Electronic Supplementary Material (ESI) for Green Chemistry.

One-pot Synthesis of Pyrrolidones from Levulinic Acid and Amines /Nitroarenes /Nitriles over Ir-PVP Catalyst

Chandan Chaudhari,*[a] Masaya Shiraishi,[b] Yoshihide Nishida,[a] Katsutoshi Sato,[a,c] Katsutoshi Nagaoka*[a]

[a]Department of Chemical Systems Engineering, Graduate School of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8603, Japan

[b]Department of Integrated Science and Technology, Faculty of Science and Engineering, Oita University, 700 Dannoharu, Oita 870-1192, Japan

[c]Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, Katsura, Kyoto 615-8520, Japan

*Corresponding authors.
E-mail address: nagaoka.katsutoshi@material.nagoya-u.ac.jp
E-mail address: chaudhari.chandan.subhash@d.mbox.nagoya-u.ac.jp

Experimental Section

General

All chemicals obtained from Tokyo Chemical Industry, Fujifilm Wako Pure Chemical Industries and Sigma-Aldrich were used as received.

Catalyst preparation

Polyvinylpyrrolidone-stabilized metal nanoparticles (Ir, Pt, Pd, Ru, and Rh) catalysts were prepared using microwave-assisted reduction method.[1] In a typical procedure, 0.04-0.25 mmol of metal chloride and 0.2-1.25 mmol of polyvinylpyrrolidone were dissolved in reductant. The mixture was purged with Ar and heated at 165 °C by microwave radiation for 15 min. The resulting solution was washed with diethyl ether and acetone, and separated by subjected to centrifugation. The catalyst was dried at 40 ^{o}C for 12 h under vacuum**.** PVP free Ir catalyst was prepared from Ir-PVP by decomposing PVP at 500 ^{o}C for 0.5 h in H_2 flow. The reaction mixture was introduced to Ir metal without exposing metal to air.

Table S1. Preparation procedure of various metal NPs

Metal	Metal conc. (mmol)	PVP conc. (mmol)	Reductant	Particle size (nm)	M-PVP[a] (%)
Ir	0.25	1.25	Triethylene glycol	1.7 ± 0.4	82
Pt	0.05	0.25	Ethylene glycol	3.7 ± 0.5	72
Pd	0.04	0.2	30 % EtOH-H_2O	3.4 ± 0.5	83
Ru	0.25	1.25	EtOH	3.0 ± 0.9	84
Rh	0.25	1.25	EtOH	3.6 ± 0.6	83

Catalyst characterization

Transmission electron microscopy (TEM) and high-resolution scanning transmission electron microscopy (STEM) were obtained with an electron microscope JEM-2100Plus and JEM-ARM200F, JEOL, Japan operated at 200 kV and 120 kV respectively. The amount of PVP on metal nanoparticles was calculated by using thermogravimetric analysis (ThermoPlus; Rigaku, Japan) from room temperature to 1000°C under air (flow rate: 200 mL/min).

General procedure for reductive amination

All reactions were carried out in 10-mL autoclave with glass tube equipped with a magnetic stirrer. In a standard run, amine, nitroarene, or nitrile (1 mmol) and levulinic acid or 2-formylbenzoic acid (2 mmol) were added to the reactor. For solid substrates, 1 mL of methanol was also added. Then, the reactor was purged with H_2 gas and heated to 30 °C in an autoclave with continuous stirring. After completion of the reaction, the catalyst was separated from the reaction mixture by a syringe microfilter. The conversion of substrate and yield of product were calculated by gas chromatography using internal standard. For indoprofen, conversion and yield of indoprofen were obtained by ^{1}H NMR n analysis using 1, 3, 5-trimethoxybenzene as an internal standard.

Table S2. Previous reports of reductive amination of levulinic acid with H_2

Catalyst	H_2 (bar)	Temp. (°C)	Substrates	Ref.
Ir complex	5	110	amines	11
Pd/ZrO_2	5	90	amines	12a
CNF_{30}@Ni@CNTs	30	130	amines	12b
Ru-PP/CNTs	30	120	amines	12c
Ru/C	35	150	amines	12d
$Pt/P\text{-}TiO_2$	1	25	amines	12e
Ru@GOIL	15	130	amines	12g
FeNi	85	150	amines	12h
Pt/TiO_2-NT	10	120	amines, nitroarenes	13
$Pt\text{-}MoO_x/TiO_2$	3–7	100–110	amines, nitriles	14
Ir-PVP	**5–10**	**30**	**amines, nitroarenes, nitriles**	**This work**

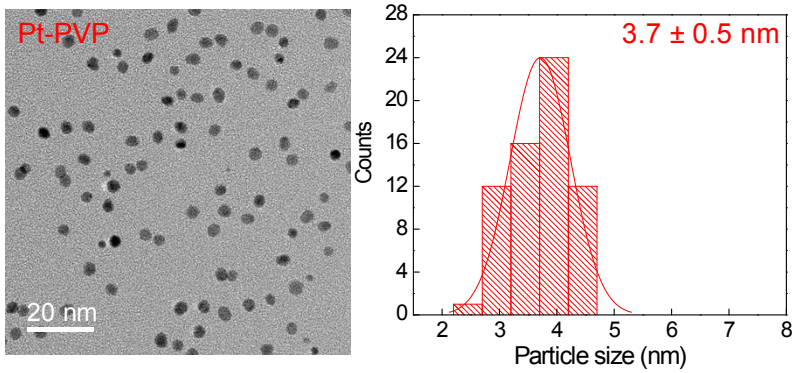


Figure S1. Transmission electron micrograph (TEM) of Pt-PVP

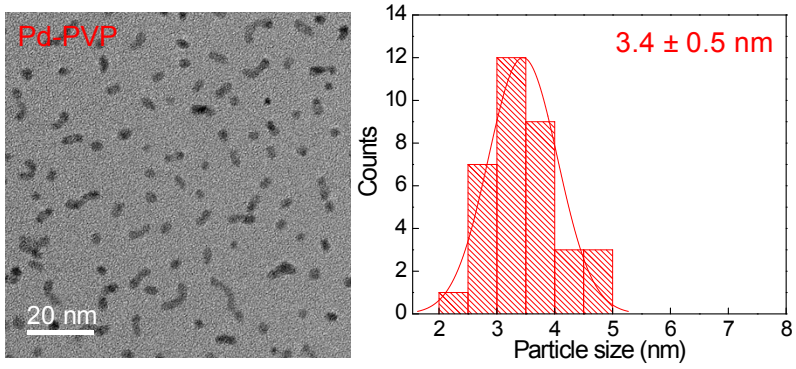


Figure S2. Transmission electron micrograph (TEM) of Pd-PVP

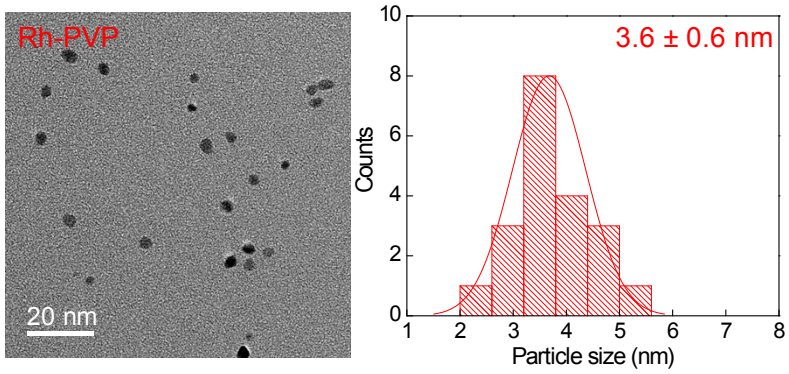


Figure S3. Transmission electron micrograph (TEM) of Rh-PVP

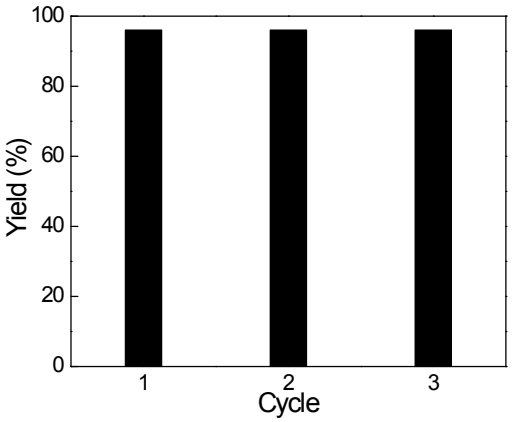


Figure S4. Recycle study for reductive amination LA with aniline over Ir-PVP catalyst.

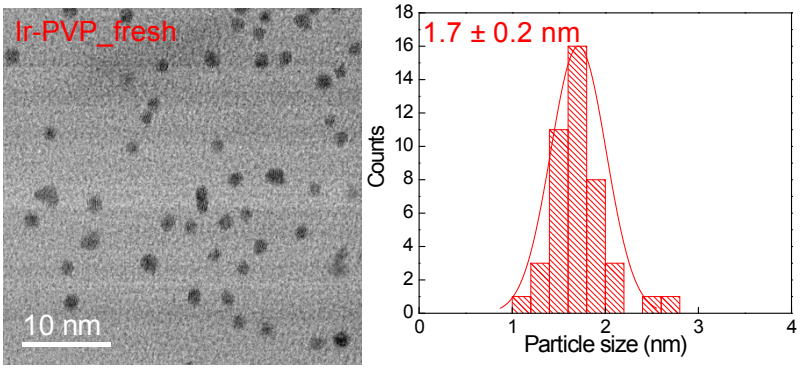


Figure S5. High-resolution scanning transmission electron micrograph of fresh Ir-PVP catalyst

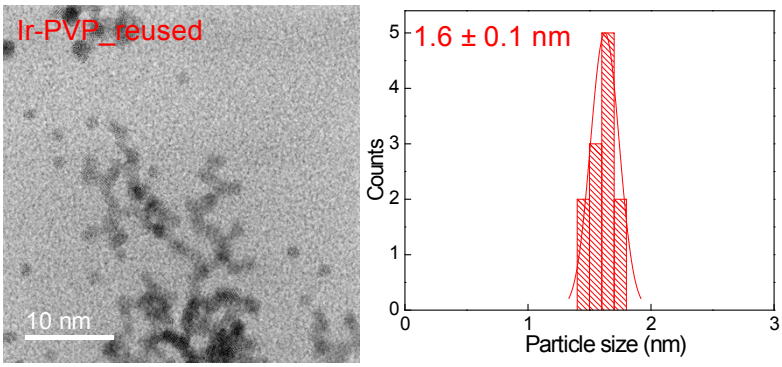


Figure S6. High-resolution scanning transmission electron micrograph of recovered Ir-PVP catalyst

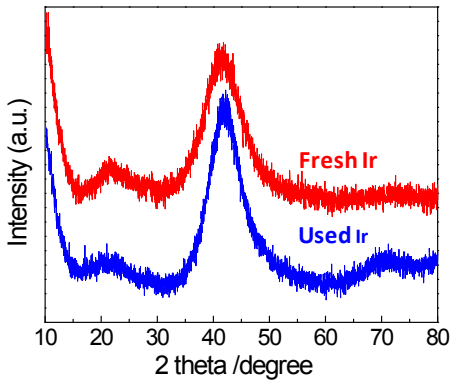


Figure S7. XRD pattern of fresh and used Ir catalyst

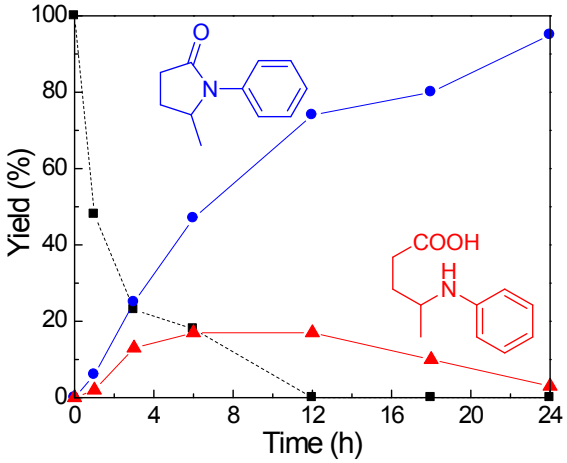
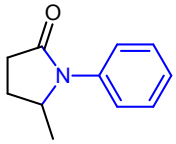


Figure S8. Time-yield profile for reductive amination of levulinic acid with aniline in the presence of Ir-PVP: yield of pyrrolidone (●), uncyclized intermediate (▲), and aniline (■).

NMR and GCMS analysis

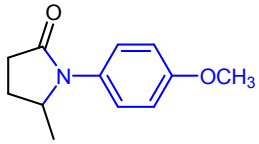
^{1}H and ^{13}C NMR spectra were recorded using at ambient temperature on Brucker Ascend operating at 500.05 and 125.75 MHz, respectively. All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. All chemical shifts are reported relative to tetramethylsilane and *d*-solvent peaks ($CDCl_3$ or DMSO-d_6). Abbreviations used in the NMR experiments: s, singlet d, doublet; t, triplet; m, multiplet. GC-MS spectra were recorded by SHIMADZU QP2010.

5-methyl-1-phenylpyrrolidin-2-one[2] (Table 1, entry 1)



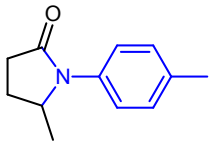
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33-7.26 (m, 4H), 7.15-7.12 (m, 1H), 4.25-4.19 (m, 1H), 2.62-2.45 (m, 2H), 2.34-2.26 (m, 1H), 1.73-1.62 (m, 1H), 1.12 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 174.7, 137.3, 129.0, 125.9, 124.2, 55.9, 31.2, 26.7, 20.1. GC-MS m/e 175.

1-(4-methoxyphenyl)-5-methylpyrrolidin-2-one[2] (Table 1, entry 2)



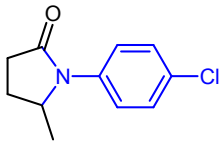
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.15 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 3.90 (d, *J* = 14.8 Hz, 1H), 3,79 (s, 3H), 2.52-2.45 (m, 1H), 2.41-2.35 (m, 1H), 2.17-2.10 (m, 1H), 1.61-1.54 (m, 1H), 1.13 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 174.9, 158.9, 129.2, 128.8, 113.9, 55.2, 52.7, 30.3, 26.6, 19.5. GC-MS m/e 205.

5-methyl-1-(4-methylphenyl)pyrrolidin-2-one[2] (Table 1, entry 3)



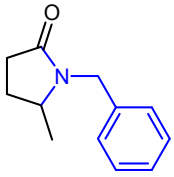
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.24-7.19 (m, 4H), 4.29-4.22 (m, 1H), 2.68-2.52 (m, 2H), 2.40-2.34 (m, 4H), 1.79-1.72 (m, 1H), 1.19 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 174.5, 135.8, 134.7, 129.6, 124.3, 55.9, 31.9, 26.7, 20.9, 20.1. GC-MS m/e 189.

1-(4-chlorophenyl)-5-methylpyrrolidin-2-one[2] (Table 1, entry 4)



^{1}H NMR (500 MHz, $CDCl_3$): δ 7.36-7.32 (m, 4H), 4.31-4.25 (m, 1H), 2.70-2.52 (m, 2H), 2.42-2.34 (m, 1H), 1.89-1.73 (m, 1H), 1.20 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 174.6, 135.9, 131.1, 129.0, 125.1, 55.6, 31.1, 26.6, 19.9. GC-MS m/e 209.

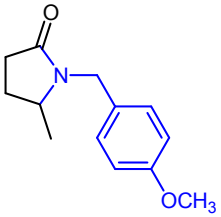
1-benzyl-5-methylpyrrolidin-2-one[2] (Table 1, entry 5 and Table 2, entry 1)



^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33-7.22 (m, 5H), 4.94 (d, *J* = 15.0 Hz, 1H), 3.98 (d, *J* = 15.0 Hz, 1H), 3.57-3.49 (m, 1H), 2.56-2.40 (m, 2H), 2.17-2.12 (m, 1H), 1.62-1.56 (m, 1H), 1.15 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.5, 136.5, 128.6, 127.9, 127.4,

53.0, 43.9, 30.1, 26.6, 19.5. GC-MS m/e 189.

1-[(4-methoxyphenyl)methyl]-5-methylpyrrolidin-2-one[3] (Table 1, entry 6 and Table 2, entry 2)

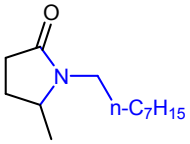


^{1}H NMR (500 MHz, $CDCl_3$): δ 7.08 (d, *J* = 8.4 Hz, 2H), 6.76 (d, *J* = 8.6 Hz, 2H), 4.82 (d, *J* = 14.8 Hz, 1H), 3.82 (d, *J* = 14.9 Hz, 1H), 3.71 (s, 3H), 3.47-3.39 (m, 1H), 2.35-2.24 (m, 2H), 2.08-2.02 (m, 1H), 1.54-1.45 (m, 1H), 1.13 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.2, 158.9, 129.3, 128.7, 114.0, 55.2, 52.7, 43.3, 30.2, 26.5, 19.5. GC-MS m/e 219.

1-(cyclohexylmethyl)-5-methylpyrrolidin-2-one[3] (Table 1, entry 7)

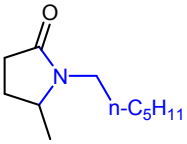
^{1}H NMR (500 MHz, $CDCl_3$): δ 3.63-3.56 (m, 1H), 3.41-3.36 (m, 1H), 2.67-2.63 (m, 1H), 2.38-2.24 (m, 2H), 2.14-2.08 (m, 1H), 1.66-1.56 (m, 4H), 1.52-1.46 (m, 3H), 1.17-1.05 (m, 6H), 0.94-0.79 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.1, 53.7, 52.9, 46.0, 35.7, 31.1, 30.5, 30.2, 26.7, 26.3, 25.8, 25.6, 19.4. GC-MS m/e 195.

5-methyl-1-octylpyrrolidin-2-one[2] (Table 1, entry 8)



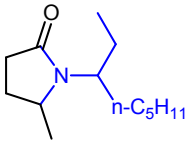
^{1}H NMR (500 MHz, $CDCl_3$): δ 3.65-3.58 (m, 1H), 3.52-3.47.94 (m, 1H), 2.86-2.80 (m, 1H), 2.39-2.24 (m, 2H), 2.14-2.07 (m, 1H), 1.54-1.42 (m, 2H), 1.39-1.32 (m, 1H), 1.24-1.07 (m, 14H), 0.8 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.0, 53.4, 40.1, 31.1, 30.2, 29.2, 29.1, 27.3, 26.9, 26.7, 22.6, 19.7, 14.0. GC-MS m/e 211.

5-methyl-1-hexylpyrrolidin-2-one[2] (Table 1, entry 9)



^{1}H NMR (500 MHz, $CDCl_3$): δ 3.65-3.59 (m, 1H), 3.53-3.47 (m, 1H), 2.86-2.81 (m, 1H), 2.39-2.22 (m, 2H), 2.16-2.07 (m, 1H), 1.54-1.41 (m, 2H), 1.39-1.32 (m, 1H), 1.21-1.07 (m, 9H), 0.8 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.0, 53.4, 40.1, 31.4, 30.2, 27.3, 26.7, 26.5, 22.5, 19.7, 13.9. GC-MS m/e 183.

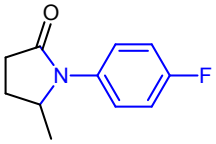
5-methyl-1-(octan-3-yl)pyrrolidin-2-one (Table 1, entry 10)



^{1}H NMR (500 MHz, $CDCl_3$): δ 3.65-3.60 (m, 1H), 3.54-3.45 (m, 1H), 2.83-2.64 (m, 2H), 2.45-2.28 (m, 2H), 2.16-2.12 (m, 2H), 1.58-1.51 (m, 2H), 1.37-1.18 (m, 6H), 1.1 (t, *J* = 6.3 Hz, 3H), 0.86-0.78 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.4, 53.4, 43.3, 31.4,

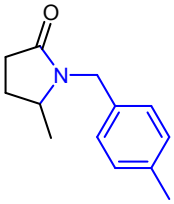
30.1, 28.0, 26.6, 26.5, 23.4, 22.9, 19.3, 13.9, 10.9. GC-MS m/e 211.

1-(4-Fluorophenyl)-5-methylpyrrolidin-2-one[2] (Table 1, entry 4)



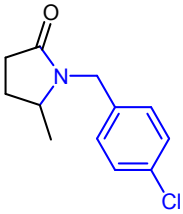
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.32-7.28 (m, 2H), 7.10-7.06 (m, 2H), 4.27-4.20 (m, 1H), 2.63-2.57 (m, 2H), 2.36-2.41 (m, 1H), 1.78-1.74 (m, 1H), 1.08 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 174.8 161.5, 159.5, 133.3, 126.2, 126.1, 115.9, 115.7, 56.1, 31.0, 26.7, 20.1. GC-MS m/e 193.

5-methyl-1-[(4-methylphenyl)methyl]pyrrolidin-2-one[4] (Table 3, entry 3)



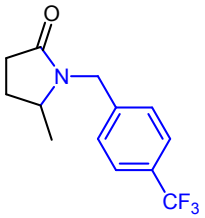
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.18 (d, *J* = 7.9 Hz, 2H), 7.06 (d, *J* = 7.7 Hz, 2H), 4.85 (d, *J* = 14.9 Hz, 1H), 3.83 (d, *J* = 14.9 Hz, 1H), 3.47-3.41 (m, 1H), 2.37-2.26 (m, 2H), 2.25 (s, 3H), 2.07-2.02 (m, 1H), 1.54-1.47 (m, 1H), 1.06 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.2, 137.1, 133.6, 129.2, 127.9, 52.7, 43.6, 30.2, 26.5, 21.0, 19.5. GC-MS m/e 203.

1-[(4-chlorophenyl)methyl]-5-methylpyrrolidin-2-one[2] (Table 3, entry 4)



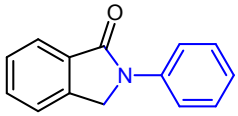
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.26 (d, *J* = 8.3 Hz, 2H), 7.15 (d, *J* = 8.2 Hz, 2H), 4.83 (d, *J* = 15.1 Hz, 1H), 3.98 (d, *J* = 15.1 Hz, 1H), 3.53-3.47 (m, 1H), 2.51-2.37 (m, 2H), 2.18-2.11 (m, 1H), 1.62-1.55 (m, 1H), 1.13 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.0, 135.4, 133.2, 129.3, 128.6, 52.9, 43.3, 30.1, 26.6, 19.6. GC-MS m/e 223.

5-methyl-1-{[4-(trifluoromethyl)phenyl]methyl}pyrrolidin-2-one[3] (Table 3, entry 5)



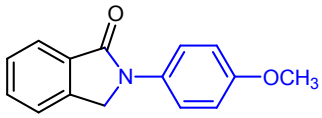
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.49 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 4.96 (d, *J* = 15.3 Hz, 1H), 4.03 (d, *J* = 15.3 Hz, 1H), 3.50-3.43 (m, 1H), 2.49-2.32 (m, 2H), 2.15-2.06 (m, 1H), 1.59-1.52 (m, 1H), 1.08 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.5, 140.9, 129.6, 128.1, 125.6, 125.5, 53.2, 43.6, 30.0, 26.7, 19.6. GC-MS m/e 257.

2-phenyl-2,3-dihydro-1H-isoindol-1-one[3] (Table 3, entry 1)



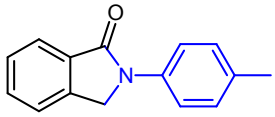
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.85 (d, *J* = 7.5 Hz, 1H), 7.81-7.78 (m, 2H), 7.54-7.51 (m, 1H), 7.45-7.42 (m, 2H), 7.38-7.34 (m, 2H), 7.09-7.13 (m, 1H), 4.79 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.5, 140.1, 139.5, 133.2, 132.0, 129.1, 128.4, 124.6, 124.1, 122.6, 119.5, 50.7. GC-MS m/e 209.

2-(4-methoxyphenyl)-2,3-dihydro-1H-isoindol-1-one[3] (Table 3, entry 2)



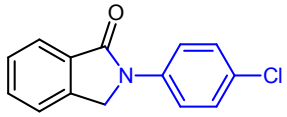
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, *J* = 7.4 Hz, 1H), 7.43-7.34 (m, 2H), 7.31-7.25 (m, 1H), 7.18-7.12 (m, 2H), 6.71-6.68 (m, 2H), 4.65 (m, 2H) 3.7 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.4, 159.1, 141.2, 132.7, 131.4, 131.3, 129.5, 128.0, 123.8, 122.7, 114.1, 55.2, 49.3. GC-MS m/e 239.

2-(4-methylphenyl)-2,3-dihydro-1H-isoindol-1-one (Table 3, entry 3)



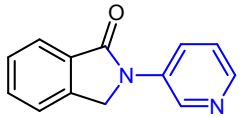
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, *J* = 7.2 Hz, 1H), 7.76-7.39 (m, 2H), 7.61-7.58 (m, 1H), 7.52-7.50 (m, 2H), 7.23 (d, *J* = 8.6 Hz, 2H), 4.83 (m, 2H) 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.3, 140.1, 136.9, 134.2, 133.3, 131.9, 129.6, 128.3, 124.0, 122.5, 119.6, 50.8, 20.8. GC-MS m/e 223.

2-(4-chlorophenyl)-2,3-dihydro-1H-isoindol-1-one[3] (Table 3, entry 4)



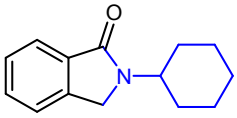
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.83 (d, *J* = 8.3 Hz, 1H), 7.77-7.74 (m, 2H), 7.51-7.51 (m, 1H), 7.45-7.42 (m, 2H), 7.32-7.29 (m, 2H), 4.75 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.5, 139.8, 138.1, 132.9, 132.3, 129.5, 129.1, 128.5, 124.2, 122.6, 120.4, 50.6. GC-MS m/e 243.

2-(pyridin-3-yl)-2,3-dihydro-1H-isoindol-1-one (Table 3, entry 5)



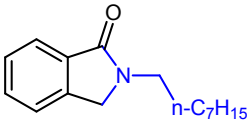
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.85 (m, 1H), 8.47-8.45 (m, 1H), 8.36-8.34 (m, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.59-7.54 (m, 1H), 7.49-7.43 (m, 2H), 7.31-7.27 (m, 1H), 4.83 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.9, 145.3, 140.0, 139.9, 136.3, 132.6, 132.4, 128.6, 126.6, 124.3, 123.7, 122.8, 50.1. GC-MS m/e 210.

2-cyclohexyl-2,3-dihydro-1H-isoindol-1-one[5] (Table 3, entry 6)



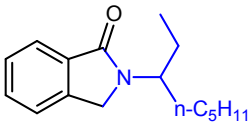
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (m, 1H), 7.55-7.52 (m, 1H), 7.47-7.42 (m, 2H), 4.61 (m, 2H), 3.64-3.59 (m, 1H), 2.01-1.40 (m, 10H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 169.4, 141.7, 132.3, 130.9, 127.7, 123.4, 122.1, 55.6, 48.6, 30.5, 24.9, 24.5. GC-MS m/e 215.

2-octyl-2,3-dihydro-1H-isoindol-1-one[2] (Table 3, entry 7)



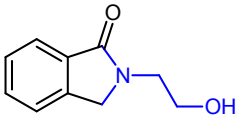
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.76 (d, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.38-7.35 (m, 2H), 4.30 (m, 2H), 3.66-3.62 (m, 1H), 3.54-3.51 (m, 1H), 1.64-1.55 (m, 2H), 1.30-1.10 (m, 10H), 0.79 (t, *J* = 7.0 Hz, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.4, 141.1, 133.1, 131.0, 127.9, 123.6, 122.6, 49.8, 42.4, 31.7, 29.2, 29.1, 28.4, 26.8, 22.6, 14.0. GC-MS m/e 245.

2-(octan-3-yl)-2,3-dihydro-1H-isoindol-1-one (Table 3, entry 8)



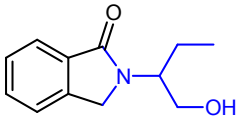
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07-8.05 (m, 1H), 7.99 (t, *J* = 8.0 Hz, 1H), 7.39-7.33 (m, 2H), 4.67 (m, 2H), 3.66-3.61 (m, 1H), 1.35-1.20 (m, 4H), 1.12-0.96 (m, 6H), 0.92-0.80 (m, 6H) ; ^{13}C NMR (125 MHz, $CDCl_3$): δ 169.0, 141.1, 132.7, 131.1, 127.6, 123.7, 122.6, 50.6, 38.4, 30.2, 28.1, 23.5, 22.7, 13.9, 10.1. GC-MS m/e 245.

2-(2-hydroxyethyl)-2,3-dihydro-1H-isoindol-1-one[6] (Table 3, entry 9)



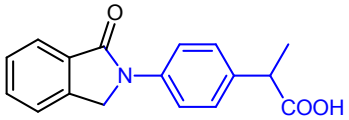
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.47-7.43 (m, 2H), 4.53 (m, 2H), 3.93-3.92 (m, 2H), 3.74-3.72 (m, 2H), 2.88 (br s, 1H) ; ^{13}C NMR (125 MHz, $CDCl_3$): δ 169.7, 141.4, 132.5, 131.4, 128.0, 123.6, 122.6, 61.6, 51.7, 46.1. GC-MS m/e 177.

2-(1-hydroxybutan-2-yl)-2,3-dihydro-1H-isoindol-1-one (Table 3, entry 10)



^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89-7.84 (m, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.31-7.23 (m, 2H), 5.1 (br s, 1H), 4.63 (m, 2H), 3.64-3.59 (m, 3H), 1.72-1.54 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$): δ 171.6, 141.5, 132.4, 131.5, 128.0, 123.6, 122.7, 64.8, 58.2, 49.3, 21.0, 9.9. GC-MS m/e 205.

2-(4-(1-Oxoisoindolin-2-yl)phenyl)propanoic acid (Indoprofen)[7]



^{1}H NMR (500 MHz, DMSO-d6): δ 7.89 – 7.84 (m, 2H), 7.77 (d, J = 7.6 Hz, 1H), 7.67 – 7.61 (m, 2H), 7.52 (m, 1H), 7.35 (d, J = 8.6 Hz, 2H), 4.96 (s, 2H), 3.70 (m, 1H), 1.39 (d, J = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d6): δ 175.8, 167.0, 141.3, 138.6, 137.4, 132.9, 132.5, 128.5, 128.3, 123.6, 123.6, 119.8, 50.8, 44.6, 18.2.

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