.8 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.49 (estimated by the effective carbon number concept^{S2}). MS (EI): m/z (%): 110 (59) [M^+], 82 (100), 67 (15), 54 (53), 53 (12).^{S3}

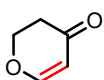


2-Phenyl-2-cyclohexen-1-one (CAS No. 4556-09-6), Table 2, entry 12, 83% GC yield, 46% isolated yield (39.9 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column temp., 280 $^{\circ}$ C, progress rate, 1 $^{\circ}$ C \cdot min $^{-1}$ (10 min), 10 $^{\circ}$ C \cdot min $^{-1}$ (12 min), 20 $^{\circ}$ C \cdot min $^{-1}$ (4 min), injection temp., 280 $^{\circ}$ C; detection temp., 300 $^{\circ}$ C; retention time, 23.2 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.91 (estimated by the effective carbon number concept^{S2}). 1H NMR (500 MHz, $CDCl_3$): δ 7.38–7.28 (m, 5H), 7.02 (t, J = 4.5 Hz, 1H), 2.60–2.56 (m, 2H), 2.55–2.50 (m, 2H), 2.12–2.06 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 24.00, 26.70, 39.24,

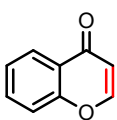
127.76, 128.20, 128.80, 136.73, 140.54, 148.14, 197.19. MS (EI): m/z (%): 173 (11), 172 (88) [M^+], 144 (78), 130 (26), 129 (25), 128 (24), 117 (21), 116 (96), 115 (100), 103 (20), 102 (15), 89 (14), 77 (11), 63 (14), 51 (14).^{S11}



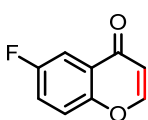
2,6-Dimethyl-2-cyclohexen-1-one (CAS No. 40790-56-5), Table 2 entry 13, 20% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column temp., 280 $^{\circ}$ C, progress rate, 1 $^{\circ}$ C \cdot min $^{-1}$ (10 min), 10 $^{\circ}$ C \cdot min $^{-1}$ (12 min), 20 $^{\circ}$ C \cdot min $^{-1}$ (4 min), injection temp., 280 $^{\circ}$ C; detection temp., 300 $^{\circ}$ C; retention time, 11.3 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.58 (estimated by the effective carbon number concept^{S2}). MS (EI): m/z (%): 124 (34) [M^+], 82 (100), 54 (38).^{S12}



2,3-Dihydro-4H-pyran-4-one (CAS No. 84302-42-1), Table 2, entry 14, 53 % GC yield. 37% isolated yield (47.5 mg as mixture with hexane and ethyl acetate). GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column temp., 280 $^{\circ}$ C, progress rate, 1 $^{\circ}$ C \cdot min $^{-1}$ (10 min), 10 $^{\circ}$ C \cdot min $^{-1}$ (12 min), 20 $^{\circ}$ C \cdot min $^{-1}$ (4 min), injection temp., 280 $^{\circ}$ C; detection temp., 300 $^{\circ}$ C; retention time, 7.5 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.24 (estimated by the effective carbon number concept^{S2}). 1H NMR (500 MHz, $CDCl_3$): δ 7.36 (d, J = 6.0 Hz, 1H), 5.42 (d, J = 6.0 Hz, 1H), 4.52 (t, J = 7.0 Hz, 2H), 2.61 (t, J = 7.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 36.77, 68.39, 107.78, 163.64, 191.98.^{S13} MS (EI): m/z (%): 98 (100) [M^+], 87 (14), 71 (21), 70 (79), 69 (97), 44 (29), 43 (29), 41 (12), 29 (18), 28 (33), 27 (18), 26 (14).

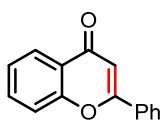


Chromone (CAS No. 491-38-3), Table 2, entry 15, 84% GC yield. 55% isolated yield (42.4 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column temp., 280 $^{\circ}$ C, progress rate, 1 $^{\circ}$ C \cdot min $^{-1}$ (10 min), 10 $^{\circ}$ C \cdot min $^{-1}$ (12 min), 20 $^{\circ}$ C \cdot min $^{-1}$ (4 min), injection temp., 280 $^{\circ}$ C; detection temp., 300 $^{\circ}$ C; retention time, 20.1 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.58 (estimated by the effective carbon number concept^{S2}). 1H NMR (500 MHz, $CDCl_3$): δ 8.21 (dd, J = 8.0 and 1.5 Hz, 1H), 7.87 (d, J = 6.0 Hz, 1H), 7.69–7.64 (m, 1H), 7.49–7.45 (m, 1H), 7.43–7.38 (m, 1H), 6.35 (d, J = 6.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 113.12, 118.35, 125.01, 125.41, 125.92, 139.94, 155.52, 156.66, 177.81.^{S14} MS (EI): m/z (%): 147 (10), 146 (100) [M^+], 120 (23), 118 (61), 92 (43), 90 (15), 89 (12), 64 (17), 63 (23), 50 (12).^{S15}

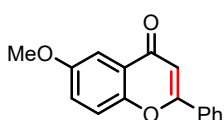


6-Fluoro-4-chromone (CAS No. 105300-38-7), Table 2, entry 16, >99% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm \times 60 m, GL Science Inc.; carrier gas (N_2) flow rate, 2.4 mL \cdot min $^{-1}$; initial column temp., 70 $^{\circ}$ C; final column

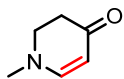
temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 19.8 min; relative sensitivity for quantification (vs biphenyl, internal standard), 1.08 (estimated by the effective carbon number concept^{S2}). MS (EI): *m/z* (%): 165 (11), 164 (100) [*M*⁺], 138 (30), 136 (53), 110 (40), 108 (15), 107 (14), 82 (27), 81 (16), 63 (11).^{S15}



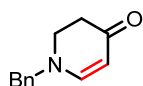
Flavone (CAS No. 525-82-6), Table 2, entry 17, >99% GC yield, 66% isolated yield (75.5 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 22.0 min; relative sensitivity for quantification (vs biphenyl, internal standard), 1.08 (estimated by the effective carbon number concept^{S2}). ¹H-NMR (500 MHz, CDCl₃): δ 8.21 (dd, *J* = 8.0 and 1.5 Hz, 1H), 7.91–7.88 (m, 2H), 7.70–7.65 (m, 1H), 7.56–7.47 (m, 4H), 7.41–7.37 (m, 1H), 6.98 (s, 1H); ¹³CNMR (125 MHz, CDCl₃): δ 107.63, 118.20, 124.03, 125.32, 125.75, 126.36, 129.14, 131.71, 131.80, 138.88, 156.31, 163.44, 171.24, 178.50.^{S16} MS (EI): *m/z* (%): 223 (16), 222 (100) [*M*⁺], 221 (34), 165 (15), 120 (74), 102 (13), 97 (18), 92 (57), 82 (17), 64 (18), 63 (16).^{S15}



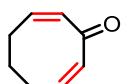
6-Methoxy-4-flavone (CAS No. 26964-24-9), Table 2, entry 18, >99% GC yield, 73% isolated yield (92.2 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 30.1 min; relative sensitivity for quantification (vs biphenyl, internal standard), 1.08 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 7.89–7.86 (m, 2H), 7.56 (d, *J* = 3.5 Hz, 1H), 7.53–7.44 (m, 4H), 7.28–7.24 (m, 2H), 6.98 (s, 1H), 3.88 (s, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 56.00, 104.97, 106.89, 119.63, 124.00, 126.30, 129.11, 131.59, 131.91, 151.12, 157.07, 163.18, 178.34.^{S17} MS (EI): *m/z* (%): 253 (17), 252 (100) [*M*⁺], 251 (83), 223 (19), 222 (29), 150 (62), 135 (18), 122 (14), 107 (34), 102 (10), 79 (34), 51 (15).^{S15}



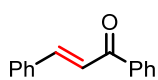
1-Methyl-2,3-dihydropyridin-4(1H)-one (CAS No. 35488-00-7), Table 2, entry 19, 50% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 17.5 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.39 (estimated by the effective carbon number concept^{S2}). MS (EI): *m/z* (%): 111 (100) [*M*⁺], 83 (28), 82 (62), 55 (62), 54 (12).^{S15}



1-Phenylmethyl-2,3-dihydropyridin-4(1H)-one (CAS No. 35487-98-0), Table 2, entry 20, 98% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 25.8 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.89 (estimated by the effective carbon number concept^{S2}). MS (EI): *m/z* (%): 187 (40) [*M*⁺], 96 (21), 91 (100), 65 (18)^{S15}



2,7-cyclooctadien-1-one (CAS No. 1073-76-3), Table 2, entry 21, 55% GC yield. GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 15.8 min; relative sensitivity for quantification (vs biphenyl, internal standard), 0.57 (estimated by the effective carbon number concept^{S2}). MS (EI): *m/z* (%): 122 (26) [*M*⁺], 94 (38), 91 (10), 81 (100), 80 (43), 79 (74), 77 (24), 68 (23), 66 (39), 65 (10), 55 (12), 53 (78), 51 (14).^{S18}



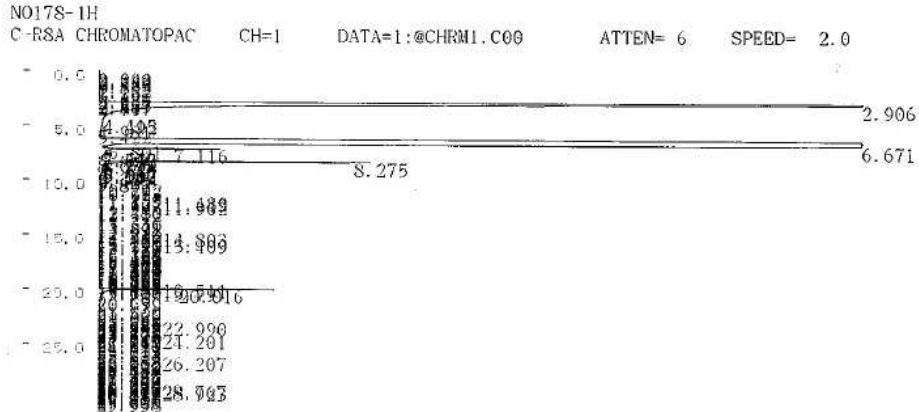
Chalcone (CAS No. 94-41-7), Table 2, entry 22, >99% GC yield, 74% isolated yield (79.7 mg). GC conditions and analysis: TC-5 capillary column, 0.25 mm × 60 m, GL Science Inc.; carrier gas (N₂) flow rate, 2.4 mL·min⁻¹; initial column temp., 70 °C; final column temp., 280 °C, progress rate, 1 °C·min⁻¹ (10 min), 10 °C·min⁻¹ (12 min), 20 °C·min⁻¹ (4 min), injection temp., 280 °C; detection temp., 300 °C; retention time, 26.3 min; relative sensitivity for quantification (vs biphenyl, internal standard), 1.16 (estimated by the effective carbon number concept^{S2}). ¹H NMR (500 MHz, CDCl₃): δ 8.03–7.98 (m, 2H), 7.82–7.77 (m, 1H), 7.64–7.58 (m, 2H), 7.56–7.45 (m, 4H), 7.40–7.36 (m, 3H); ¹³C NMR (125 MHz, CDCl₃): δ 122.09, 128.55, 128.59, 128.71, 129.04, 130.64, 132.89, 134.93, 138.25, 144.87, 190.51.^{S19} MS (EI): *m/z* (%): 209 (12), 208 (79) [*M*⁺], 207 (100), 179 (21), 178 (11), 165 (12), 131 (44), 130 (15), 105 (35), 103 (46), 102 (15), 89 (12), 77 (99), 76 (13), 51 (35), 50 (10).^{S20}

Additional References

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GC chromatogram of aerobic α,β -desaturation of cyclohexanone to cyclohexenone (Table 1, entry 1)



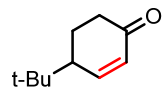
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**** CALCULATION REPORT ****

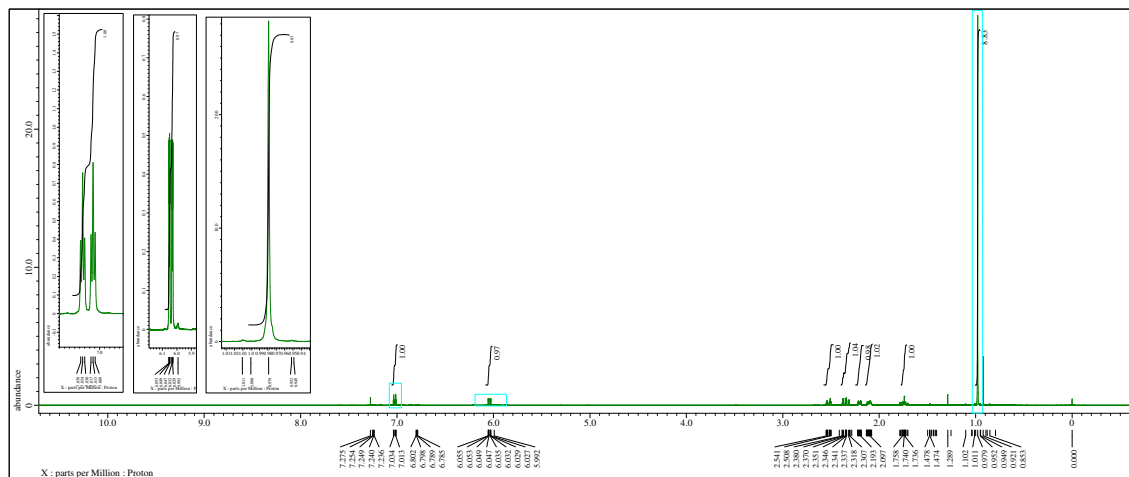
CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
I	15	2.906	35348604	7681086	SV		89.3566	Ethanol
	20	6.671	4008614	222983	S		10.1332	DMA
	22	7.116	44285	9833	T		0.1119	cyclohexanone
	29	8.275	99703	22492	SV		0.252	cyclohexenone
	95	20.016	57835	14734	S		0.1462	biphenyl
TOTAL			39559036	7951127			100	

¹H NMR and ¹³C NMR spectra

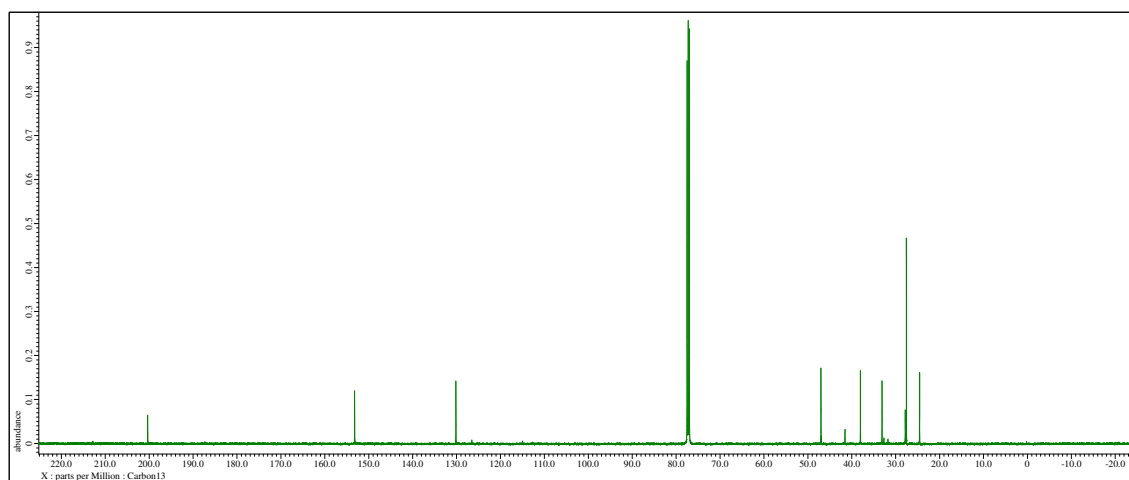
4-(*tert*-Butyl)-2-cyclohexen-1-one (**2c**)



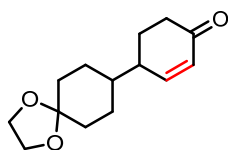
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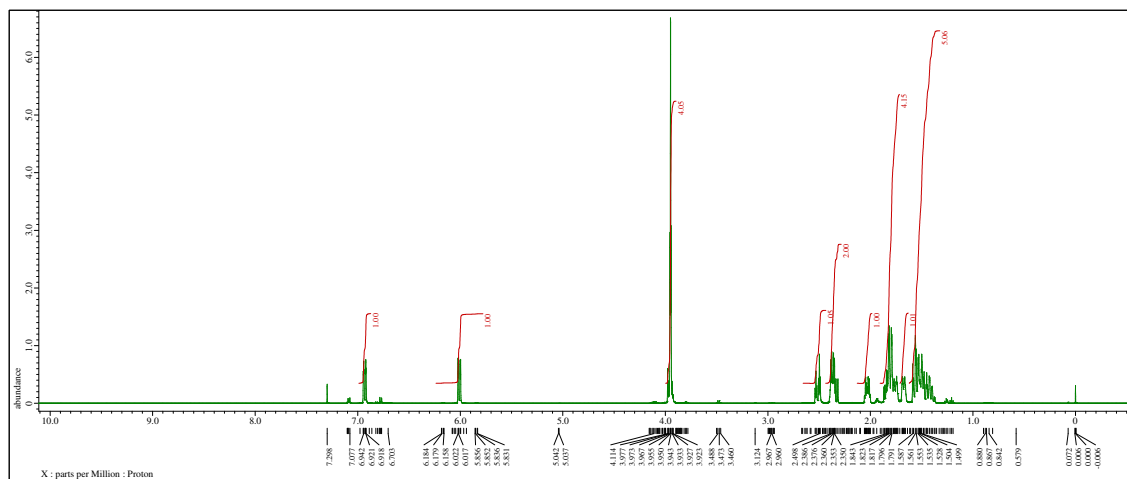
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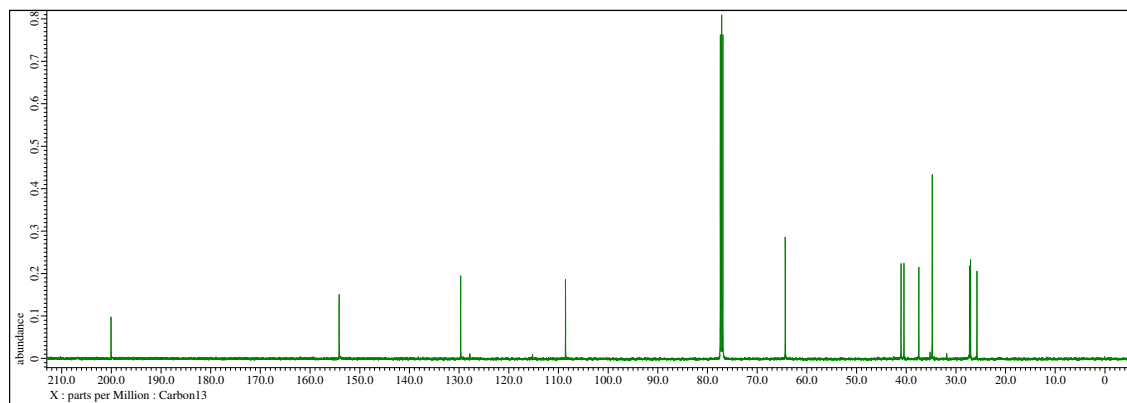
4-(1,4-Dioxaspiro[4.5]decan-8-yl)cyclohex-2-en-1-one (**2d**)



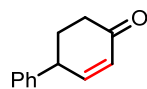
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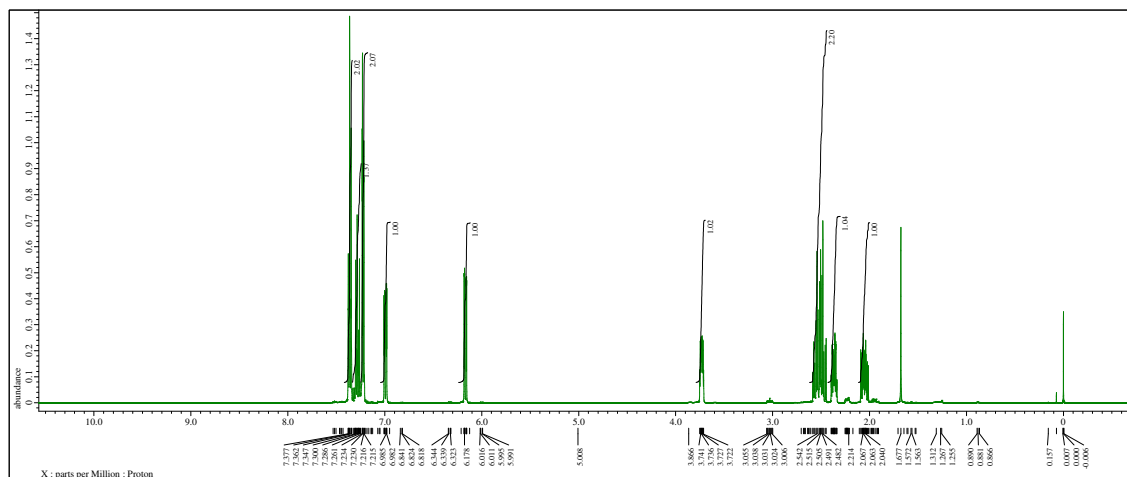
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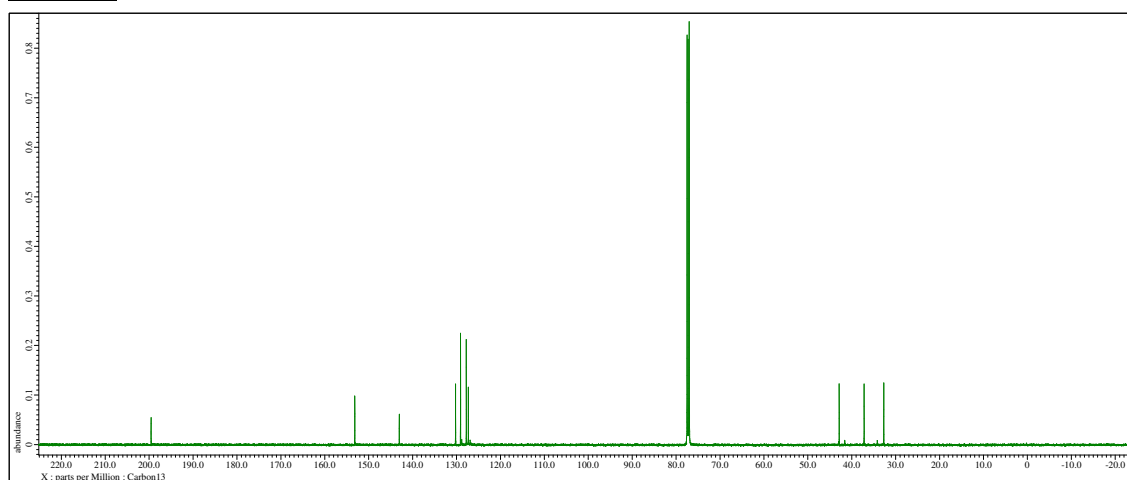
4-Phenyl-2-cyclohexen-1-one (2e)



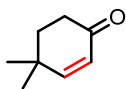
¹H NMR



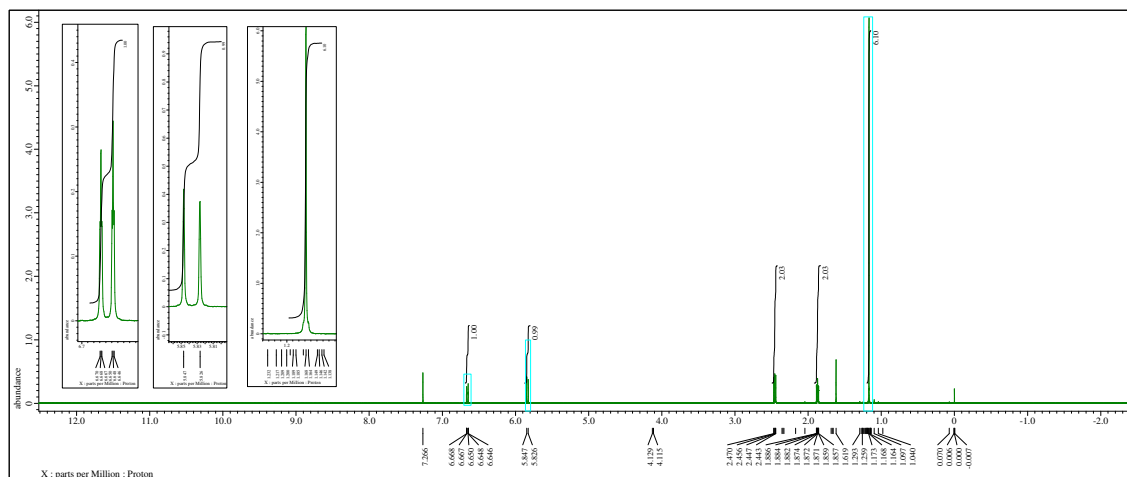
¹³C NMR



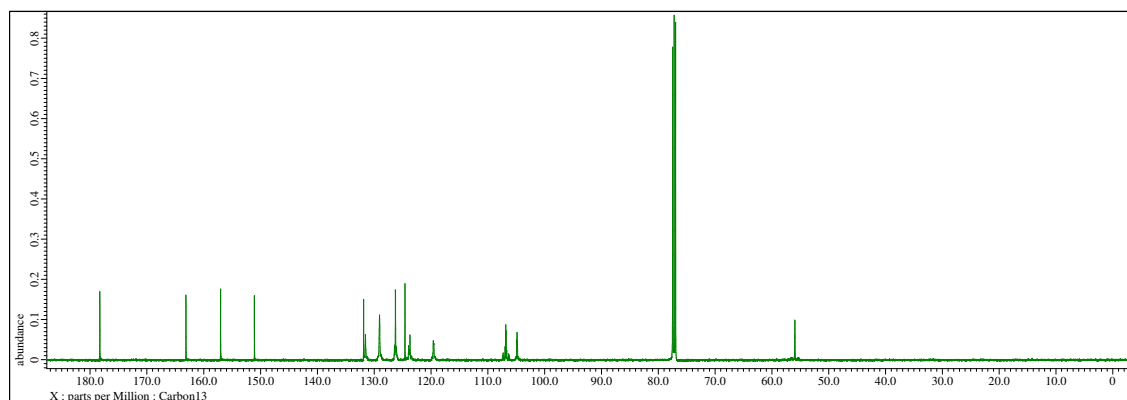
4,4-Dimethyl-2-cyclohexen-1-one (2g)



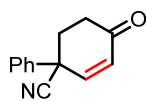
¹H NMR



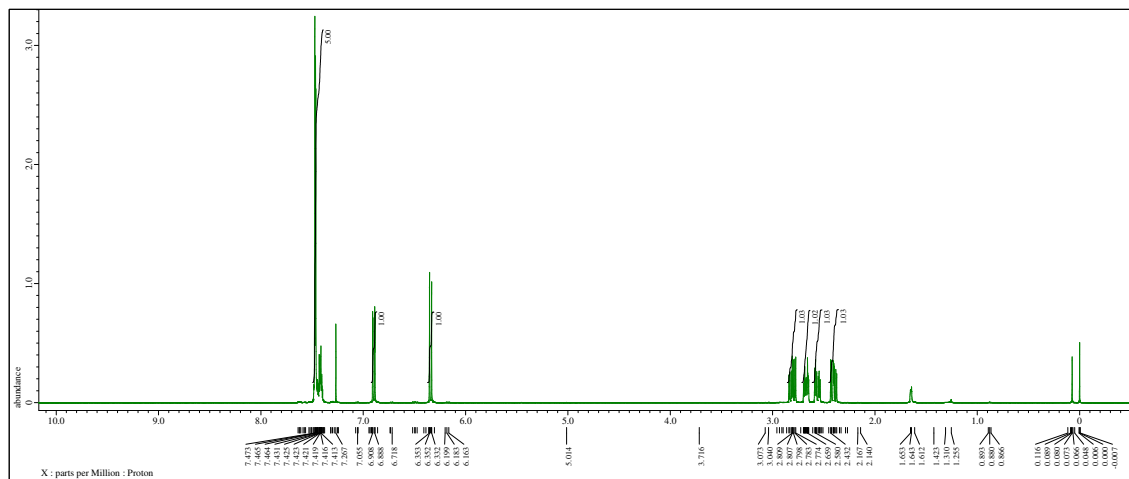
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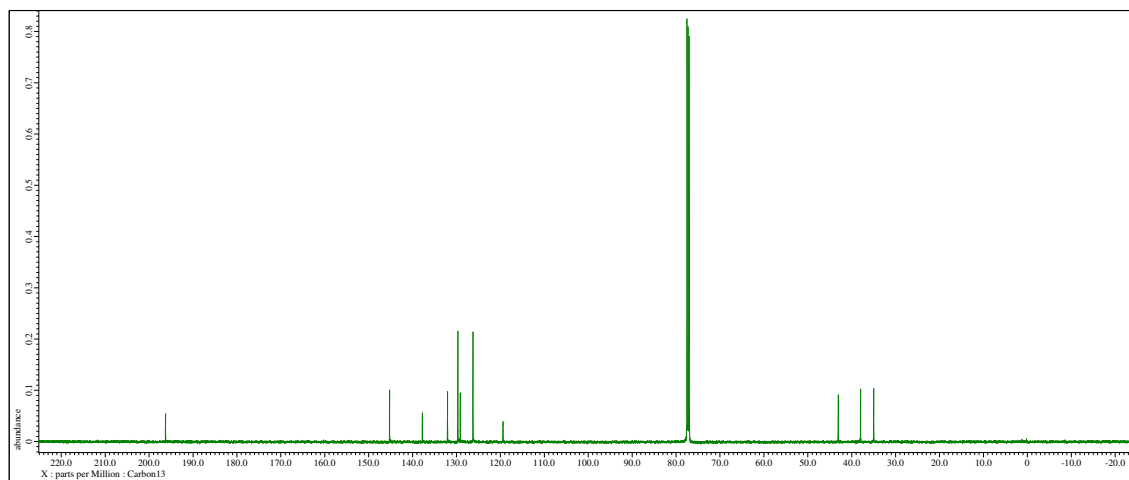
4-Cyano-4-phenyl-2-cyclohexen-1-one (2h)



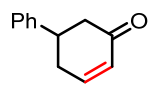
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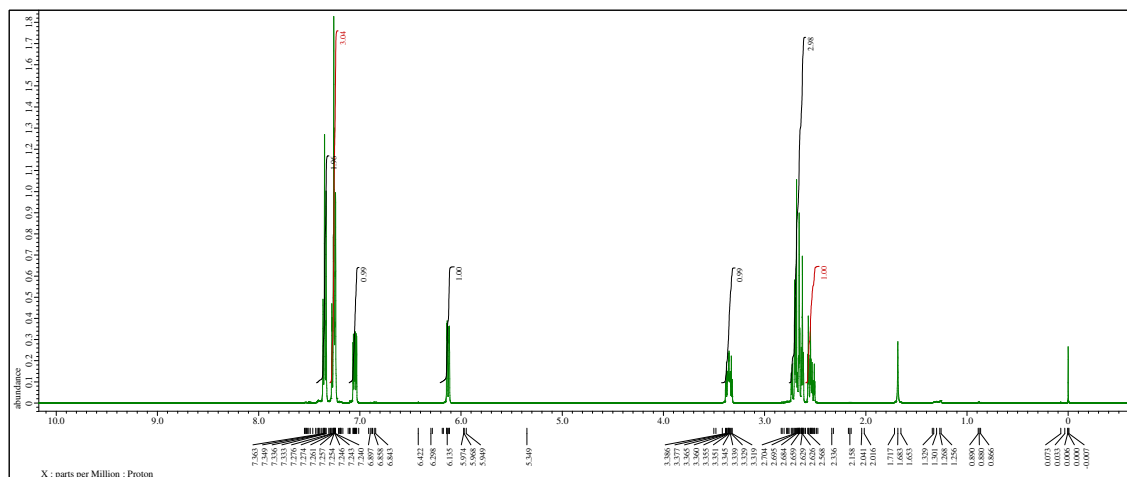
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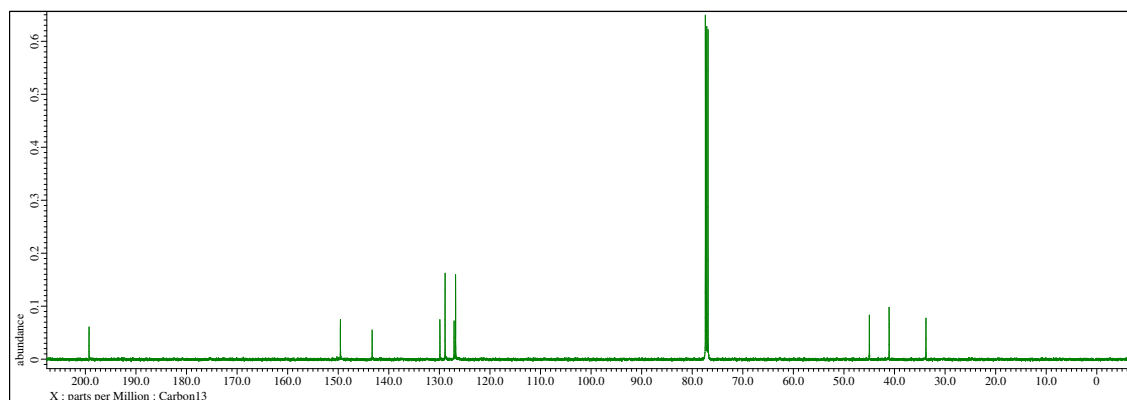
5-Phenyl-2-cyclohexen-1-one (2j)



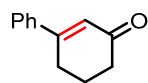
¹H NMR



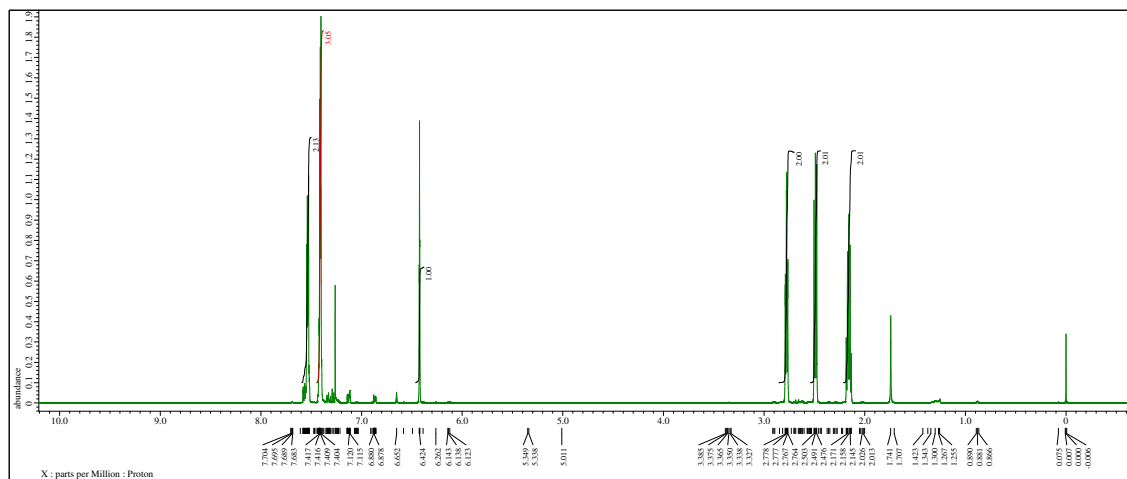
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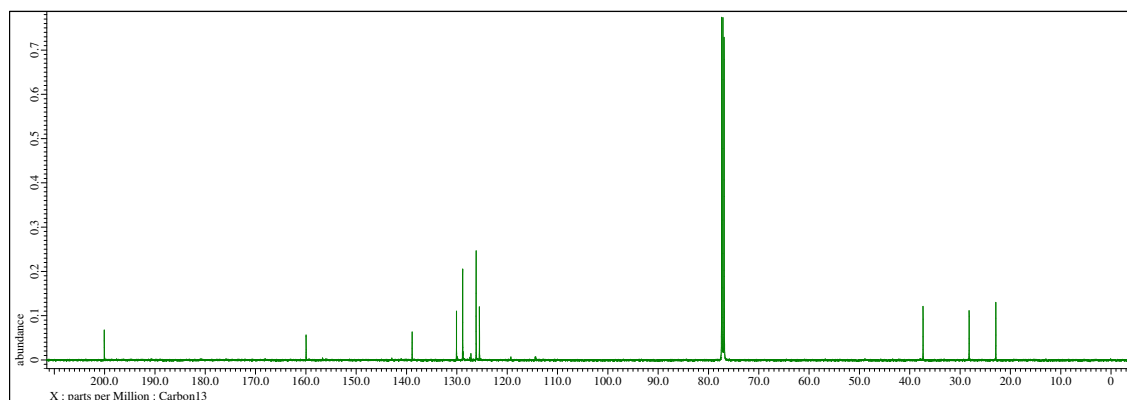
1-Phenyl-1-cyclohexen-3-one (2j')



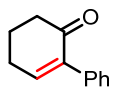
¹H NMR



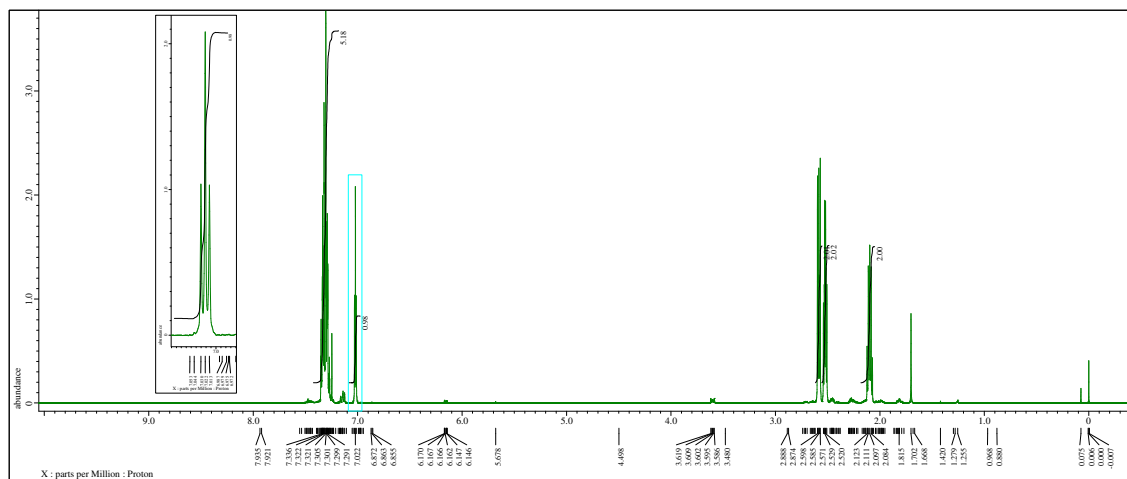
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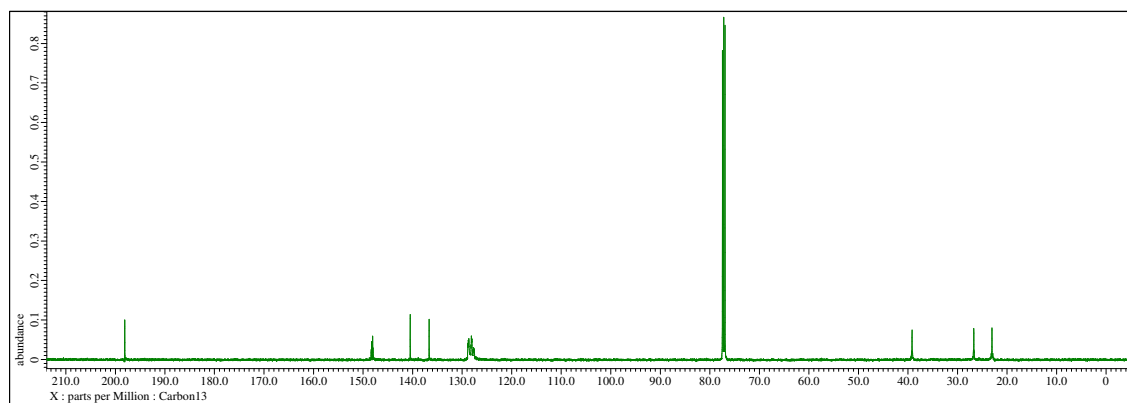
2-Phenyl-2-cyclohexen-1-one (2I)



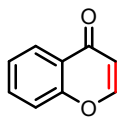
¹H NMR



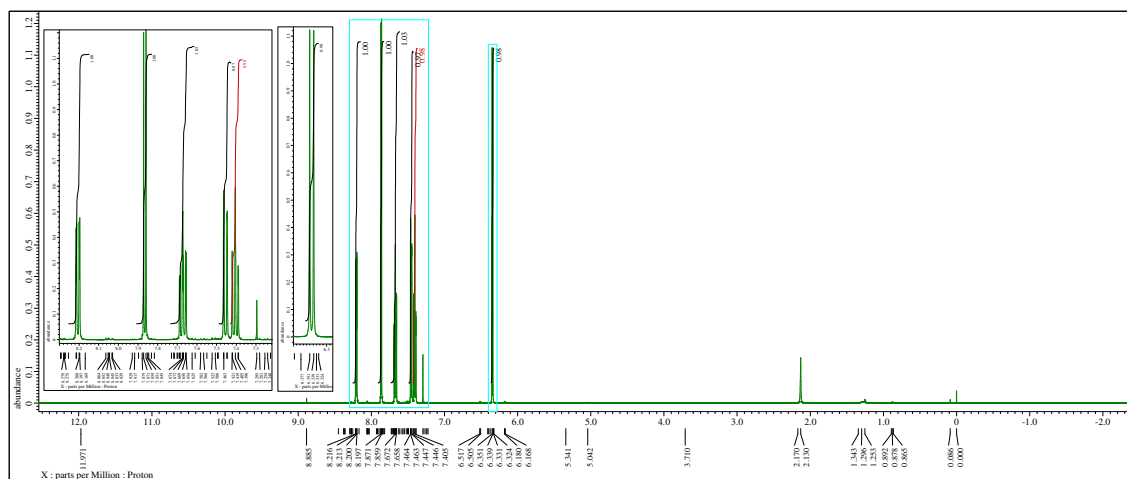
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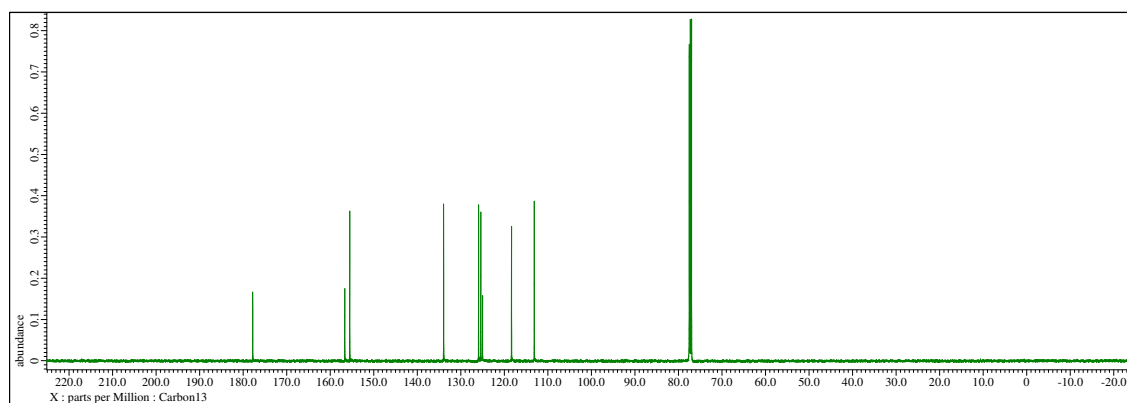
Chromone (2o)



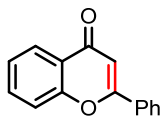
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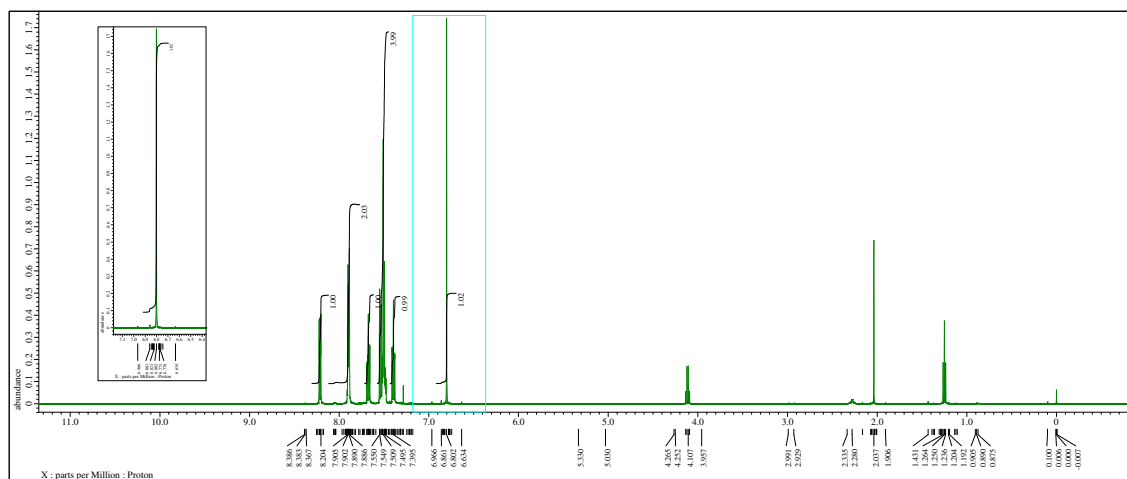
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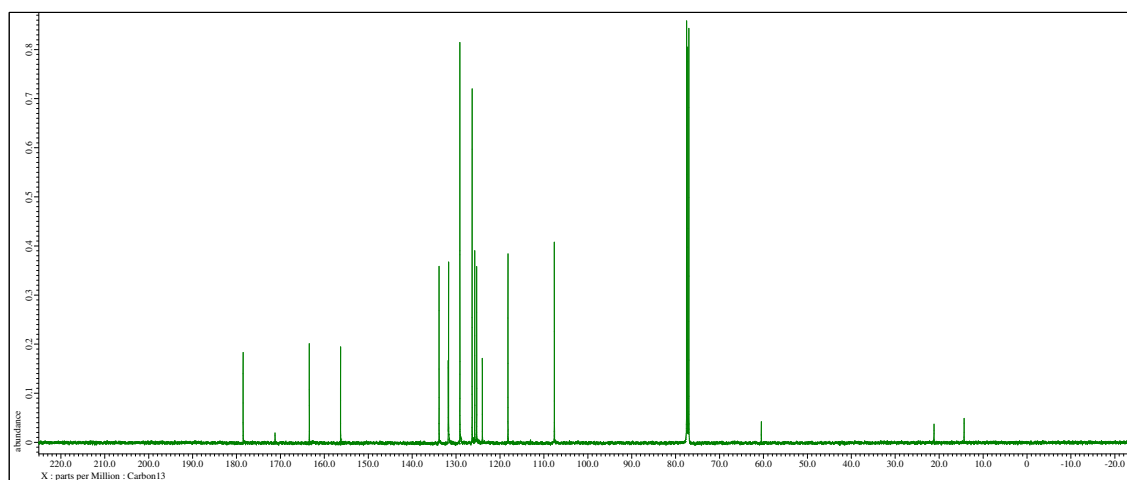
Flavone (2q)



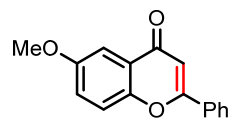
¹H NMR



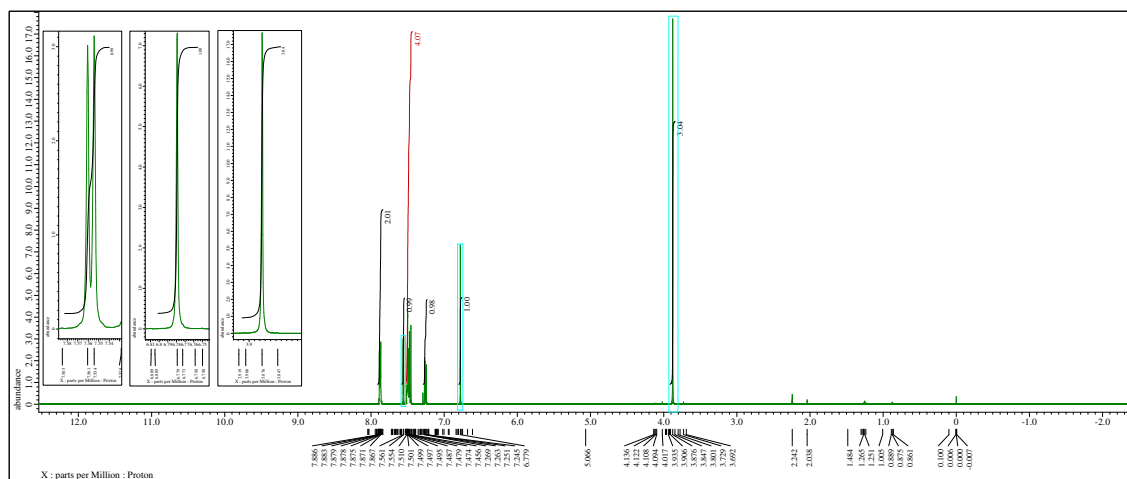
¹³C NMR



6-Methoxy-4-flavone (2r)



¹H NMR



¹³C NMR

