Supporting Information
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Supporting Information

Visible-Light-Activated Enantioselective Perfluoroalkylation with a Chiral Iridium Photoredox Catalyst

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1. General Information ..............................................................................................................................................S2
2. Synthesis of Catalysts........................................................................................................................................S3
3. Synthesis of Substrates.......................................................................................................................................S10
4. Iridium-Catalyzed Photoredox Reactions .........................................................................................................S15
5. Enantioselectivities as Determined by Chiral HPLC .........................................................................................S27
7. References.........................................................................................................................................................S44
1. General Information

All reactions were carried out under an atmosphere of argon with magnetic stirring. Catalysis reactions were performed in a Schlenk tube (10 mL). A 21 W compact fluorescent lamp (CFL) is served as light source. The photocatalyst $\Lambda$-Ir$^1$ was synthesized according to our published procedures. Solvents were distilled under nitrogen from calcium hydride (CH$_3$CN, CH$_2$Cl$_2$), sodium/benzophenone (THF), or magnesium turnings/iodine (MeOH). Reagents that were purchased from commercial suppliers were used without further purification. Flash column chromatography was performed with silica gel 60 M from Macherey-Nagel (irregular shaped, 230–400 mesh, pH 6.8, pore volume: 0.81 mL x g$^{-1}$, mean pore size: 66 Å, specific surface: 492 m$^2$ x g$^{-1}$, particle size distribution: 0.5% < 25 μm and 1.7% > 71 μm, water content: 1.6%). $^1$H NMR, $^{19}$F NMR and proton decoupled $^{13}$C NMR spectra were recorded on Bruker Avance 300 (300 MHz) spectrometers at ambient temperature. NMR standards were used as follows: $^1$H NMR spectroscopy: δ = 7.26 ppm (CDCl$_3$), δ = 5.32 ppm (CD$_2$Cl$_2$). $^{19}$F NMR spectroscopy: δ = 0 ppm (CFCl$_3$). $^{13}$C{$^1$H} NMR spectroscopy: δ = 77.0 ppm (CDCl$_3$), δ = 53.8 ppm (CD$_2$Cl$_2$). IR spectra were recorded on a Bruker Alpha FT-IR spectrophotometer. High-resolution mass spectra were recorded on a Bruker En Apex Ultra 7.0 TFT-MS instrument using ESI/FD/APCI technique. CD spectra were recorded on a JASCO J-810 CD spectropolarimeter (600-200 nm, 1 nm bandwidth, 50 nm/min scanning speed, accumulation of 3 scans). Chiral HPLC chromatography was performed with an Agilent 1200 or Agilent 1260 HPLC system. Optical rotations were measured on a Krüss P8000-T polarimeter with $[\alpha]_D^{22}$ values reported in degrees with concentrations reported in g/100 mL.
2. Synthesis of Catalysts

Catalysts $\Lambda$-Ir2 and $\Delta$-Ir2 were synthesized according to the following route.

2.1 Synthesis of Ligand

![Chemical Reaction]

4-( tert-Butyl)-N-(3-( tert-butyl)phenyl)benzothioamide (S1)

Compound S1 was synthesized following a published procedure with slight modifications.\(^2\) Na$_2$S·9H$_2$O (1.5 g, 6.25 mmol) was added to a mixture of sulfur (1.0 g, 31.2 mmol) and 3-( tert-butyl)aniline (5.6 g, 37.5 mmol) in DMF (25 mL). The suspension was stirred at 115 °C for 0.5 h under nitrogen. Afterwards, the mixture was cooled to room temperature, 4-( tert-butyl)benzaldehyde (4.1 g, 25 mmol) was added and the mixture was stirred at 115 °C for 24 h under nitrogen. After cooling to room temperature, the resulting solution was quenched with saturated NH$_4$Cl aqueous solution and extracted with ethyl acetate. The organic fraction was thoroughly washed with water and dried with Na$_2$SO$_4$. After concentration, the residue was purified by silica gel column ($n$-hexane/EtOAc = 40:1) to yield thioamide S1 as a yellow solid (4.72 g, 58%).

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 9.06 (brs, 1H), 7.83-7.76 (m, 3H), 7.72-7.62 (m, 1H), 7.51-7.27 (m, 4H), 1.35 (s, 18H).

$^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 197.8, 154.7, 152.3, 140.6, 138.9, 128.5, 126.5, 125.5, 123.7, 120.6, 120.5, 34.83, 34.78, 31.2, 31.1.

IR (film): $\nu$ (cm$^{-1}$) 3173, 2957, 2867, 1595, 1512, 1472, 1419, 1336, 1274, 1240, 1199, 1112, 999, 907, 843, 747, 701.

HRMS (ESI, $m/z$) calcd for C$_{21}$H$_{27}$NSNa [M+Na]$^+$: 348.1756, found: 348.1755.
**5-(tert-Butyl)-2-(4-(tert-butyl)phenyl)benzo[d]thiazole (S2)**

Compound S2 was synthesized following a published procedure with slight modifications. A mixture of S1 (2.1 g, 6.46 mmol), PdCl₂ (115 mg, 0.65 mmol), CsF (491 mg, 3.2 mmol), DMSO (13 mL) was stirred under O₂ atmosphere at 120 °C for 4 hours. Then the reaction was heated to 140 °C for 15 h. Afterwards, the mixture was cooled to room temperature, the resulting solution was quenched with saturated NH₄Cl aqueous solution and extracted with ethyl acetate. The organic fraction was thoroughly washed with water and dried with Na₂SO₄. After concentration, the residue was purified by silica gel column (n-hexane/EtOAc = 50:1) to yield ligand S2 as a white solid (1.065 g, 51%).

1H NMR (300 MHz, CDCl₃) δ 8.11 (d, J = 1.5 Hz, 1H), 8.03 (dt, J₁ = 8.4 Hz, J₂ = 2.1 Hz, 2H), 7.81 (d, J = 8.4 Hz, 1H), 7.51 (dt, J₁ = 8.7 Hz, J₂ = 2.1 Hz, 2H), 7.46 (dd, J₁ = 8.7 Hz, J₂ = 2.1 Hz, 1H), 1.42 (s, 9H), 1.38 (s, 9H).

13C NMR (75 MHz, CDCl₃) δ 168.2, 154.6, 154.4, 150.0, 131.9, 131.1, 127.3, 125.9, 123.2, 120.9, 119.6, 35.0, 34.9, 31.5, 31.2.

IR (film): ν (cm⁻¹) 3069, 2958, 2865, 1598, 1541, 1473, 1402, 1361, 1310, 1258, 1204, 1107, 1020, 966, 925, 877, 832, 812, 734, 702, 659, 609, 541, 459, 409.


### 2.2 Synthesis of racemic catalyst

![Synthesis of racemic catalyst](image)

**Iridium Dimer Complex (S3)**

Phenyl benzothiazole ligand (S2) (790 mg, 2.44 mmol) was added to iridium chloride hydrate (420 mg, 1.19 mmol) in a mixture of 2-ethoxyethanol/water (3:1, 52.9 mL). The reaction mixture was heated at 130 °C for 24 h under nitrogen atmosphere. The resulting precipitate was collected by centrifugation and dried to yield the iridium dimer (S3) as a red solid (624 mg, 60% yield).
**Rac-Ir2 complex**

A mixture of Iridium dimer (S3) (583 mg, 0.335 mmol) and AgPF₆ (253 mg, 1.0 mmol) in CH₃CN (22.4 mL) was purged with nitrogen for 5 min and then heated at 60 °C overnight. The reaction mixture was cooled to room temperature and concentrated to dryness. The residue was subjected to a flash silica gel chromatography (DCM/MeCN = 500:1 to 50:1) to obtain the racemic catalyst Rac-Ir2 as a yellow solid (711 mg, 100% yield).

**1H NMR (300 MHz, CD₂Cl₂) δ 8.40 (d, J = 1.5 Hz, 2H), 8.00 (d, J = 9.0 Hz, 2H), 7.71 (dd, J₁ = 8.7 Hz, J₂ = 1.8 Hz, 2H), 7.58 (d, J = 8.1 Hz, 2H), 7.01 (dd, J₁ = 8.1 Hz, J₂ = 1.8 Hz, 2H), 6.14 (d, J = 1.5 Hz, 2H), 2.39 (s, 6H), 1.45 (s, 18H), 0.88 (s, 18H).**

**13C NMR (75 MHz, CD₂Cl₂) δ 204.5, 178.4, 176.0, 173.7, 165.6, 161.7, 153.0, 151.9, 148.9, 148.2, 146.3, 144.7, 144.2, 140.1, 58.8, 58.1, 54.9, 54.1, 27.3.**

**IR (film): ν (cm⁻¹) 2957, 2869, 1584, 1463, 1435, 1366, 1295, 1267, 1203, 1151, 1111, 995, 935, 839, 730, 673, 641, 598, 556, 458.**
2.3 Synthesis of chiral catalyst

Auxiliary complexes \((S)\)\text{-}Aux-\(\Lambda\)\text{-}Ir2 and \((S)\)\text{-}Aux-\(\Delta\)\text{-}Ir2

A mixture of \textbf{Rac-Ir2} (400.0 mg, 0.376 mmol), the chiral auxiliary \((S)\)\text{-}Aux (166.4 mg, 0.752 mmol) and triethylamine (95.1 mg, 0.940 mmol) in DCM (37.6 mL) was purged with argon for 5 min and then stirred for 4 hours. The reaction mixture was concentrated to dryness. The residue was subjected to a flash silica gel chromatography (EtOAc/\(n\)-hexane = 1:10) to separate the two diastereomers. The first eluting diastereomer was assigned as \((S)\)\text{-}Aux-\(\Lambda\)\text{-}Ir2 (an orange solid, 161 mg, 41%) and the second eluting diastereomer as \((S)\)\text{-}Aux-\(\Delta\)\text{-}Ir2 (an orange solid, 173 mg, 44%). The absolute configurations of \((S)\)\text{-}Aux-\(\Lambda\)\text{-}Ir and \((S)\)\text{-}Aux-\(\Delta\)\text{-}Ir2 were assigned by comparison with CD spectra of the published analogous complexes\(^1\) and further confirmed by an X-ray crystal structure of \(\Delta\text{-}Ir2\) which was obtained by the follow-up transformation.

\((S)\)\text{-}Aux-\(\Lambda\)\text{-}Ir2:

\(^1\)H NMR (300 MHz, CD\(_2\)Cl\(_2\) ) \(\delta\) 9.01 (d, \(J = 1.5\) Hz, 1H), 7.88-7.82 (m, 2H), 7.74 (d, \(J = 8.4\) Hz, 1H), 7.66 (d, \(J = 8.1\) Hz, 1H), 7.56 (d, \(J = 8.4\) Hz, 1H), 7.51 (d, \(J = 2.1\) Hz, 1H), 7.49 (d, \(J = 2.1\) Hz, 1H), 7.22 (dd, \(J_1 = 7.8\) Hz, \(J_2 = 1.8\) Hz, 1H), 7.00-6.90 (m, 4H), 6.59 (dd, \(J_1 = 8.4\) Hz, \(J_2 = 1.2\) Hz, 1H), 6.15-6.07 (m, 1H), 6.06 (d, \(J = 1.8\) Hz, 1H), 4.44 (dt, \(J_1 = 10.2\) Hz, \(J_2 = 2.4\) Hz, 1H), 3.37 (dd,
$J_1 = 11.4$ Hz, $J_2 = 9.9$ Hz, 1H), 3.00 (dt, $J_1 = 11.7$ Hz, $J_2 = 2.1$ Hz, 1H), 1.50 (s, 9H), 1.20 (s, 9H), 1.01 (s, 9H), 0.97 (s, 9H), 0.90-0.80 (m, 1H), 0.34 (d, $J = 6.9$ Hz, 3H), 0.15 (d, $J = 6.9$ Hz, 3H).

$^1$H NMR (300 MHz, CD$_2$Cl$_2$) $\delta$ 8.86 (d, $J = 1.5$ Hz, 1H), 7.92 (d, $J = 1.5$ Hz, 1H), 7.86 (d, $J = 8.4$ Hz, 1H), 7.79 (d, $J = 8.4$ Hz, 1H), 7.62-7.48 (m, 3H), 7.47 (dd, $J_1 = 8.4$ Hz, $J_2 = 1.8$ Hz 1H), 7.04-6.90 (m, 3H), 6.60-6.53 (m, 2H), 6.31-6.22 (m, 2H), 3.67-3.59 (m, 1H), 2.93 (dd, $J_1 = 11.4$ Hz, $J_2 = 4.8$ Hz, 1H), 2.59 (dd, $J_1 = 11.4$ Hz, $J_2 = 9.6$ Hz, 1H), 1.95-1.83 (m, 1H), 1.28 (s, 9H), 1.17 (s, 9H), 1.05 (s, 9H), 1.01 (s, 9H), 0.94-0.88 (m, 1H), 0.86 (d, $J = 6.9$ Hz, 3H), 0.12 (d, $J = 6.9$ Hz, 3H).

$^1$H NMR (75 MHz, CD$_2$Cl$_2$) $\delta$ 181.3, 180.5, 169.3, 168.2, 153.59, 153.55, 152.7, 152.4, 151.9, 151.7, 151.0, 150.3, 140.3, 139.6, 133.3, 132.4, 132.2, 129.3, 128.4, 128.3, 126.1, 125.5, 124.2, 123.9, 123.7, 122.1, 121.7, 121.2, 119.3, 118.9, 118.4, 117.6, 112.9, 83.3, 35.5, 35.3, 34.7, 34.6, 31.8, 31.4, 31.2, 31.1, 30.1, 21.0, 17.8.

IR (film): $\nu$ (cm$^{-1}$) 3058, 2958, 2966, 1582, 1556, 1523, 1436, 1356, 1288, 1258, 1196, 1147, 1108, 994, 934, 882, 845, 806, 746, 671, 637, 596, 555, 463.

HRMS (APCI, m/z) calcd for C$_{54}$H$_{65}$Ir$_{3}$N$_{3}$O$_{3}$ [M+H]$^+$: 1058.3756, found: 1058.3769.

CD (MeOH): $\lambda$, nm ($\Delta\varepsilon$, M$^{-1}$cm$^{-1}$) 488 (+12), 348 (--48), 325 (+38), 271 (--4), 256 (+7), 245 (+2), 228 (+66), 216 (--96).
CD spectra of complexes (S)-Aux-Λ-Ir2 and (S)-Aux-Δ-Ir2. Recorded in CH3OH (0.2 mM).

**Chiral catalysts Λ-Ir2 and Δ-Ir2**

A suspension of the auxiliary complex (S)-Aux-Λ-Ir2 (150 mg, 0.142 mmol) or (S)-Aux-Δ-Ir2 (150 mg, 0.142 mmol) in MeCN (5.7 ml, 25 mM) was added trifluoroacetic acid (97.2 mg, 0.852 mmol) under argon in the dark. The reaction mixture was concentrated to dryness and dissolved in MeCN. NH4PF6 (462.9 mg, 2.84 mmol) was added to the solution. After stirring for 15 min, the reaction mixture was concentrated to dryness and subjected to a flash silica gel chromatography (CH2Cl2/CH3CN = 100:1 to 30:1) to give the enantiopure catalyst Λ-Ir2 (143.7 mg, 95%) or Δ-Ir2 (146.3 mg, 97%) as a yellow solid. The absolute configurations were verified by CD spectroscopy and confirmed by a crystal structure of Δ-Ir2.

CD (MeOH) for Λ-Ir2: λ, nm (Δε, M⁻¹cm⁻¹) 465 (−12), 363 (+56), 347 (+39), 338 (+47), 293 (−53), 259 (+6), 242 (−35), 236 (−25), 229 (−45), 216 (+216).

CD (MeOH) for Δ-Ir2: λ, nm (Δε, M⁻¹cm⁻¹) 465 (+10), 363 (−44), 348 (−31), 339 (−34), 294 (+44), 259 (−4), 242 (+29), 237 (+20), 229 (+36), 215 (−171).
CD spectra of complexes $\Lambda$-Ir2 and $\Delta$-Ir2. Recorded in CH$_3$OH (0.2 mM).
3. Synthesis of Substrates

2-Acyl imidazoles 1a’, 1a-g and the corresponding Weinreb amides were synthesized according to our recently published procedures (method A).\textsuperscript{4} 2-Acyl imidazole 1h was synthesized according to a reported procedure with some modifications (method B).\textsuperscript{5}

**General procedure for method A.** To a solution of 1-(o-tolyl)-1H-imidazole (1.1 eq.) in THF at −78 °C was added n-BuLi (1.1 eq.) dropwise. The reaction was stirred at −78 °C for 30 min, then stirred at room temperature for 30 min. The corresponding Weinreb amide (1.0 eq. in THF) was added dropwise to the flask after the reaction was cooled back down to −78 °C. The overall concentration of Weinreb amide was 0.4 M. The reaction was allowed to warm to room temperature slowly (over a period of 3-4 h) and stirred overnight. The reaction was quenched with AcOH (6.0 eq.) at room temperature and extracted with EtOAc. The organic layer was washed with aqueous saturated NaHCO\textsubscript{3} and brine. The combined organic layers were dried over anhydrous Na\textsubscript{2}SO\textsubscript{4}, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/hexane = 1:3) to produce 1a-g.

The experimental data of 1a-d, 1f-g are shown below. The other 2-acyl imidazoles (1a\textsuperscript{4}, 1e\textsuperscript{6}) have been reported previously.

**2-Phenyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)ethanone (1a)**

75% yield. A white solid.
$^1$H NMR (300 MHz, CDCl$_3$) δ 7.40-7.16 (m, 9H), 7.15-7.01 (m, 2H), 4.50 (d, $J = 15.3$ Hz, 1H), 4.40 (d, $J = 15.3$ Hz, 1H), 1.90 (s, 3H).

$^{13}$C NMR (75 MHz, CDCl$_3$) δ 188.3, 143.2, 137.7, 134.4, 134.3, 130.6, 129.9, 129.8, 128.9, 128.3, 126.71, 126.67, 126.5, 126.2, 45.3, 16.9.

IR (film): $\nu$ (cm$^{-1}$) 3105, 3030, 2914, 1685, 1592, 1494, 1452, 1390, 1306, 1208, 1147, 1079, 1023, 991, 958, 912, 887, 840, 789, 761, 721, 696, 590, 542, 512, 480, 454.

HRMS (ESI, $m/z$) calcd for C$_{18}$H$_{16}$N$_2$O$_2$Na [M+Na]$^+$: 299.1155, found: 299.1156.

2-(4-Methoxyphenyl)-1-(1-(o-tolyl)-1H-imidazol-2-yl)ethanone (1b)

![Diagram of 2-(4-Methoxyphenyl)-1-(1-(o-tolyl)-1H-imidazol-2-yl)ethanone (1b)]

72% yield. A white solid.

$^1$H NMR (300 MHz, CDCl$_3$) δ 7.40-7.21 (m, 6H), 7.14-7.07 (m, 2H), 6.89-6.80 (m, 2H), 4.45 (d, $J = 15.0$ Hz, 1H), 4.35 (d, $J = 15.6$ Hz, 1H), 3.79 (s, 3H), 1.92 (s, 3H).

$^{13}$C NMR (75 MHz, CDCl$_3$) δ 188.7, 158.6, 143.3, 137.9, 134.5, 130.9, 130.7, 129.8, 129.0, 126.7, 126.5, 126.4, 126.3, 113.9, 55.2, 44.5, 17.0.

IR (film): $\nu$ (cm$^{-1}$) 3158, 3186, 2916, 1668, 1607, 1583, 1509, 1488, 1460, 1447, 1394, 1302, 1261, 1239, 1179, 1146, 1114, 1087, 1057, 1037, 975, 941, 916, 830, 818, 787, 768, 714, 671, 615, 567, 549, 530, 518, 458, 445, 419.

HRMS (ESI, $m/z$) calcd for C$_{19}$H$_{18}$N$_2$O$_2$Na [M+Na]$^+$: 329.1260, found: 329.1263.

2-(4-Chlorophenyl)-1-(1-(o-tolyl)-1H-imidazol-2-yl)ethanone (1c)

![Diagram of 2-(4-Chlorophenyl)-1-(1-(o-tolyl)-1H-imidazol-2-yl)ethanone (1c)]

72% yield. A white solid.
$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.37 (d, $J = 1.0$ Hz, 1H), 7.35-7.31 (m, 1H), 7.30-7.20 (m, 6H), 7.11 (d, $J = 1.0$ Hz, 1H), 7.08 (dd, $J_1 = 7.7$ Hz, $J_2 = 1.4$ Hz, 1H), 4.45 (d, $J = 15.3$ Hz, 1H), 4.36 (d, $J = 15.4$ Hz, 1H), 1.90 (s, 3H).

$^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 187.8, 143.0, 137.7, 134.4, 132.79, 132.75, 131.2, 130.7, 130.0, 129.1, 128.5, 126.9, 126.6, 126.2, 44.7, 17.0.

IR (film): $\nu$ (cm$^{-1}$) 3111, 3029, 2913, 1684, 1591, 1494, 1451, 1392, 1306, 1145, 1079, 1023, 958, 912, 841, 788, 764, 718, 591, 543, 454.

HRMS (ESI, m/z) calcd for C$_{18}$H$_{15}$ClN$_2$O Na$^{+}$: 333.0765, found: 333.0766.

2-(2-Chlorophenyl)-1-(1-(o-tolyl)-1H-imidazol-2-yl)ethanone (1d)

62% yield. A white solid.

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.39 (d, $J = 1.0$ Hz, 1H), 7.37-7.20 (m, 5H), 7.20-7.14 (m, 3H), 7.13 (d, $J = 1.0$ Hz, 1H), 4.77 (d, $J = 17.6$ Hz, 1H), 4.57 (d, $J = 17.7$ Hz, 1H), 1.99 (s, 3H).

$^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 187.0, 143.0, 137.7, 134.7, 134.5, 132.9, 132.1, 130.7, 129.9, 129.3, 129.0, 128.4, 126.6, 126.5, 126.2, 43.6, 17.1.

IR (film): $\nu$ (cm$^{-1}$) 3089, 1683, 1501, 1488, 1472, 1460, 1444, 1400, 1344, 1309, 1150, 1094, 1050, 1032, 963, 948, 915, 811, 802, 787, 766, 751, 717, 692, 678, 598, 573, 554, 535, 504, 459, 448, 436.

HRMS (ESI, m/z) calcd for C$_{18}$H$_{15}$ClN$_2$O Na$^{+}$: 333.0765, found: 333.0766.

1-(1-(o-Tolyl)-1H-imidazol-2-yl)butan-1-one (1f)

93% yield. A white solid.
$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.34-7.15 (m, 4H), 7.07-6.96 (m, 2H), 3.12-2.94 (m, 2H), 1.90 (s, 3H), 1.68-1.52 (m, 2H), 0.88 (t, $J$ = 7.4 Hz, 3H).

$^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 191.4, 143.5, 138.0, 134.4, 130.7, 129.6, 129.0, 126.5, 126.24, 126.17, 40.9, 17.4, 17.1, 13.7.

IR (film): $\nu$ (cm$^{-1}$) 3102, 2961, 2877, 1685, 1457, 1407, 1400, 1301, 1211, 1149, 1025, 967, 886, 766, 699.

HRMS (ESI, $m/z$) calcd for C$_{14}$H$_{17}$N$_2$O $[M+H]^+$: 229.1335, found: 229.1335.

1-(1-(o-Tolyl)-1H-imidazol-2-yl)hexan-1-one (1g)

91% yield. A colorless oil.

$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.43-7.24 (m, 4H), 7.16-7.05 (m, 2H), 3.22-3.04 (m, 2H), 1.99 (s, 3H), 1.70-1.61 (m, 2H), 1.38-1.28 (m, 4H), 0.92-0.84 (m, 3H).

$^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 191.6, 143.5, 138.1, 134.5, 130.7, 129.6, 129.0, 126.5, 126.3, 126.2, 38.9, 31.4, 23.6, 22.4, 17.1, 13.8.

IR (film): $\nu$ (cm$^{-1}$) 3108, 2927, 2862, 1681, 1496, 1452, 1404, 1303, 1141, 1037, 956, 910, 762, 714.

HRMS (ESI, $m/z$) calcd for C$_{16}$H$_{21}$N$_2$O $[M+H]^+$: 257.1648, found: 257.1647.

**Method B:**

Procedure for the preparation of 1h. To a solution of 1-(o-tolyl)-1H-imidazole (948 mg, 6.0 mmol) in THF (15 mL) at $-78 \, ^{\circ}C$ was added $n$-BuLi (2.4 mL, 2.5 M in hexane, 6.0 mmol) dropwise. The reaction was stirred at $-78 \, ^{\circ}C$ for 1 h, then stirred at room temperature for 30 min. The
tert-butyl chloroacetate (1.3 mL, 7.5 mmol) was added at one portion to the flask after the reaction was cooled back down to −78 °C. The reaction was allowed to warm to room temperature slowly (over a period of 3-4 h) and stirred overnight. The reaction was quenched with water at room temperature and extracted with EtOAc. The combined organic layers were dried over anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/hexane = 1:3) to produce S1h (1.0 g, yield: 72%) as a white solid.

To a mixture of S1h (936 mg, 4.0 mmol) and K₂CO₃ (552 mg, 4.0 mmol) in DMF (8.0 mL) at 0 °C were added p-cresol (648 mg, 6.0 mmol). The reaction mixture was stirred at room temperature for overnight. The reaction was quenched with water (8 mL) at room temperature and extracted with DCM (4 × 10 mL). The combined organic layers were dried over anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (EtOAc/hexane = 1:3) to afford 1h (713 mg, yield: 58%) as a white solid.

1-(1-(o-Tolyl)-1H-imidazol-2-yl)-2-(p-tolyloxy)ethanone (1h)

![Structure of 1h](image)

$^1$H NMR (300 MHz, CDCl₃) δ 7.28-7.10 (m, 4H), 7.06-6.98 (m, 2H), 6.94 (d, $J = 8.4$ Hz, 2H), 6.72 (d, $J = 8.7$ Hz, 2H), 5.42 (d, $J = 17.7$ Hz, 1H), 5.31 (d, $J = 17.7$ Hz, 1H), 2.15 (s, 3H), 1.88 (s, 3H).

$^{13}$C NMR (75 MHz, CDCl₃) δ 184.5, 155.9, 141.2, 137.1, 134.4, 130.7, 130.4, 130.1, 129.8, 129.2, 126.7, 126.5, 126.3, 114.4, 69.8, 20.3, 17.0.

IR (film): $\nu$ (cm⁻¹) 3134, 2922, 1697, 1506, 1459, 1424, 1404, 1337, 1295, 1262, 1214, 1178, 1144, 1081, 1013, 946, 911, 822, 803, 787, 771, 720, 704, 678, 561, 536, 508, 459, 448.

4. Iridium-Catalyzed Photoredox Reactions

**General procedure:** A dried 10 mL Schlenk tube was charged with the catalyst \( \Lambda\text{-Ir}2 \) or \( \Delta\text{-Ir}2 \) (2 or 4 mol%), \( \text{NaHCO}_3 \) (25.2 mg, 0.3 mmol, 1.5 equiv) and the corresponding 2-acyl imidazole 1 (0.2 mmol, 1.0 equiv). The tube was purged with nitrogen and MeOH/THF (4:1, 0.5 mL) was added via syringe, followed by \( \text{CnFmI} \). The reaction mixture was degassed via freeze-pump-thaw for three cycles. After the mixture was thoroughly degassed, the vial was sealed and positioned approximately 5 cm from a 21 W compact fluorescent lamp. The reaction was stirred at room temperature for the indicated time (monitored by TLC) under nitrogen atmosphere. Afterwards, the mixture was diluted with \( \text{CH}_2\text{Cl}_2 \) (8 mL). The combined organic layers were concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (hexane/EtOAc = 30:1 to 10:1) to afford the products 3a-n. Racemic samples were obtained by carrying out the reactions with \( \text{rac-Ir}2 \). The enantiomeric excess was determined by chiral HPLC analysis.
(S)-3,3,4,4,5,6,6,6-Nonafluoro-2-phenyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)hexan-1-one (2a)

According to the general procedure, the reaction of 2-acyl imidazole 1a (55.3 mg, 0.20 mmol) and C₄F₉I (415.1 mg, 1.20 mmol) catalyzed by Δ-Ir₂ (4.3 mg, 0.004 mol) gave 2a as a yellow oil (78.3 mg, yield: 79%) after 46 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak AD-H column, ee = 99% (HPLC: AD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, tᵣ (major) = 5.7 min, tᵣ (minor) = 5.0 min). [α]D²² = −134.6° (c 0.4, CH₂Cl₂).

³¹H NMR (300 MHz, CD₂Cl₂) δ 7.59-7.54 (m, 2H), 7.46-6.94 (m, 9H), 6.44-6.27 (m, 1H), 2.00 (s, 3H), 1.62 (s, 3H, other rotamer).

¹³C NMR (75 MHz, CD₂Cl₂) δ 181.6, 142.3, 137.9 (d, J = 3.3 Hz), 135.1 (d, J = 27.5 Hz), 131.2 (d, J = 5.9 Hz), 131.1, 131.0 (d, J = 3.5 Hz), 129.7 (d, J = 3.9 Hz), 129.3 (d, J = 12.5 Hz), 129.2, 128.7 (d, J = 9.6 Hz), 127.1 (d, J = 9.7 Hz), 126.6 (d, J = 21.6 Hz), 52.4-51.6 (m), 16.9 (d, J = 15.4 Hz).

¹⁹F NMR (282 MHz, CD₂Cl₂) δ −81.92 - −82.44 (m, 3F), −110.84 - −115.21 (m, 2F), −121.21-−122.07 (m, 2F), −125.66 - −128.36 (m, 2F).

IR (film): ν (cm⁻¹) 3115, 3067, 3036, 2978, 1694, 1497, 1456, 1401, 1350, 1214, 1129, 1026, 971, 866, 813, 763, 739, 707, 645, 578, 550, 525, 455.


(S)-3,3,4,4,5,6,6,7,7,8,8,8-Tridecafluoro-2-phenyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)octan-1-one (3a)

According to the general procedure, the reaction of 2-acyl imidazole 1a (55.3 mg, 0.20 mmol) and C₆F₁₃I (535.2 mg, 1.20 mmol) catalyzed by Δ-Ir₂ (4.3 mg, 0.004 mol) gave 3a as a yellow oil (103.5 mg, yield: 87%) after 46 hours. Enantiomeric excess established by HPLC analysis using a
Chiralpak AD-H column, ee = 99% (HPLC: AD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, t_r (major) = 4.2 min, t_r (minor) = 4.7 min). [α]_D^22 = −100.9° (c 0.3, CH₂Cl₂).

^1H NMR (300 MHz, CD₂Cl₂) δ 7.59-7.51 (m, 2H), 7.46-6.93 (m, 9H), 6.42-6.24 (m, 1H), 1.99 (s, 3H), 1.67 (s, 3H, other rotamer).

^13C NMR (75 MHz, CD₂Cl₂) δ 181.6, 142.9 (d, J = 3.6 Hz), 137.9 (d, J = 2.6 Hz), 135.1 (d, J = 27.0 Hz), 131.2 (d, J = 7.6 Hz), 131.1, 131.0 (d, J = 4.3 Hz), 129.7 (d, J = 3.5 Hz), 129.3 (d, J = 11.7 Hz), 129.2, 128.7 (d, J = 9.2 Hz), 127.1 (d, J = 9.5 Hz), 126.7 (d, J = 21.8 Hz), 52.6-51.8 (m), 16.9 (d, J = 9.1 Hz).

^19F NMR (282 MHz, CD₂Cl₂) δ −81.97 - −82.11 (m, 3F), −110.62 - −114.90 (m, 2F), −120.62 - −120.94 (m, 2F), −122.43 - −123.11 (m, 2F), −123.57 - −124.12 (m, 2F), −126.98 - −127.43 (m, 2F).

IR (film): ν (cm⁻¹) 3068, 3037, 2973, 1695, 1497, 1457, 1401, 1234, 1196, 1142, 1027, 975, 910, 862, 810, 766, 736, 703, 633, 527, 454.

HRMS (FD, m/z) calcd for C_{37}H_{15}F_{13}N₂O [M]^+: 594.0977, found: 594.0992.

(R)-3,3,4,4,5,6,7,8,8,8- Tridecafluoro-2-(4-methoxyphenyl)-1-(1-(o-toly)-1H-imidazol-2-yl)octan-1-one (3b)

According to the general procedure, the reaction of 2-acyl imidazole 1b (61.3 mg, 0.20 mmol) and C₆F₁₃I (535.2 mg, 1.20 mmol) catalyzed by Λ-Ir2 (4.3 mg, 0.004 mol) gave 3b as a yellow oil (111.8 mg, yield: 90%) after 48 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak AD-H column, ee = 99% (HPLC: AD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, t_r (major) = 4.4 min, t_r (minor) = 5.4 min). [α]_D^22 = −123.5° (c 1.1, CH₂Cl₂).

^1H NMR (300 MHz, CD₂Cl₂) δ 7.52-6.85 (m, 10H), 6.37-6.18 (m, 1H), 3.78 (s, 3H), 1.99 (s, 3H), 1.64 (s, 3H, other rotamer).

^13C NMR (75 MHz, CD₂Cl₂) δ 181.9 (d, J = 4.2 Hz), 160.8, 143.1-142.9 (m), 138.1, 135.2 (d, J = 28.6 Hz), 132.4, 131.2 (d, J = 6.1 Hz), 130.9 (d, J = 2.1 Hz), 129.7 (d, J = 3.5 Hz), 128.6 (d, J = 7.8 Hz), 127.1 (d, J = 9.5 Hz), 126.7 (d, J = 21.6 Hz), 121.4 (d, J = 3.4 Hz), 114.7, 55.6, 51.8-51.1 (m), 594.0992.
According to the general procedure, the reaction of 2-acyl imidazole 1c (62.2 mg, 0.20 mmol) and C₆F₁₃I (535.2 mg, 1.20 mmol) catalyzed by Λ-Ir2 (4.3 mg, 0.004 mol) gave 3c as a yellow oil (78.6 mg, yield: 63%) after 72 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak AD-H column, ee = 96% (HPLC: AD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, tᵣ (major) = 4.2 min, tᵣ (minor) = 4.9 min). [α]D²² = −96.9° (c 0.9, CH₂Cl₂).

³¹P NMR (300 MHz, CD₂Cl₂) δ 7.57-7.50 (m, 2H), 7.48-6.95 (m, 8H), 6.44-6.26 (m, 1H), 1.99 (s, 3H), 1.65 (s, 3H, other rotamer).

¹³C NMR (75 MHz, CD₂Cl₂, mixture of rotamers) δ 181.3, 142.7, 137.8 (d, J = 2.9 Hz), 135.6 (d, J = 1.7 Hz), 135.1, 135.0 (d, J = 29.0 Hz), 132.5, 132.2, 131.3, 131.2, 131.1, 129.9, 129.8, 129.7, 129.5, 129.4, 129.0, 128.9, 128.6, 128.3, 127.2, 127.1, 127.0, 126.8, 126.5, 51.7-51.0 (m), 16.9 (d, J = 4.8 Hz).

¹⁹F NMR (282 MHz, CD₂Cl₂) δ −81.03 - −81.32 (m, 3F), −109.92 - −114.91 (m, 2F), −119.69 - −120.19 (m, 2F), −121.45 - −122.62 (m, 2F), −122.81 - −123.43 (m, 2F), −126.11 - −126.65 (m, 2F).

IR (film): v (cm⁻¹) 3116, 2964, 2928, 2860, 1694, 1610, 1494, 1456, 1400, 1309, 1233, 1196, 1142, 1055, 1021, 976, 859, 769, 714, 657, 552, 452.

According to the general procedure, the reaction of 2-acyl imidazole 1d (62.2 mg, 0.20 mmol) and C₆F₁₃I (535.2 mg, 1.20 mmol) catalyzed by Λ-Ir₂ (4.3 mg, 0.004 mol) gave 3d as a yellow oil (93.1 mg, yield: 74%) after 72 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OD-H column, ee = 98% (HPLC: OD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, tᵣ (major) = 6.9 min, tᵣ (minor) = 6.3 min). [α]D²² = −152.6 (c 1.0, CH₂Cl₂).

¹H NMR (300 MHz, CD₂Cl₂) δ 7.74-7.67 (m, 1H), 7.52-6.94 (m, 10H), 2.00 (s, 3H), 1.69 (s, 3H, other rotamer).

¹³C NMR (75 MHz, CD₂Cl₂) δ 181.4-181.1 (m), 143.1 (d, J = 2.8 Hz), 137.9 (d, J = 2.6 Hz), 136.5 (d, J = 4.1 Hz), 135.1 (d, J = 35.6 Hz), 131.7 (d, J = 10.8 Hz), 131.3 (d, J = 2.6 Hz), 131.2 (d, J = 5.2 Hz), 130.7 (d, J = 3.9 Hz), 130.5 (d, J = 7.4 Hz), 129.7 (d, J = 2.0 Hz), 129.0 (d, J = 7.5 Hz), 127.6 (d, J = 2.2 Hz), 127.4 (d, J = 4.7 Hz), 127.1 (d, J = 11.9 Hz), 126.7 (d, J = 23.7 Hz), 47.8-46.8 (m), 16.9.

⁹F NMR (282 MHz, CD₂Cl₂) δ −80.95 - −81.40 (m, 3F), −109.16 - −114.44 (m, 2F), −119.23 - −121.05 (m, 2F), −121.58 - −122.31 (m, 2F), −122.82 - −123.38 (m, 2F), −126.17 - −126.74 (m, 2F).

IR (film): ν (cm⁻¹) 3070, 2978, 2930, 1694, 1496, 1459, 1401, 1353, 1311, 1233, 1196, 1141, 1029, 974, 865, 812, 754, 709, 653, 547.

HRMS (FD, m/z) calcd for C₂₄H₁₄ClF₁₃N₂O [M⁺]: 628.0587, found: 628.0614.

(R)-2-(2-Chlorophenyl)-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-(1-(o-tolyl)-1H-imidazol-2-yl)octan-1-one (3e)

According to the general procedure, the reaction of 2-acyl imidazole 1e (42.9 mg, 0.20 mmol) and
C₆F₁₃I (535.2 mg, 1.20 mmol) catalyzed by Λ-Ir₂ (8.6 mg, 0.008 mol) gave 3e as a yellow oil (86.0 mg, yield: 82%) after 24 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OJ-H column, ee = 97% (HPLC: OJ-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1.0 mL/min, 25 °C, tᵣ (major) = 4.4 min, tᵣ (minor) = 7.0 min). [α]D²² = −1.5° (c 1.1, CH₂Cl₂).

¹H NMR (300 MHz, CD₂Cl₂) δ 7.46-7.26 (m, 4H), 7.22-7.08 (m, 2H), 5.23-5.05 (m, 1H), 1.99 (s, 3H), 1.94 (s, 3H, other rotamer), 1.41 (t, J = 7.4 Hz, 3H).

¹³C NMR (75 MHz, CD₂Cl₂) δ 185.2, 143.1, 138.1 (d, J = 5.1 Hz), 135.2 (d, J = 22.7 Hz), 131.2 (d, J = 5.0 Hz), 130.9 (d, J = 4.4 Hz), 129.7, 128.6 (d, J = 6.1 Hz), 127.1 (d, J = 13.3 Hz), 126.8 (d, J = 8.0 Hz), 42.2-41.5 (m), 17.1 (d, J = 30.3 Hz) 11.3 (d, J = 5.1 Hz).

¹⁹F NMR (282 MHz, CD₂Cl₂) δ −81.15 (t, J = 9.7 Hz, 3F), −113.35 - -116.35 (m, 2F), −120.38 - -121.25 (m, 2F), −121.65 - -122.30 (m, 2F), −122.75 - -123.35 (m, 2F), −126.05 - -126.50 (m, 2F).

IR (film): ν (cm⁻¹) 2925, 2859, 1693, 1497, 1457, 1404, 1351, 1309, 1234, 1197, 1143, 1018, 948, 905, 766, 704, 626, 529, 465.


(R)-2-Ethyl-3,3,4,4,5,5,6,6,7,7,8,8-tridecafluoro-1-(1-(o-tolyl)-1H-imidazol-2-yl)octan-1-one (3f)

According to the general procedure, the reaction of 2-acyl imidazole 1f (45.7 mg, 0.20 mmol) and C₆F₁₃I (535.2 mg, 1.20 mmol) catalyzed by Λ-Ir₂ (8.6 mg, 0.008 mol) gave 3f as a yellow oil (64.3 mg, yield: 59%) after 62 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OD-H column, ee = 99% (HPLC: OD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1.0 mL/min, 25 °C, tᵣ (major) = 4.5 min, tᵣ (minor) = 4.9 min). [α]D²² = −22.1° (c 0.8, CH₂Cl₂).

¹H NMR (300 MHz, CD₂Cl₂) δ 7.46-7.24 (m, 4H), 7.22-7.18 (m, 1H), 7.17-7.06 (m, 1H), 5.15-4.96 (m, 1H), 2.04-1.90 (m, 2H), 1.99 (s, 3H), 1.94 (s, 3H, other rotamer), 0.92 (q, J = 8.0 Hz, 3H).

¹³C NMR (75 MHz, CD₂Cl₂) δ 185.2, 144.3, 138.2 (d, J = 3.4 Hz), 135.2 (d, J = 21.6 Hz), 131.2 (d, J = 9.0 Hz), 131.0 (d, J = 3.5 Hz), 129.7, 128.6, 127.0 (d, J = 11.6 Hz), 126.8 (d, J = 8.0 Hz), S20
48.5-47.8 (m), 20.2-20.0 (m), 17.1 (d, J = 34.5 Hz) 11.6 (d, J = 5.4 Hz).

19F NMR (282 MHz, CD2Cl2) δ –81.89 (t, J = 9.7 Hz, 3F), –113.45 - -115.64 (m, 2F), –120.38 - -121.25 (m, 2F), –121.65 - -122.30 (m, 2F), –122.75 - -123.35 (m, 2F), –126.75 - -126.45 (m, 2F).

IR (film): ν (cm⁻¹) 2928, 2861, 1691, 1498, 1457, 1405, 1317, 1233, 1197, 1142, 1053, 904, 766, 740, 714, 647, 531, 459.


(R)-2-Butyl-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-(1-(o-tolyl)-1H-imidazol-2-yl)octan-1-one (3g)

According to the general procedure, the reaction of 2-acyl imidazole 1g (51.3 mg, 0.20 mmol) and C₆F₁₃I (535.2 mg, 1.20 mmol) catalyzed by Λ-Ir2 (8.6 mg, 0.008 mol) gave 3g as a yellow oil (70.2 mg, yield: 61%) after 72 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OD-H column, ee = 98% (HPLC: OD-H, 254 nm, hexane/isopropanol = 99.5:0.5, flow rate 0.5 mL/min, 25 °C, tₘ (major) = 13.5 min, tᵢ (minor) = 14.5 min). [α]D²² = −34.5° (c 0.4, CH₂Cl₂).

1H NMR (300 MHz, CD₂Cl₂) δ 7.46-7.25 (m, 4H), 7.22-7.07 (m, 2H), 5.22-5.03 (m, 1H), 2.03-1.82 (m, 2H), 1.99 (s, 3H), 1.94 (s, 3H, other rotamer), 1.45-1.15 (m, 4H), 0.85 (t, J = 7.1 Hz, 3H).

13C NMR (75 MHz, CD₂Cl₂) δ 185.3, 144.2, 138.1 (d, J = 3.8 Hz), 135.2 (d, J = 24.5 Hz), 131.2 (d, J = 8.4 Hz), 131.0 (d, J = 2.8 Hz), 129.7, 128.6 (d, J = 1.6 Hz), 127.0 (d, J = 12.4 Hz), 126.8 (d, J = 8.6 Hz), 47.1-46.4 (m), 29.4 (d, J = 9.4 Hz), 26.4-26.2 (m), 22.9 (d, J = 1.2 Hz), 17.1 (d, J = 34.2 Hz) 13.8.

19F NMR (282 MHz, CD₂Cl₂) δ –81.30 (t, J = 9.9 Hz, 3F), –110.60 - -115.40 (m, 2F), –119.38 - -121.25 (m, 2F), –121.65 - -122.40 (m, 2F), –122.75 - -123.35 (m, 2F), –126.20 - -126.65 (m, 2F).

IR (film): ν (cm⁻¹) 2961, 2930, 2869, 1691, 1498, 1457, 1405, 1234, 1197, 1142, 1053, 904, 766, 716, 644, 531.

HRMS (FD, m/z) calcd for C₂₂H₁₀F₁₃N₂O [M]⁺: 574.1290, found: 574.1263.
(R)-3,3,4,4,5,6,6,7,7,8,8,8-Tridecafluoro-1-(1-(o-tolyl)-1H-imidazol-2-yl)-2-(p-tolylxyloxy)octan-1-one (3h)

According to the general procedure, the reaction of 2-acyl imidazole 1h (61.3 mg, 0.20 mmol) and C₆F₁₃I (535.2 mg, 1.20 mmol) gave 3h as a yellow oil (78.1 mg, yield: 62%) after 62 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak AD-H column, ee = 98% (HPLC: AD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, tᵢ (major) = 6.0 min, tᵢ (minor) = 5.0 min). [α]D²² = −30.6° (c 1.0, CH₂Cl₂).

¹H NMR (300 MHz, CD₂Cl₂) δ 7.49-7.26 (m, 5H), 7.22-7.03 (m, 3H), 6.97-6.84 (m, 3H), 2.27 (s, 3H), 1.949 (s, 3H), 1.87 (s, 3H, other rotamer).

¹³C NMR (75 MHz, CD₂Cl₂) δ 180.3, 154.6, 143.2, 137.3, 135.3, 134.9, 132.9, 132.1, 131.8, 131.4, 131.3, 131.2, 130.6, 130.0, 129.9, 129.0, 128.2, 127.2, 127.03, 126.98, 126.9, 126.7, 118.0, 115.7, 73.5, 37.6, 32.4, 30.5, 30.2, 29.9, 27.6, 23.2, 20.6, 17.2, 16.8, 14.3.

¹⁹F NMR (282 MHz, CD₂Cl₂) δ −81.65 - −82.65 (m, 3F), −115.20 - −118.05 (m, 2F), −121.50 - −124.90 (m, 6F), −125.90 - −128.45 (m, 2F).

IR (film): ν (cm⁻¹) 3118, 3035, 2928, 2865, 1702, 1610, 1506, 1456, 1403, 1315, 1197, 1144, 902, 812, 766, 714, 525.

HRMS (FD, m/z) calcd for C₂₅H₁₇F₁₃N₂O₂ [M⁺]: 624.1082, found: 624.1103.

(R)-3,3,3-Trifluoro-2-phenyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)propan-1-one (3i)

According to the general procedure, the reaction of 2-acyl imidazole 1a (53.3 mg, 0.20 mmol) and trifluoriodomethane (391.8 mg, 2.00 mmol) catalyzed by Λ-Ir2 (4.3 mg, 0.004 mol) gave 3i as a yellow oil (29.8 mg, yield: 43%) after 44 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak IC column, ee = 93% (HPLC: IC, 254 nm, hexane/isopropanol = 99:1, flow rate 1...
mL/min, 25 °C, t<sub>r</sub> (major) = 6.1 min, t<sub>r</sub> (minor) = 5.7 min). [α]<sub>D</sub><sup>22</sup> = −303.0° (c 0.4, CH<sub>2</sub>Cl<sub>2</sub>).

1H NMR (300 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 7.54-7.47 (m, 2H), 7.46-6.97 (m, 9H), 6.17-6.04 (m, 1H), 2.03 (s, 3H), 1.70 (s, 3H, other rotamer).

13C NMR (75 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 182.1, 137.9, 135.2, 134.9, 131.3, 131.2, 131.0, 130.5, 130.3, 129.7, 129.4, 129.3, 128.9, 128.5, 127.1, 127.0, 126.9, 126.8, 126.5, 123.0, 56.2-55.2 (m), 17.1 (d, J = 20.8 Hz).

19F NMR (282 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ –67.33 (d, J = 7.9 Hz, 3F).

IR (film): ν (cm<sup>−1</sup>) 3114, 3065, 3035, 2963, 2928, 1692, 1497, 1455, 1402, 1328, 1257, 1153, 1120, 1027, 976, 861, 822, 764, 739, 698, 674, 588, 522, 455.

HRMS (FD, m/z) calcd for C<sub>19</sub>H<sub>15</sub>F<sub>3</sub>N<sub>2</sub>O [M]: 344.1137, found: 344.1120.

(R)-3,3,4,4,5,5,5-Heptafluoro-2-methyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)pentan-1-one (3j)

![Chemical Structure]

According to the general procedure, the reaction of 2-acyl imidazole 1e (42.9 mg, 0.20 mmol) and 1,1,1,2,2,3,3-heptafluoro-3-iodopropane (355.1 mg, 1.20 mmol) catalyzed by Λ-Ir<sub>2</sub> (4.3 mg, 0.004 mmol) gave 3j as a yellow oil (40.7 mg, yield: 53%) after 45 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OJ-H column, ee = 95% (HPLC: OJ-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, t<sub>r</sub> (major) = 14.6 min, t<sub>r</sub> (minor) = 20.6 min). [α]<sub>D</sub><sup>22</sup> = −11.5° (c 0.5, CH<sub>2</sub>Cl<sub>2</sub>).

1H NMR (300 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 7.45-7.25 (m, 4H), 7.22-7.08 (m, 2H), 5.20-5.02 (m, 1H), 1.93 (s, 3H), 1.93 (s, 3H, other rotamer), 1.40 (t, J = 7.4 Hz, 3H).

13C NMR (75 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 185.1, 142.9, 138.0 (d, J = 5.3 Hz), 135.1 (d, J = 23.2 Hz), 131.1 (d, J = 4.2 Hz), 130.8 (d, J = 5.1 Hz), 129.6, 128.6 (d, J = 5.7 Hz), 127.0 (d, J = 13.3 Hz), 126.7 (d, J = 8.6 Hz), 41.9-41.1 (m), 17.0 (d, J = 27.1 Hz), 11.2 (d, J = 5.0 Hz).

19F NMR (282 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ –80.47 - –81.47 (td, J<sub>2</sub> = 11.0 Hz, J<sub>2</sub> = 1.7 Hz, 3F), –114.45 - –117.36 (m, 2F), –125.09 - –125.36 (m, 2F).

IR (film): ν (cm<sup>−1</sup>) 3114, 2924, 2855, 1693, 1497, 1457, 1404, 1346, 1306, 1222, 1180, 1116, 1070, 1008, 949, 914, 762, 711, 672, 631, 535, 453.
HRMS (FD, m/z) calcd for C_{16}H_{15}F_{2}N_{2}O [M]^+: 382.0916, found: 382.0904.

(R)-3,3,4,4,5,5,6,6,6-Nonafluoro-2-methyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)hexan-1-one (3k)

According to the general procedure, the reaction of 2-acyl imidazole 1e (42.9 mg, 0.20 mmol) and 1,1,2,2,3,3,4,4,4-nonafluoro-4-iodobutane (345.9 mg, 1.20 mmol) catalyzed by Λ-Ir2 (4.3 mg, 0.004 mol) gave 3k as a yellow oil (42.2 mg, yield: 49%) after 24 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OJ-H column, ee = 95% (HPLC: OJ-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, t_r (major) = 14.6 min, t_r (minor) = 20.6 min). [α]_D^{22} = -4.5° (c 0.5, CH_2Cl_2).

{^1}H NMR (300 MHz, CD_2Cl_2) δ 7.45-7.26 (m, 4H), 7.18-7.08 (m, 2H), 5.22-5.04 (m, 1H), 1.98 (s, 3H), 1.93 (s, 3H, other rotamer), 1.40 (t, J = 7.4 Hz, 3H).
{^{13}}C NMR (75 MHz, CD_2Cl_2) δ 185.1, 143.0, 138.1 (d, J = 4.7 Hz), 135.1 (d, J = 23.9 Hz), 131.2 (d, J = 5.0 Hz), 130.9 (d, J = 4.6 Hz), 129.7, 128.6 (d, J = 5.2 Hz), 127.0 (d, J = 13.9 Hz), 125.7 (d, J = 7.6 Hz), 42.1-41.2 (m), 17.0 (d, J = 29.1 Hz), 11.2 (d, J = 5.3 Hz).
{^{19}}F NMR (282 MHz, CD_2Cl_2) δ -80.47 - -81.47 (m, 3F), -113.64 - -116.76 (m, 2F), -121.07 - -122.98 (m, 2F), -125.06 - -127.62 (m, 2F).
IR (film): ν (cm⁻¹) 3116, 2956,2928, 1693, 1497, 1458, 1405, 1346, 1307, 1212, 1131, 1016, 946, 907, 874, 840, 762, 712, 527, 458.
HRMS (FD, m/z) calcd for C_{17}H_{15}F_{6}N_{2}O [M]^+: 432.0884 found: 432.0883.

(R)-3,3,4,4,5,5,6,6,6,7,7,7,8,8,8,9,9,10,10-Heptadecafluoro-2-methyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)decan-1-one (3l)

According to the general procedure, the reaction of 2-acyl imidazole 1e (42.9 mg, 0.20 mmol) and
1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-8-iodooctane (655.0 mg, 1.20 mmol) catalyzed by Δ-Ir2 (4.3 mg, 0.004 mol) gave 3l as a yellow oil (80.0 mg, yield: 63%) after 24 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OJ-H column, ee = 95% (HPLC: OJ-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, tR(major) = 4.2 min, tR(minor) = 6.1 min). \([\alpha]D^{22} = +2.5^\circ\text{ (c 0.9, CH}_2\text{Cl}_2)\).

\(^1\)H NMR (300 MHz, CD\(_2\)Cl\(_2\)) \(\delta\) 7.45-7.25 (m, 4H), 7.22-7.08 (m, 2H), 5.22-5.04 (m, 1H), 1.98 (s, 3H), 1.93 (s, 3H, other rotamer), 1.41 (t, \(J = 7.4\) Hz, 3H).

\(^13\)C NMR (75 MHz, CD\(_2\)Cl\(_2\)) \(\delta\) 185.1, 143.0, 138.1 (d, \(J = 5.7\) Hz), 135.1 (d, \(J = 22.8\) Hz), 131.2 (d, \(J = 4.3\) Hz), 130.9 (d, \(J = 5.0\) Hz), 129.7, 128.6 (d, \(J = 5.9\) Hz), 127.0 (d, \(J = 13.4\) Hz), 126.7 (d, \(J = 7.8\) Hz), 42.2-41.4 (m), 17.0 (d, \(J = 31.4\) Hz), 11.3 (d, \(J = 5.7\) Hz).

\(^19\)F NMR (282 MHz, CD\(_2\)Cl\(_2\)) \(\delta\) –88.14 - –88.33 (m, 3F), –113.41 - –116.53 (m, 2F), –119.37 - –121.79 (m, 2F), –121.66 - –123.68 (m, 6F), –122.75 - –123.19 (m, 2F), –126.15 - –126.58 (m, 2F).

IR (film): \(\nu\) (cm\(^{-1}\)) 3115, 2924, 2854, 1694, 1498, 1458, 1405, 1202, 1144, 1011, 950, 908, 766, 708, 652, 529, 459.

HRMS (FD, \(m/z\) calcd for C\(_{21}\)H\(_13\)F\(_7\)N\(_2\)O [M]\(^+\): 632.0756, found: 632.0785.

\((S)-3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-Henicosafluoro-2-methyl-1-(1-(o-tolyl)-1H-imidazol-2-yl)dodecan-1-one\) (3m)

According to the general procedure, the reaction of 2-acyl imidazole 1e (42.9 mg, 0.20 mmol) and 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-henicosafluoro-10-iododecane (775.2 mg, 1.20 mmol) catalyzed by Δ-Ir2 (8.6 mg, 0.008 mol) in MeOH/THF (0.8mL/0.2mL) gave 3m as a yellow solid (75.1 mg, yield: 51%) after 44 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OJ-H column, ee = 95% (HPLC: OJ-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, tR(major) = 5.4 min, tR(minor) = 3.8 min). \([\alpha]D^{22} = +4.6^\circ\text{ (c 0.8, CH}_2\text{Cl}_2)\).

\(^1\)H NMR (300 MHz, CD\(_2\)Cl\(_2\)) \(\delta\) 7.45-7.26 (m, 4H), 7.22-7.07 (m, 2H), 5.22-5.05 (m, 1H), 1.98 (s, 3H), 1.93 (s, 3H, other rotamer), 1.41 (t, \(J = 7.2\) Hz, 3H).

\(^13\)C NMR (75 MHz, CD\(_2\)Cl\(_2\)) \(\delta\) 185.2, 143.0, 138.1 (d, \(J = 4.7\) Hz), 135.1 (d, \(J = 23.5\) Hz), 131.2 (d,
Enantiomeric, the reaction of 9H-imidazol-1-yl)propan-1-one (3n)

According to the general procedure, the reaction of 2-acyl imidazole 1e (42.9 mg, 0.20 mmol) and 1-(difluoriodomethyl)-2,3,4,5,6-pentafluorobenzene (413.0 mg, 1.20 mmol) catalyzed by \( \Lambda\text{-Ir} \)} (4.3 mg, 0.004 mol) gave 3n as a yellow oil (80.0 mg, yield: 93%) after 15 hours. Enantiomeric excess established by HPLC analysis using a Chiralpak OD-H column, ee > 99.5% (HPLC: OD-H, 254 nm, hexane/isopropanol = 99:1, flow rate 1 mL/min, 25 °C, \( t_r \) (major) = 8.6 min, \( t_r \) (minor) = 9.5 min). \( [\alpha]_D^{22} = +70.6^\circ \) (c 0.9, CH2Cl2).

\(^1\)H NMR (300 MHz, CD2Cl2) \( \delta \) 7.44-7.22 (m, 4H), 7.16-7.02 (m, 2H), 5.16-4.98 (m, 1H), 1.95 (s, 3H), 1.89 (s, 3H, other rotamer), 1.39 (t, \( J = 6.9 \) Hz, 3H).

\(^{13}\)C NMR (75 MHz, CD2Cl2) \( \delta \) 186.6, 143.1, 138.0 (d, \( J = 5.9 \) Hz), 131.1 (d, \( J = 8.4 \) Hz), 130.7, 138.0 (d, \( J = 3.9 \) Hz), 129.6, 128.3 (d, \( J = 12.4 \) Hz), 127.0 (d, \( J = 10.7 \) Hz), 126.6 (d, \( J = 7.1 \) Hz), 49.0-47.9 (m), 17.0 (d, \( J = 37.3 \) Hz), 11.0 (dt, \( J_1 = 20.1, J_2 = 4.6 \) Hz).

\(^{19}\)F NMR (282 MHz, CD2Cl2) \( \delta \) –87.75 - –93.05 (m, 1F), –95.75 - –98.85 (m, 1F), –137.40 - –141.55 (m, 2F), –150.60 - –152.70 (m, 1F), –160.45 - –163.80 (m, 2F).

IR (film): \( \nu \) (cm\(^{-1}\)) 3117, 2926, 2891, 1688, 1654, 1498, 1457, 1402, 1336, 1190, 1084, 988, 943, 908, 832, 764, 710, 546, 458.

HRMS (FD, \( m/z \)) calcd for C20H13F7N2O [M]+: 430.0916, found: 430.0920.
5. Enantioselectivities as Determined by Chiral HPLC

Enantiomeric purities of the reaction products were determined with a Daicel Chiralpak AD-H, OD-H, OJ-H or IC (250 × 4.6 mm) HPLC column on an Agilent 1200 or 1260 Series HPLC System using hexane/isopropanol as a mobile phase. The column temperature was 25 °C and UV-absorption was measured at 254 nm.

![HPLC traces of rac-2a (reference) and (S)-2a](image)

**Figure S1.** HPLC traces of rac-2a (reference) and (S)-2a
Figure S2. HPLC traces of rac-3a (reference) and (S)-3a.
Figure S3. HPLC traces of rac-3b (reference) and (R)-3b.
**Figure S4.** HPLC traces of rac-3c (reference) and (R)-3c.
Figure S5. HPLC traces of rac-3d (reference) and (R)-3d.
Figure S6. HPLC traces of rac-3e (reference) and (R)-3e.

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Totals: 886.30118 58.33996
Figure S7. HPLC traces of rac-3f (reference) and (R)-3f.

Signal 1: VWD1 A, Wavelength=254 nm

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Totals: 793.01934 106.93971
**Figure S8.** HPLC traces of rac-3g (reference) and (R)-3g.
Figure S9. HPLC traces of rac-3h (reference) and (R)-3h.

Signal 1: VWD1 A, Wavelength=254 nm

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Figure S10. HPLC traces of rac-3i (reference) and (R)-3i.

93% ee
Figure S11. HPLC traces of rac-3j (reference) and (R)-3j.
Figure S12. HPLC traces of rac-3k (reference) and (R)-3k.
Figure S13. HPLC traces of rac-3l (reference) and (R)-3l.

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type Width Area Height Area
# [min] [min] mAU *s [mAU] %
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1  4.177 MM  0.3480 2819.94385 135.04567  97.3051
2  6.123 MM  0.5946  78.09837  2.18894  2.6949

Totals: 2898.04221 137.23461
**Figure S14.** HPLC traces of rac-3m (reference) and (S)-3m.
Figure S15. HPLC traces of rac-3n (reference) and (R)-3n

> 99.5% ee
6. Single-Crystal X-Ray Diffraction Study

Single crystals of Δ-Ir2 suitable for X-ray diffraction were obtained by slow diffusion from a solution of Δ-Ir2 (20 mg) in toluene (2.0 mL) layered with n-hexane (0.5 mL) at room temperature for several days in a glass tube.

X-ray data were collected with a Bruker 3 circuit D8 Quest diffractometer with MoKa radiation (microfocus tube with multilayer optics) and Photon 100 CMOS detector at 110 K. Scaling and absorption correction was performed by using the SADABS software package of Bruker. Structures were solved using direct methods in SHELXS or SHELXT and refined using the full matrix least squares procedure in SHELXL-2014. The hydrogen atoms were placed in calculated positions and refined as riding on their respective C atom, and Uiso(H) was set at 1.2 Ueq(Csp2) and 1.5 Ueq(Csp3). The absolute configurations of compound Δ-Ir2 has been determined. Crystal data and details of the structure determination are presented in the Supplementary Table S1.

Figure S16. Crystal structure of Δ-Ir2. ORTEP drawing with 30% probability thermal ellipsoids.
Table S1. Crystal data and structure refinement for test_0m.

Crystal data

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7. References


7. SADABS, Bruker AXS Inc., Madison, Wisconsin, USA, **2014**.

8. Sheldrick, G. M. *SHELXT*, Universität Göttin gen, Göttingen, Germany, **2014**.

9. Sheldrick, G. M. *SHELXL*, Universität Göttin gen, Göttingen, Germany, **2014**.

10. APEX2, Bruker AXS Inc., Madison, Wisconsin, USA, **2014**.

11. SAINT, Bruker AXS Inc., Madison, Wisconsin, USA, **2013**.


14. Brandenburg, K. *Diamond - Crystal and Molecular Structure Visualization*, Crystal Impact - Dr. H. Putz & Dr. K. Brandenburg GbR, Bonn, Germany, **2014**.