Palladium and Visible-Light Mediated Carbonylative Suzuki-Miyaura Coupling of Unactivated Alkyl Halides and Aryl Boronic Acids

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General information

All reagents were purchased at the highest commercial quality and used without further purification. Yields refer to isolated, homogenous and spectroscopically pure material, unless otherwise stated. Blue light-emitting diodes (2 W, $\lambda = 465$ nm) and white light-emitting diodes (2 W, 3200K) were used for irradiation of the reaction mixture. Crude reaction mixtures were purified by silica gel chromatography (E. Merck silica gel, particle size 0.043–0.063 mm). The luminous emittance was measured at the surface of the reaction vessel (a distance of 7 cm) to 12 900 lux (all LED lists) and 4500 lux (single LED list) with a lux meter (Lux light meter, CL-J18-11-C3). Thin layer chromatography was carried out using E. Merck silica plates (60F-254) with UV light (254 nm) as the visualization agent. Analytical reversed phase HPLC-MS (ESI) was performed on a Dionex Ultimate 3000 system using MeCN/0.05% HCOOH in H$_2$O as the mobile phase with MS detection, equipped with a C18 (Phenomenex Kinetex SB C18 (4.8 × 50 mm)) column using a UV diode array detector. Purity determinations were performed on the same instrument with UV detection at 245 nm. Low resolution GC-MS (EI) analyses were performed with a CP-3800 column using a 70−300 °C temperature gradient and electron impact ionization at 70 eV. Accurate mass values were determined on a mass spectrometer equipped with an electron-impact ion source and TOF detector. $^1$H NMR spectra were recorded at 400 MHz and $^{13}$C($^1$H) NMR spectra at 100 MHz. The chemical shifts for $^1$H NMR and $^{13}$C($^1$H) NMR spectra were referenced to tetramethylsilane via residual solvent signals ($^1$H: CHCl$_3$ δ 7.26, CD$_3$OD δ 3.31, CDCl$_3$ δ 77.16, CD$_3$OD δ 49.00).

General procedure for optimization of carbonylative Suzuki coupling

At the initiation of the optimization, 1 (0.25 mmol), 2 (0.375 mmol), potassium carbonate (K$_2$CO$_3$, 0.25 mmol), Pd(PPh$_3$)$_2$Cl$_2$ (5 mol%), fac-Ir(ppy)$_3$ (1 mol%) and Hantzsch ester (0.5 mmol) was added to the reaction chamber (C$_{rxn}$), followed by benzene and water (2:1, 2 mL total volume). To the carbon monoxide chamber (C$_{CO}$), molybdenum hexacarbonyl (Mo(CO)$_6$, 0.75 mmol) was added followed by acetonitrile (2 mL). All solvents were sonicated for 15 min before addition to the H-tube. After capping of C$_{rxn}$ and C$_{CO}$, DBU (1.5 mmol) was added to C$_{CO}$. C$_{rxn}$ was then subjected to visible light radiation for 24 h. Both chambers were held at room temperature. After 24 h, the contents of C$_{rxn}$ was filtered and washed with dichloromethane. The filtrate was concentrated in vacuo. Anisole (1 eq) was used as the internal standard for calculation of the NMR yield. In experiments with anisole as solvent, 1-hexene (1 eq) was used as the internal standard. See table S1 for all experiments.

Table S1. Full optimization of reaction parameters

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<th>Entry</th>
<th>Solvent C$_{rxn}$</th>
<th>Catalyst/ligand</th>
<th>Base</th>
<th>Reductant</th>
<th>Temperature</th>
<th>NMR yield$^a$</th>
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<td>S1</td>
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<td>RT</td>
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<td>Benzenes/water 7:1</td>
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<td>K$_2$CO$_3$</td>
<td>HE (2 eq)</td>
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<td>-</td>
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[52]
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<td>Water</td>
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<td>RT</td>
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<td>RT</td>
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<td>RT</td>
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<td>S27</td>
<td>Benzene / acetonitrile / water 4:1:1</td>
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<td>K₂CO₃</td>
<td>HE (2 eq)</td>
<td>RT</td>
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<tr>
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<td>HE (2 eq)</td>
<td>RT</td>
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<td>K₂CO₃</td>
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<td>RT</td>
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<td>K₂CO₃</td>
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<td>RT</td>
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<td>RT</td>
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<td>Pd(dpff) Cl₂, fac-Ir(ppy)₃</td>
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<td>RT</td>
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<td>HE (2 eq)</td>
<td>RT</td>
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<td>S38</td>
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<td>K₂CO₃</td>
<td>HE</td>
<td>70 °C</td>
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S3
**Reaction conditions:** Chamber<sub>rin</sub> 0.25 mmol 1, 1.5 eq 2, 5 mol% [Pd], 1 eq K<sub>2</sub>CO<sub>3</sub>, 1 mol% fac-Ir(ppy)₃, 2 ml solvent Chamber<sub>CO</sub> 2.5 eq Mo(CO)₆, 5 eq DBU, 2 ml MeCN. Solvents were sonicated for 15 min before addition to H-tube. a Yield determined by H NMR. b Determined by visual inspection of GC. c 2 mol% fac-Ir(ppy)₃ d 5 mol% ligand. e 10 mol% ligand. f 10 mol% Pd(PPh₃)₄. g 3 eq water. h N₂ vacuum sparging for 5 minutes instead of sonication of solvent. i 7.5 mol% Pd(PPh₃)₄. j 3 mol solvent in C<sub>rin</sub> and C<sub>CO</sub>. k 3.33 ml solvent in C<sub>rin</sub> and C<sub>CO</sub>. l 4 ml solvent in C<sub>rin</sub> and C<sub>CO</sub>. m 5 ml solvent in C<sub>rin</sub> and C<sub>CO</sub>. n Increase in concentration, 0.3 mmol of cyclohexyl iodide. o 3 eq of cyclohexyl iodide. p 1 eq phenyl boronic acid. q 5 eq phenyl boronic acid. r 1 eq of naphthalene. s 7 mol% ligand. t Heating both chambers to 50°C. u Reaction run without light.

**Abbreviations:** ppy = 2-phenylpyridinato-C<sub>2</sub>; HE = Hantzsch ester, RT = room temperature, BBBDP = 4,4'-diter-butyl-2,2'-bipyridine, TBA = tributylamine.
**Synthesis of alkyl iodides**

1-[[4-Methyl[phenyl]sulfonyl]piperidin-4-ol\(^1\) **CAS: 80213-12-3**

4-Hydroxy piperidine (2.0 mmol) was dissolved in water (5 mL), to which Na\(_2\)CO\(_3\) (1.3 eq) and \(p\)-tolidene sulfonfyl chloride (1.6 eq) was added. The reaction mixture was diluted with diethylether (15 mL) and left to stir at room temperature for 24 h. After completion, the reaction mixture was extracted with 3x20 mL ethyl acetate. The combined organic phases were washed with 30 mL brine, dried over Na\(_2\)SO\(_4\) filtered and concentrated in vacuo. Purified with silica column chromatography using a gradient (3:1 \(i\)-hexane:ethyl acetate + 1% triethylamine to ethyl acetate + 1% triethylamine). Spectral data were in agreement with literature values. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.66 – 7.61 (m, 2H), 7.33 – 7.29 (m, 2H), 3.78 – 3.70 (m, 1H), 3.35 – 3.26 (m, 2H), 2.87 – 2.79 (m, 2H), 2.43 (s, 3H), 1.96 – 1.87 (m, 2H), 1.69 – 1.59 (m, 2H), 1.46 (s, 1H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 143.7, 133.2, 129.8, 127.8, 66.0, 43.3, 33.4, 21.7. MS-ESI [M+H\(^+\)]: \(m/z\) 256.2. HPLC purity > 99%.

4-Iodo-1-[[4-methyl[phenyl]sulfonyl]piperidin-4-ol\(^2\) **CAS: 289890-80-8**

1-[[4-methyl[phenyl]sulfonyl]piperidin-4-ol (1.6 mmol) was dissolved in dichloromethane (10 mL), before addition of PPh\(_3\) (1.6 eq) and imidazole (1.6 eq). The reaction mixture was stirred at -10°C for 5 minutes before addition of \(I_2\) (2.0 eq). The ice-bath was then removed and the mixture stirred at ambient temperature overnight. The reaction mixture was then diluted with H\(_2\)O (10 mL) and extracted with 2x10 mL diethylether. The combined organic phases were dried over Na\(_2\)SO\(_4\), filtered and concentrated in vacuo. Purification with silica column chromatography eluting with 3:1 \(i\)-hexane:ethyl acetate + 1% triethylamine afforded the title compound as a beige solid (413.6 mg, 72%). \(R_t = 0.88\) (3:1 \(i\)-hexane:ethyl acetate + 1% triethylamine). Spectral data were in agreement with literature values. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.65 (d, \(J = 8.3\) Hz, 2H), 7.34 (d, \(J = 8.0\) Hz, 2H), 4.33 – 4.25 (m, 1H), 3.21 – 3.12 (m, 2H), 3.02 – 2.95 (m, 2H), 2.45 (s, 3H), 2.16 – 2.08 (m, 4H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 143.9, 133.3, 129.9, 127.7, 45.8, 36.6, 25.7, 21.7. MS-ESI [M+H\(^+\)]: \(m/z\) 365.9. HPLC purity > 99%.

3-Iodobutylbenzene\(^2,3\) **CAS: 59456-20-1**

4-Phenyl-2-butanol (6 mmol), PPh\(_3\) (1 eq), imidazole (1.5 eq) and \(I_2\) (1.3 eq) were dissolved in dichloromethane (15 mL) at -10°C and left to stir for 4 h at room temperature. The reaction mixture was concentrated in vacuo and purified with silica column chromatography eluting with 7:1 \(i\)-hexane:ethyl acetate. Isolated as a yellow oil (1.5 g, 96%). \(R_t = 0.70\) (29:1 \(i\)-hexane:ethyl acetate). Spectral data were in agreement with literature values. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.32 – 7.27 (m, 2H), 7.23 – 7.18 (m, 3H), 4.17 – 4.06 (m, 1H), 2.90 – 2.80 (m, 1H), 2.75 – 2.64 (m, 1H), 2.21 – 2.09 (m, 1H), 1.95 (d, \(J = 6.8\) Hz, 3H), 1.93 – 1.83 (m, 1H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 140.9, 128.6, 128.6, 126.2, 44.5, 36.0, 29.8, 29.1. EI-MS: \(m/z\) 260.0.

2-Iodoctane\(^3,4\) **CAS: 557-36-8**

2-Octanol (7.7 mmol), PPh\(_3\) (1 eq), imidazole (2 eq) and \(I_2\) (1.2 eq) were dissolved in dichloromethane (25 mL) at -10°C and left to stir for 3 days at room temperature. The reaction mixture was filtered and concentrated in vacuo and purified with silica column chromatography eluting with 7:1 \(i\)-hexane:ethyl acetate. Isolated as a colorless oil (1.2 g, 67%). \(R_t = 0.89\) (29:1 \(i\)-hexane:ethyl acetate). Spectral data were in agreement with literature values. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 4.19 (dqd, \(J = 8.5, 6.8, 5.1\) Hz, 1H), 1.92 (d, \(J = 6.8\) Hz, 3H), 1.89 – 1.79 (m, 1H), 1.65 – 1.56 (m, 1H), 1.54 – 1.44 (m, 1H), 1.40 – 1.25 (m, 7H), 1.25 – 1.09 (m, 7H).
0.93 – 0.85 (m, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 43.1, 31.8, 31.0, 29.8, 29.1, 28.6, 22.7, 14.2. EI-MS: m/z 240.1.

General procedure for carbonylative Suzuki coupling – investigation of scope
Conditions as in entry S63, table S1. To C$_{rxn}$ was added the appropriate alkyl iodide or alkyl bromide (0.3 mmol), boronic acid (1.5 eq), Pd(PPh$_3$)$_4$ (5 mol%) and K$_2$CO$_3$ (1 eq) followed by benzene/water (2:1, 4 mL total volume). To C$_{CO}$ was added Mo(CO)$_6$ (2.5 eq) followed by acetonitrile (4 mL). After capping, both chambers were subjected to 5 minutes of N$_2$/vacuum sparging. When finished, DBU (5 eq) was added to C$_{CO}$ and the double chamber system was positioned in a Dry-Syn heating block with C$_{CO}$ heated at 70°C and C$_{rxn}$ held at room temperature whilst subjected to visible light for 24 h. Thereafter, 5% citric acid (aq.) was added to the reaction mixture and the mixture was extracted with dichloromethane (3x10 mL). The organic phase was washed with brine (10 mL), dried over MgSO$_4$, filtered and concentrated in vacuo. Extracted product was purified with silica column chromatography, with 0.5%-1% ethyl acetate in i-hexane or n-pentane as the eluent.

Experimental set-up
The double-chamber system can be seen in figure S1a and the experimental set-up in figure S1b. For a full description of the reaction set-up please see S. Y. Chow et. al. Chem. Eur. J. 2016, 22, 9155–9161

![Image](image_url)

Figure S1. a) Double-chamber system, C$_{CO}$ is the left chamber and C$_{rxn}$ is the right chamber. b) Experimental set-up.
Cyclohexylphenylmethanone \(^5\) (4) CAS: 712-50-5

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as crystals (37 mg, 65% from cyclohexyl iodide; 20 mg, 35% from cyclohexyl bromide; 22 mg, 39% from cyclohexyl bromide (\(C_{60}\) and \(C_{60}\) heated to 50°C)). \(R_f = 0.52\) (29:1 \(i\)-hexane:ethyl acetate). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.98 – 7.91 (m, 2H), 7.57 – 7.51 (m, 1H), 7.49 – 7.41 (m, 2H), 3.26 (tt, \(J = 11.5, 3.2\) Hz, 1H), 1.94 – 1.80 (m, 4H), 1.78 – 1.70 (m, 1H), 1.56 – 1.24 (m, 5H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 204.1, 136.5, 132.9, 128.7, 128.4, 45.8, 29.6, 26.1, 26.0. El-MS: \(m/z\) 188.1.

2-Methyl-1,4-diphenylbutan-1-one \(^5\) (5) CAS: 108974-08-9

Synthesized according to the general procedure. Isolated as a colorless oil (45 mg, 65%). \(R_f = 0.25\) (29:1 \(i\)-hexane:ethyl acetate). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.99 – 7.95 (m, 2H), 7.68 – 7.62 (m, 1H), 7.57 – 7.51 (m, 2H), 7.40 – 7.35 (m, 2H), 7.32 – 7.23 (m, 3H), 3.57 (h, \(J = 6.8\) Hz, 1H), 2.79 – 2.72 (m, 2H), 2.33 – 2.22 (m, 1H), 1.92 – 1.81 (m, 1H), 1.34 (d, \(J = 6.9\) Hz, 3H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 204.2, 141.9, 136.7, 133.0, 128.7, 128.6, 128.5, 128.4, 126.1, 39.9, 35.3, 33.6, 17.4. El-MS: \(m/z\) 238.1. HRMS found: 239.1427 calc: 239.1436.

2-Methyl-1-phenyloctan-1-one \(^6\) (6) CAS: 132719-12-1

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (43 mg, 64%). \(R_f = 0.1\) (1% EtOAc in \(i\)-Hexane). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.98 – 7.93 (m, 2H), 7.58 – 7.52 (m, 1H), 7.50 – 7.44 (m, 2H), 3.46 (h, \(J = 6.8\) Hz, 1H), 1.85 – 1.74 (m, 1H), 1.49 – 1.37 (m, 1H), 1.35 – 1.21 (m, 8H), 1.19 (d, \(J = 6.8\) Hz, 3H), 0.90 – 0.80 (m, 3H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 204.8, 136.9, 132.9, 128.7, 128.4, 40.7, 33.9, 31.8, 29.5, 27.5, 22.7, 17.4, 14.2. El-MS: \(m/z\) 218.2.

Cyclopentylphenylmethanone \(^7\) (7) CAS: 5422-88-8

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (34 mg, 64%). \(R_f = 0.75\) (7:1 \(i\)-hexane:EtOAc). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.00 – 7.95 (m, 2H), 7.58 – 7.52 (m, 1H), 7.49 – 7.41 (m, 2H), 3.72 (p, \(J = 7.9\) Hz, 1H), 1.98 – 1.87 (m, 4H), 1.80 – 1.61 (m, 4H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 203.0, 137.1, 132.8, 128.6, 128.6, 46.5, 30.1, 26.5. El-MS: \(m/z\) 174.1.

Phenyl(1-tosylpiperidin-4-yl)methanone \(^8\) (8) CAS: 922504-26-5

Synthesized according to the general procedure. Isolated as a yellow solid (63 mg, 60%). \(R_f = 0.42\) (3:1 \(i\)-hexane:ethyl acetate + 1% triethylamine). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.87 – 7.82 (m, 2H), 7.69 – 7.64 (m, 2H), 7.57 – 7.52 (m, 1H), 7.46 – 7.40 (m, 2H), 7.37 – 7.32 (m, 2H), 3.80 – 3.73 (m, 2H), 3.23 – 3.14 (m, 1H), 2.57 – 2.48 (m, 2H), 2.45 (s, 3H), 1.98 – 1.81 (m, 4H). \(^1^3\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 201.5, 143.8, 135.7, 133.4, 133.2, 129.8, 128.9, 128.3, 127.9, 45.7, 42.4, 28.0, 21.7. ESI-MS: 344.1 HRMS found: 344.1315 calc: 344.1309. HPLC purity > 99%.

1-Phenylnonan-1-one \(^9\) (9) CAS: 6008-36-2
Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (36 mg, 55% from 1-iodooctane; 20 mg and 27 mg, 30% and 40% from 1-bromoocotane (24 h and 55 h irradiation)). Rf = 0.44 (29:1 i-hexane:ethyl acetate). 1H NMR (400 MHz, CDCl3) δ 8.07 – 7.83 (m, 2H), 7.58 – 7.52 (m, 1H), 7.48 – 7.41 (m, 2H), 2.96 (t, J = 7.3 Hz, 2H), 1.80 – 1.65 (m, 2H), 1.42 – 1.20 (m, 10H), 0.91 – 0.83 (m, 3H). 13C NMR (101 MHz, CDCl3) δ 200.8, 137.2, 133.0, 128.7, 128.2, 38.8, 32.0, 29.6, 29.5, 29.3, 24.5, 22.8, 14.3. EI-MS: m/z 218.2.

1-Phenylpentan-1-one9 (10) CAS: 1674-37-8
Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (44 mg, 71% from 1-iodoheptane, 25 mg, 42% from 1-bromohexane). Rf = 0.37 (29:1 i-Hexane:EtOAc). 1H NMR (400 MHz, CDCl3) δ 7.98 – 7.94 (m, 2H), 7.58 – 7.52 (m, 1H), 7.49 – 7.41 (m, 2H), 2.96 (t, J = 7.4 Hz, 2H), 1.78 – 1.68 (m, 2H), 1.43 – 1.23 (m, 8H), 0.92 – 0.84 (m, 3H). 13C NMR (101 MHz, CDCl3) δ 200.8, 137.2, 133.0, 128.7, 128.2, 38.8, 31.9, 29.5, 29.3, 24.5, 22.8, 14.3. EI-MS: m/z 204.1.

3-Methyl-1-phenylbutan-1-one10 (11) CAS: 582-62-7
Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (24 mg, 50%). Rf = 0.16 (1% EtOAc in i-Hexane). 1H NMR (400 MHz, CDCl3) δ 7.97 – 7.93 (m, 2H), 7.58 – 7.52 (m, 1H), 7.49 – 7.43 (m, 2H), 2.84 (d, J = 6.9 Hz, 2H), 2.30 (dp, J = 13.5, 6.7 Hz, 1H), 1.00 (d, J = 6.7 Hz, 6H). 13C NMR (101 MHz, CDCl3) δ 200.4, 137.5, 132.3, 128.7, 128.2, 47.7, 25.3, 22.9. EI-MS: m/z 162.1.

1,4-Diphenylbutan-1-one8 (12) CAS: 5407-91-0
Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (45 mg, 67% from 3-iodo-1-phenylpropane; 28 mg and 33 mg, 41% and 48% from 3-bromo-1-phenylpropane (24 h and 55 h irradiation)). Rf = 0.31 (29:1 i-hexane:ethyl acetate). 1H NMR (400 MHz, CDCl3) δ 7.95 – 7.91 (m, 2H), 7.58 – 7.53 (m, 1H), 7.49 – 7.42 (m, 2H), 7.33 – 7.27 (m, 2H), 7.25 – 7.19 (m, 3H), 2.99 (t, J = 7.3 Hz, 2H), 2.73 (t, J = 7.4 Hz, 2H), 2.15 – 2.05 (m, 2H). 13C NMR (101 MHz, CDCl3) δ 200.3, 141.8, 137.1, 133.1, 128.7, 128.5, 128.1, 126.1, 37.8, 35.3, 25.8. EI-MS: m/z 224.1.

5-Chloro-1-phenylpentan-1-one11 (13) CAS: 942-93-8
Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a white solid (42 mg, 71% from 1-chloro-4-iodobutane; 36 mg, 61% from 1-chloro-4-bromobutane). Rf = 0.73 (7:1 i-hexane:ethyl acetate). 1H NMR (400 MHz, CDCl3) δ 7.98 – 7.93 (m, 2H), 7.60 – 7.53 (m, 1H), 7.50 – 7.43 (m, 2H), 3.64 – 3.54 (m, 2H), 3.07 – 2.97 (m, 2H), 1.98 – 1.82 (m, 4H). 13C NMR (101 MHz, CDCl3) δ 199.8, 137.0, 133.2, 128.8, 128.1, 44.9, 37.7, 32.2, 21.6. EI-MS: m/z 196.1, 198.1.

((3R,5R,7R)-Adamantan-1-yl)[phenyl]methanone12 (14) CAS: 31919-47-8
Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a white solid (45 mg, 61% from 1-iodoadamantane, 25 mg, 32% from 1-bromoadamantane). Rf = 0.28 (29:1 i-
hexane:ethyl acetate). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.56 – 7.52 (m, 2H), 7.46 – 7.36 (m, 3H), 2.10 – 2.04 (m, 3H), 2.03 – 1.98 (m, 6H), 1.81 – 1.69 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 210.4, 139.7, 130.3, 128.1, 127.2, 47.0, 39.2, 36.7, 28.3. El-MS: $m/z$ 240.2.

4-Methyl-1-phenylpentan-1-one$^9$ (18) CAS: 2050-07-9

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (18 mg, 34%). $R_t$ = 0.40 (29:1 i-hexane:ethyl acetate). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.98 – 7.94 (m, 2H), 7.58 – 7.53 (m, 1H), 7.49 – 7.43 (m, 2H), 2.99 – 2.94 (m, 2H), 1.66 – 1.61 (m, 3H), 0.96 – 0.93 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 201.0, 137.2, 133.0, 128.7, 128.2, 36.8, 33.4, 28.0, 22.6. El-MS: $m/z$ 176.1.

1-Phenylnon-8-en-1-one (19) CAS: 148056-64-8

Synthesized according to the general procedure. Isolated as a colorless oil (17 mg, 26%). $R_t$ = 0.42 (29:1 i-hexane:ethyl acetate). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.98 – 7.93 (m, 2H), 7.58 – 7.52 (m, 1H), 7.49 – 7.43 (m, 2H), 5.86 – 5.74 (m, 1H), 5.01 – 4.91 (m, 2H), 2.96 (tt, $J$ = 7.5 Hz, 2H), 2.07 – 2.01 (m, 2H), 1.78 – 1.70 (m, 2H), 1.44 – 1.34 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 200.7, 139.2, 137.2, 133.0, 128.7, 128.2, 114.4, 38.7, 33.9, 29.3, 29.1, 28.9, 24.4. El-MS: $m/z$ 216.1 HRMS found: 216.1520 calc: 216.1514.

[1,1'-Biphenyl]-2-yl(cyclo-hexyl)methanone (20) CAS: 963-92-8

Synthesized according to the general procedure. Isolated as a colorless oil (34 mg, 43%). $R_t$ = 0.41 (29:1 i-hexane:ethyl acetate). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.52 – 7.47 (m, 1H), 7.44 – 7.36 (m, 6H), 7.35 – 7.30 (m, 2H), 2.10 (tt, $J$ = 11.4, 3.3 Hz, 1H), 1.64 – 1.54 (m, 2H), 1.53 – 1.45 (m, 3H), 1.29 – 1.16 (m, 2H), 1.13 – 1.00 (m, 1H), 0.93 – 0.80 (m, 2H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 211.8, 140.8, 140.7, 139.8, 130.1, 129.9, 128.9, 128.6, 128.0, 127.7, 127.3, 50.3, 29.0, 25.7, 25.6. El-MS: $m/z$ 264.1 HRMS found: 265.1597 calc: 265.1592.

Cyclohexyl(naphthalen-2-yl)-methanone (21) CAS: 10404-26-9

Synthesized according to the general procedure. Isolated as a white solid (43 mg, 59%). $R_t$ = 0.33 (29:1 i-hexane:ethyl acetate). $^1$H NMR (400 MHz, CDCl$_3$) δ 8.46 (d, $J$ = 1.7 Hz, 1H), 8.02 (dd, $J$ = 8.6, 1.8 Hz, 1H), 8.00 – 7.95 (m, 1H), 7.92 – 7.85 (m, 2H), 7.62 – 7.52 (m, 2H), 3.43 (tt, $J$ = 11.3, 3.3 Hz, 1H), 1.99 – 1.84 (m, 4H), 1.82 – 1.73 (m, 1H), 1.63 – 1.39 (m, 4H), 1.37 – 1.24 (m, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 204.0, 135.6, 133.8, 132.7, 129.7, 129.7, 128.6, 128.4, 127.9, 126.8, 124.5, 45.8, 29.7, 26.1, 26.1. El-MS: $m/z$ 238.1 HRMS found: 239.1436 calc: 239.1436.

1-(p-Tolyl)octan-1-one$^{13}$ (22) CAS: 2789-44-8

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a white solid (52 mg, 79%). $R_t$ = 0.40 (29:1 i-hexane:ethyl acetate). $^1$H NMR (400 MHz, CD$_2$OD) δ 7.89 – 7.85 (m, 2H), 7.32 – 7.27 (m, 2H), 2.97 (t, $J$ = 7.3 Hz, 2H), 2.40 (s, 3H), 1.73 – 1.63 (m, 2H), 1.40 – 1.26 (m, 8H), 0.93 – 0.87 (m, 3H). $^{13}$C NMR (101 MHz, CD$_2$OD) δ 202.6, 145.3, 135.8, 130.3, 129.3, 39.4, 32.9, 30.4, 30.3, 25.7, 23.7, 21.6, 14.4. El-MS: $m/z$ 218.2.
Cyclohexyl(m-tolyl)methane \(^{14}\) (23) CAS: 3277-78-9

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (39 mg, 64%). \(R_i = 0.42\) (29:1 i-hexane:ethyl acetate). \(^1H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.76 – 7.71 (m, 2H), 7.36 – 7.32 (m, 2H), 3.29 – 3.20 (m, 1H), 2.41 (s, 3H), 1.92 – 1.81 (m, 4H), 1.78 – 1.70 (m, 1H), 1.56 – 1.23 (m, 5H). \(^13C\) NMR (101 MHz, CDCl\(_3\)) \(\delta\) 204.3, 138.5, 136.6, 133.6, 128.9, 128.6, 125.6, 45.8, 29.6, 26.1, 26.0, 21.6. El-MS: \(m/z\) 202.1.

1-(2-(Trifluoromethyl)-phenyl)octan-1-one (24) CAS: 1778855-78-9

Synthesized according to the general procedure. Isolated as a colorless oil (46 mg, 56%). \(R_i = 0.34\) (29:1 i-hexane:ethyl acetate). \(^1H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.73 – 7.68 (m, 1H), 7.62 – 7.51 (m, 2H), 7.42 – 7.38 (m, 1H), 2.83 (t, \(J = 7.4\) Hz, 2H), 1.70 (p, \(J = 7.4\) Hz, 2H), 1.38 – 1.25 (m, 8H), 0.91 – 0.84 (m, 3H). \(^13C\) NMR (101 MHz, CDCl\(_3\)) \(\delta\) 204.9, 140.8 (q, \(J = 1.9\) Hz), 131.9, 130.0, 127.0, 127.0 (q, \(J = 32.8\) Hz), 126.8 (q, \(J = 5.2\) Hz), 123.8 (q, \(J = 274.8\) Hz), 43.4, 31.8, 29.2, 29.1, 23.9, 22.8, 14.2. \(^19F\) NMR (376 MHz, CDCl\(_3\)) \(\delta\) -58.1. El-MS: \(m/z\) 272.1 HRMS found: 273.1460 calc: 273.1461.

1-(4-Fluorophenyl)octan-1-one \(^{15}\) (25) CAS: 111829-15-3

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a white solid (47 mg, 71%). \(R_i = 0.36\) (29:1 i-hexane:ethyl acetate). \(^1H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.95 – 7.88 (m, 2H), 7.09 – 7.02 (m, 2H), 2.86 (t, \(J = 7.3\) Hz, 2H), 1.65 (q, \(J = 7.4\) Hz, 2H), 1.33 – 1.17 (m, 8H), 0.85 – 0.78 (m, 3H). \(^13C\) NMR (101 MHz, CDCl\(_3\)) \(\delta\) 199.1, 165.8 (d, \(J = 254.2\) Hz), 133.6 (d, \(J = 3.1\) Hz), 130.8 (d, \(J = 9.3\) Hz), 115.7 (d, \(J = 21.7\) Hz), 38.7, 31.9, 29.5, 29.3, 24.5, 22.8, 14.2. \(^19F\) NMR (376 MHz, CDCl\(_3\)) \(\delta\) -105.7 – -105.8 (m). El-MS: \(m/z\) 222.1.

4-Chloro-1-(4-fluorophenyl)-butan-1-one \(^{16}\) (26) CAS: 3874-54-2

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a colorless oil (41 mg, 68%). \(R_i = 0.27\) (29:1 i-hexane:ethyl acetate). \(^1H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.05 – 7.98 (m, 2H), 7.18 – 7.11 (m, 2H), 3.68 (t, \(J = 6.2\) Hz, 2H), 3.16 (t, \(J = 7.0\) Hz, 2H), 2.23 (m, 2H). \(^13C\) NMR (101 MHz, CDCl\(_3\)) \(\delta\) 197.5, 165.9 (d, \(J = 254.9\) Hz), 133.3 (d, \(J = 3.2\) Hz), 130.8 (d, \(J = 9.3\) Hz), 115.9 (d, \(J = 21.8\) Hz), 44.8, 35.3, 26.8. \(^19F\) NMR (376 MHz, CDCl\(_3\)) \(\delta\) -105.0 – -105.1 (m). El-MS: \(m/z\) 200.0.

1-(4-Chlorophenyl)octan-1-one (27) CAS: 7295-52-5

Synthesized according to the general procedure. Isolated as a white solid (60 mg, 83%). \(R_i = 0.49\) (29:1 i-hexane:ethyl acetate). \(^1H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.92 – 7.87 (m, 2H), 7.46 – 7.40 (m, 2H), 2.95 – 2.89 (m, 2H), 1.76 – 1.66 (m, 2H), 1.38 – 1.23 (m, 8H), 0.91 – 0.84 (m, 3H). \(^13C\) NMR (101 MHz, CDCl\(_3\)) \(\delta\) 199.5, 139.4, 135.5, 129.6, 129.0, 38.8, 31.8, 29.4, 29.3, 24.4, 22.8, 14.2. El-MS: \(m/z\) 238.1, 240.1 HRMS found: 239.1195 calc: 239.1197.

1-(2-Methoxophenyl)octan-1-one (28) CAS: 153644-77-0

Synthesized according to the general procedure. Isolated as a white solid (19 mg, 26%). \(R_i = 0.29\) (29:1 i-hexane:ethyl acetate). \(^1H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.64 (dd, \(J = 7.7, 1.8\) Hz, 1H), 7.47 – 7.41 (m, 1H), 7.01 – 6.93 (m, 2H), 3.89 (s, 3H), 2.95 (t, \(J = 7.3\) Hz, 2H), 1.71 – 1.62 (m, 2H), 1.37 – 1.23 (m, 8H), 0.91 – 0.84 (m, 3H). \(^13C\) NMR (101 MHz, CDCl\(_3\))
\[ \delta 203.6, 158.4, 133.2, 130.3, 129.0, 120.8, 111.6, 55.6, 43.9, 31.9, 29.5, 29.3, 24.6, 22.8, 14.3. \text{El-MS: } m/z 234.1 \text{ HRMS found: 235.1700 calc: 235.1698.} \\

**1-(4-Methoxyphenyl)octan-1-one** \(^{17}\) (29) CAS: 62170-25-6

Synthesized according to the general procedure. Spectral data were in agreement with literature values. Isolated as a white solid (57 mg, 80%). \( R_f = 0.30 \) (29:1 i-hexane:ethyl acetate). \(^1^H\) NMR (400 MHz, CDCl \(_3\)) \( \delta 7.97 - 7.91 \) (m, 2H), 6.95 – 6.90 (m, 2H), 3.86 (s, 3H), 2.90 (t, \( J = 7.6 \) Hz, 2H), 1.76 – 1.66 (m, 2H), 1.39 – 1.24 (m, 8H), 0.91 – 0.85 (m, 3H). \(^1^C\) NMR (101 MHz, CDCl \(_3\)) \( \delta 199.4, 163.4, 130.5, 130.3, 113.8, 55.6, 38.5, 31.9, 29.5, 29.3, 24.8, 22.8, 14.2. \text{El-MS: } m/z 234.2.

**Cyclohexyl[dibenzo[b,d]thio-phen-4-yl]methanone** (30)

Synthesized according to the general procedure. Isolated as an oil (55 mg, 62%). \( R_f = 0.40 \) (0.5% ethyl acetate in \( n \)-pentane). \(^1^H\) NMR (400 MHz, CDCl \(_3\)) \( \delta 8.33 \) (dd, \( J = 7.7, 1.1 \) Hz, 1H), 8.15 – 8.08 (m, 2H), 7.91 – 7.86 (m, 1H), 7.53 (t, \( J = 7.7 \) Hz, 1H), 7.46 – 7.39 (m, 2H), 3.43 (tt, \( J = 11.5, 3.3 \) Hz, 1H), 1.95 – 1.80 (m, 4H), 1.75 – 1.68 (m, 1H), 1.58 (qd, \( J = 12.8, 3.2 \) Hz, 2H), 1.39 (qt, \( J = 12.7, 3.3 \) Hz, 2H), 1.27 (tt, \( J = 12.5, 3.3 \) Hz, 1H). \(^1^C\) NMR (101 MHz, CDCl \(_3\)) \( \delta 203.2, 142.6, 140.0, 137.7, 133.9, 129.6, 128.3, 127.3, 126.0, 124.6, 124.2, 122.9, 121.5, 45.5, 29.9, 26.1. \text{El-MS: } m/z 294.1 \text{ HRMS found: 295.1150 calc: 295.1130.}

**1-(2-Methylthiophenyl)octan-1-one** (31) CAS: 177885-66-5

Synthesized according to the general procedure. Isolated as a colorless oil (40 mg, 53%). \( R_f = 0.21 \) (29:1 i-hexane:ethyl acetate). \(^1^H\) NMR (400 MHz, CDCl \(_3\)) \( \delta 7.81 \) (dd, \( J = 7.8, 1.5 \) Hz, 1H), 7.48 – 7.43 (m, 1H), 7.34 – 7.31 (m, 1H), 7.21 – 7.16 (m, 1H), 2.94 (t, \( J = 7.3 \) Hz, 2H), 2.43 (s, 3H), 1.77 – 1.69 (m, 2H), 1.38 – 1.25 (m, 8H), 0.90 – 0.84 (m, 3H). \(^1^C\) NMR (101 MHz, CDCl \(_3\)) \( \delta 202.0, 142.3, 134.8, 132.1, 130.2, 125.3, 123.6, 40.2, 31.8, 29.4, 29.3, 24.6, 22.8, 16.2, 14.2. \text{El-MS: } m/z 250.1 \text{ HRMS found: 251.1472 calc: 251.1470.}

**1-(4-Fluorophenyl)-4-(4-methylpiperidin-1-yl)butan-1-one** (Melperone) CAS: 3575-80-2

\[ \text{26} \] (0.20 mmol), 4-methylpiperidine (2.0 eq), KI (0.2 eq) and NaHCO \(_3\) (2.0 eq) were dissolved in toluene (5 mL). The reaction mixture was heated to 100°C for 22 h. After completion, the reaction mixture was concentrated in vacuo and purified with silica column chromatography using a gradient (3:1 i-hexane:ethyl acetate + 1% triethylamine to ethyl acetate + 1% triethylamine). Isolated as a red solid (29 mg, 55%). \( R_f = 0.16 \)
(3:1 i-hexane:ethyl acetate + 1% trimethylamine). $^1$H NMR (400 MHz, CDCl$_3$) δ 8.02 – 7.96 (m, 2H), 7.15 – 7.08 (m, 2H), 2.95 (t, $J = 7.2$ Hz, 2H), 2.88 – 2.80 (m, 2H), 2.36 (t, $J = 7.1$ Hz, 2H), 1.97 – 1.84 (m, 4H), 1.61 – 1.54 (m, 2H), 1.38 – 1.23 (m, 1H), 1.21 – 1.08 (m, 2H), 0.89 (d, $J = 6.5$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 198.6, 166.7 (d, $J = 254.1$ Hz), 133.6 (d, $J = 2.7$ Hz), 130.7 (d, $J = 9.3$ Hz), 115.6 (d, $J = 21.7$ Hz), 58.2, 54.0, 36.4, 34.3, 30.8, 21.9 (2 carbons). MS-ESI [M+H$^+$]: m/z 264.2. HPLC purity > 99%.

Control experiments

To learn more about the reaction, a set of control experiments were conducted (table S2).

Table S2. Control experiments for the visible-light mediated carbonylative Suzuki-Miyaura cross-coupling

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst</th>
<th>Additive</th>
<th>Irradiation</th>
<th>Outcome$^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>-</td>
<td>LED</td>
<td>No product</td>
</tr>
<tr>
<td>2</td>
<td>Pd(PPh$_3$)$_4$</td>
<td>TEMPO (1 eq)</td>
<td>LED</td>
<td>No product</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>TEMPO (1 eq)</td>
<td>LED</td>
<td>No product</td>
</tr>
<tr>
<td>4</td>
<td>Pd(PPh$_3$)$_4$</td>
<td>TEMPO (1 eq)</td>
<td>LED</td>
<td>No product</td>
</tr>
<tr>
<td>5$^b$</td>
<td>Pd(PPh$_3$)$_4$</td>
<td>TEMPO (1 eq)</td>
<td>-</td>
<td>Trace</td>
</tr>
<tr>
<td>6</td>
<td>Pd(PPh$_3$)$_4$</td>
<td>-</td>
<td>Ambient light</td>
<td>Trace</td>
</tr>
<tr>
<td>7$^b$</td>
<td>Pd(PPh$_3$)$_4$</td>
<td>TEMPO (1 eq)</td>
<td>-</td>
<td>No product</td>
</tr>
<tr>
<td>8$^b$</td>
<td>Pd(PPh$_3$)$_4$</td>
<td>-</td>
<td>-</td>
<td>No product</td>
</tr>
<tr>
<td>9$^i$</td>
<td>Pd(PPh$_3$)$_4$</td>
<td>LED</td>
<td>Trace</td>
<td>Trace (of coupling product)</td>
</tr>
</tbody>
</table>

Reaction conditions: As in entry S63, table S1. $^a$ Outcome determined by GCMS- and LCMS-analysis. $^b$ Reaction performed in the dark. $^i$ No Mo(CO)$_6$. 

S12
Pressure measurement

**Figure S2.** Pressure measurement set-up. To the left, a schematic illustration and to the right, the actual set-up.

To \( C_{rxn} \) was added benzene/water 2:1 (4 mL) and to \( C_{CO} \) was added \( \text{Mo(CO)}_6 \) (0.75 mmol) followed by acetonitrile (4 mL). After capping, both chambers were subjected to 5 minute of \( \text{N}_2/\text{vacuum sparging}. \) \( C_{rxn} \) was pierced with a capillary connected to a manometer and DBU (1.5 mmol) was added to \( C_{CO} \) and the H-tube was positioned in a Dry-Syn heating block with \( C_{CO} \) heated at 70°C (figure S2). The temperature in \( C_{rxn} \) was measured to 34°C. The resulting pressure increase due to the CO release was monitored at regular time points (see table S3 and figure S3). Maximum pressure measured was 2.6 bar, reached within 20-25 minutes of the start of the reaction.

**Table S3.** Pressure measurements.

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Measurement 1 (bar)</th>
<th>Measurement 2 (bar)</th>
<th>Average pressure (bar)</th>
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</thead>
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<tr>
<td>5</td>
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<tr>
<td>60</td>
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</tr>
<tr>
<td>210</td>
<td>2,5</td>
<td>2,2</td>
<td>2,35</td>
</tr>
</tbody>
</table>
Figure S3. Graphic representation of pressure measurements. Maximum pressure reached within 20-25 minutes of the start of the reaction.
References

NMR spectra

Parameter Value
1 Solvent CDCl3
2 Temperature 298 K
3 Spectrometer Frequency 400.13 MHz
4 Nucleus 1H

Parameter Value
1 Solvent CDCl3
2 Temperature 298 K
3 Spectrometer Frequency 100.62 MHz
4 Nucleus 13C

1-[(4-Methylphenyl)sulfonyl]piperidin-4-ol CAS: 80213-12-3
4-Iodo-1-[(4-methylphenyl)sulfonyl]piperidine \( ^1 \) CAS: 289890-80-8
3-Iodobutylbenzene<sup>2,3</sup> CAS: 59456-20-1
2-Iodoctane CAS: 557-36-8
Cyclohexylphenylmethanone\(^*\) (4) CAS: 712-50-5 (from cyclohexyl iodide)
Cyclohexylphenylmethanone (4) CAS: 712-50-5 (from cyclohexl bromide)
Cyclohexylphenylmethanone \textsuperscript{5} (4) CAS: 712-50-5 (from cyclohexl bromide, heating \(\text{C}_\text{Rxn}\) and \(\text{C}_{\text{CO}}\) to 50°C)
2-Methyl-1,4-diphenylbutan-1-one (5) CAS: 108974-08-9
2-Methyl-1-phenyloctan-1-one (6) CAS: 132719-12-1
Cyclopentylphenylmethanone (7) CAS: 5422-88-8
Phenyl(1-tosylpiperidin-4-yl)methanone (8) CAS: 922504-26-5
1-Phenylnonan-1-one $^8$ (9) CAS: 6008-36-2 (from 1-iodooctane)
1-Phenylnonan-1-one \(^8\) (9) CAS: 6008-36-2 (from 1-bromooctane, 24 h irradiation)
1-Phenylnonan-1-one (9) CAS: 6008-36-2 (from 1-bromooctane, 55 h irradiation)
1-Phenyl-1-undecanone (10) CAS: 1674-37-8 (from 1-iodoheptane)
1-Phenyloctan-1-one\textsuperscript{9} (10) CAS: 1674-37-8 (from 1-bromoheptane)
3-Methyl-1-phenylbutan-1-one\textsuperscript{10} (11) CAS: 582-62-7
1,4-Diphenylbutan-1-one\textsuperscript{a} (12) CAS: 5407-91-0 (from 3-iodo-1-phenylpropane)
1,4-Diphenylbutan-1-one (12) CAS: 5407-91-0 (from 3-bromo-1-phenylpropane, 24 h irradiation)
1,4-Diphenylbutan-1-one (12) CAS: 5407-91-0 (from 3-bromo-1-phenylpropane, 55 h irradiation)
5-Chloro-1-phenylpentan-1-one\textsuperscript{11} (13) CAS: 942-93-8 (from 1-chloro-4-iodobutane)
5-Chloro-1-phenylpentan-1-one (13) CAS: 942-93-8 (from 4-bromo-1-chlorobutane)
((3r,5r,7r)-Adamantan-1-yl)(phenyl)methanone \( ^{12} \) (14) CAS: 31919-47-8 (from 1-iodoadamantane)
((3r,5r,7r)-Adamantan-1-yl)(phenyl)methanone\textsuperscript{12} \textsuperscript{(14)} CAS: 31919-47-8 (from 1-bromo adamantane)
4-Methyl-1-phenylpentan-1-one<sup>9</sup> (18) CAS: 2050-07-9
1-Phenylnon-8-en-1-one (19) CAS: 148056-64-8
[1,1'-Biphenyl]-2-yl(cyclo-hexyl)methanone (20) CAS: 963-92-8
Cyclohexyl(naphthalen-2-yl)-methanone (21) CAS: 10404-26-9
1-(p-Tolyl)octan-1-one (22) CAS: 2789-44-8
Cyclohexyl(m-tolyl)methanone (23) CAS: 3277-78-9
1-(2-(Trifluoromethyl)-phenyl)octan-1-one (24) CAS: 1778855-78-9
1-(2-(Trifluoromethyl)-phenyl)octan-1-one (24) CAS: 1778855-78-9
1-(4-Fluorophenyl)octan-1-one \textsuperscript{15} (25) CAS: 111829-15-3
1-(4-Fluorophenyl)octan-1-one (25) CAS: 111829-15-3
4-Chloro-1-(4-fluorophenyl)-butan-1-one (26) CAS: 3874-54-2
4-Chloro-1-(4-fluorophenyl)-butan-1-one$^{16}$ (26) CAS: 3874-54-2
1-(4-Chlorophenyl)octan-1-one (27) CAS: 7295-52-5
1-(2-Methoxyphenyl)octan-1-one (28) CAS: 153644-77-0
1-(4-Methoxyphenyl)octan-1-one\textsuperscript{17} (29) CAS: 62170-25-6
1-(4-Methoxyphenyl)octan-1-one\textsuperscript{17} (29) CAS: 62170-25-6 (CO-surrogate synthesis)
Cyclohexyl(dibenzo[b,d]thio-phen-4-yl)methanone (30) CAS: -
1-(2-(Methylthio)phenyl)octan-1-one (31) CAS: 1778855-66-5
1-(4-Fluorophenyl)-4-(4-methylpiperidin-1-yl)butan-1-one (Melperone) CAS: 3575-80-2