Supporting Information

Reductive Cross-Coupling of α-Oxy Halides Enabled by Thermal Catalysis, Photocatalysis, Electrocatalysis, or Mechanochemistry

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1. General Information

Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents for chromatography were HPLC grade. Anhydrous and degassed DMA used in reactions was purchased from Sigma-Aldrich in Sure/Seal™ bottle. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with F-254 indicator, visualized by irradiation with UV light. Column chromatography was performed on silica gel (particle size 0.043–0.063 mm) by using Interchim PuriFlash® 430 automatic purification system. $^1$H-NMR and $^{13}$C-NMR were recorded on Bruker DRX-500 and AMX-400 instruments in CDCl$_3$ and are reported relative to the solvent residual peaks. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s (singlet), bs (broad singlet), d (doublet), t (triplet), m (multiplet); coupling constants (J) are in Hertz (Hz). Mass spectra (EI-MS, 70 eV) were conducted on a Agilent 7890 gas chromatograph equipped with 5975C EI-MSD Triple-Axis Detector using DB5MS and HP5MS columns. HRMS analysis was performed using a Thermo LTQ Velos Orbitrap mass spectrometer (Thermo Scientific, Pittsburgh, PA, USA) equipped with an ESI source. Cyclic voltammetry (CV) was performed on BioLogic Potentiostat SP-50. Luminescence intensities were recorded using a fluoromax-4 spectrophotometer from Horiba Scientific. For the electrocatalyzed reactions at constant current modes, Matsusada R4K36-0.1-L(230V) was used as power supply. For the photoredox catalyzed reactions, Kessil PR160-440nm blue LED lamp was used as light source. For the ball milling reactions, Retsch Mixer Mill MM400 was used as the ball mill.

2. General Procedure

2.1 General procedure for the synthesis of acyl iodides and α-oxy halides:$^{[1]}$

**Acyl iodides:** A round-bottom flask was charged with a magnetic stir bar and sodium iodide (1.1 equiv.), the corresponding acyl chloride (1.0 equiv.) was added at 0 °C. Then the reaction was warmed up to room temperature and stirred for 2 hours. The mixture was then filtered to remove salts. The product was purified by distillation or used directly for the next step.

**α-oxy iodides:** To a round-bottom flask with acyl iodide (11 mmol, 1.1 equiv.), aldehyde (10 mmol, 1.0 equiv.) was added at 0 °C. The reaction was stirred at 0 °C for 0.5 h. Then it was diluted with CH$_2$Cl$_2$ and quenched with aq. NaHCO$_3$ and aq. Na$_2$S$_2$O$_3$. The mixture was extracted with CH$_2$Cl$_2$ for two times.
The combined organic layer was dried over Na$_2$SO$_4$ and concentrated under reduced pressure at room temperature to give the α-oxy iodide as a yellow oil.

**α-oxy bromides:** An oven-dried round-bottom flask charged with a magnetic stir bar and ZnCl$_2$ (0.05 equiv.) was filled with nitrogen atmosphere, followed by the addition of CH$_2$Cl$_2$ and acyl bromide (1.2 equiv.). The resulting solution was cooled to -10 °C and the mixture was stirred for 10 min. At this temperature, the aldehyde (1.0 equiv.) was added dropwise via syringe and the resulting mixture was stirred for 2 h. Then, the reaction mixture was filtered through a short column of neutral aluminium oxide, and washed with CH$_2$Cl$_2$. The filtrate was concentrated under reduced pressure. The product was purified by vacuum distillation or used directly after the determination of its purity.

### 2.2 General procedure for the nickel catalyzed cross-coupling of α-oxy halides with C(sp$^2$) and C(sp)-electrophiles utilizing metal reductant Mn

A dry 5-mL vial equipped with a Teflon-coated magnetic stir bar (10mm*3mm) was charged with aryl iodide/vinyl bromide/acyl chloride/alkynyl bromide (0.2 mmol, 1 equiv., if solid), NiCl$_2$·dme (4.4 mg, 0.02 mmol, 10 mol%), 4,7-dimethoxy-1,10-phenanthroline (d-OMe-phen) (4.8 mg, 0.02 mmol, 10 mol%), and Mn (22 mg, 0.4 mmol, 2 equiv.) in glovebox. Anhydrous and degassed DMA (2.0 mL), aryl iodide/vinyl bromide/acyl chloride/alkynyl bromide (0.2 mmol, 1 equiv., if liquid), α-oxy halides (0.6 mmol, 3 equiv), were added via syringe. The vial was capped and sealed with parafilm. The reaction mixture was stirred for 16 h at room temperature. After the reaction is completed, the mixture was transferred to a 50 mL round bottom flask. Then H$_2$O (20 mL) was added and the mixture was extracted with EtOAc (20 mL) for three times. The combined organic layer was washed with H$_2$O (20 mL) and brine (20 mL). The organic layer was dried with anhydrous Na$_2$SO$_4$, then concentrated under vacuum. The product was purified by flash column chromatography on silica gel using hexane/EtOAc as eluent.

### 2.3 General procedure for the nickel catalyzed cross-coupling of α-oxy halides with aryl iodide utilizing photocatalysis

A dry 5-mL vial equipped with a Teflon-coated magnetic stir bar (10mm*3mm) was charged with aryl iodide (0.2 mmol, 1 equiv., if solid), 3CzClIPN (6.6 mg, 0.01 mmol, 5 mol%), NiCl$_2$·dme (4.4 mg, 0.02 mmol, 10 mol%), 4,7-dimethoxy-1,10-phenanthroline (d-OMe-phen) (4.8 mg, 0.02 mmol, 10 mol%), and diethyl-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate (HE) (101mg, 0.4 mmol, 2 equiv.) in
glovebox. Anhydrous and degassed DMA (4.0 mL), aryl iodide (0.2 mmol, 1 equiv., if liquid), α-oxy bromide (0.6 mmol, 3 equiv), ‘Bu3N (240 μL, 1 mmol, 5 equiv.) were added via syringe. The vial was capped and sealed with parafilm. The reaction mixture was stirred for 16 h under irradiation with a 45 W Kessil PR160-440 nm blue LED lamp with 50 W fan cooling. After the reaction is completed, the mixture was transferred to a 50 mL round bottom flask. Then H2O (20 mL) was added and the mixture was extracted with EtOAc (20 mL) for three times. The combined organic layer was washed with H2O (20 mL) and brine (20 mL). The organic layer was dried with anhydrous Na2SO4, then concentrated under vacuum. The product was purified by flash column chromatography on silica gel using hexane/EtOAc as eluent.

2.4 General procedure for the nickel catalyzed cross-coupling of α-oxy halides with aryl/acyl halide utilizing electrocatalysis

A dry 5-mL vial equipped with a Teflon-coated magnetic stir bar (10mm*3mm) was charged with aryl iodide (0.2 mmol, 1 equiv., if solid), NiCl2·dme (4.4 mg, 0.02 mmol, 10 mol%), 4,7-dimethoxy-1,10-phenanthroline (d-OMe-phen) (4.8 mg, 0.02 mmol, 10 mol%), and ‘Bu3NPF6 (310 mg, 0.8 mmol, 4 equiv.) in glovebox. Anhydrous and degassed DMA (4.0 mL), aryl iodide/acyl chlroide (0.2 mmol, 1 equiv., if liquid), α-oxy iodide (0.6 mmol, 3 equiv) were added via syringe. Then, it was capped with a Teflon lid equipped with iron rod (4×50 mm) as the anode and nickel foam electrode (20×10×1 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 8 mA under room temperature for 16 h. After the reaction is completed, the mixture was transferred to a 50 mL round bottom flask, electrodes were washed with ethyl acetate. Then H2O (20 mL) was added and the mixture was extracted with EtOAc (20 mL) for three times. The combined organic layer was washed with H2O (20 mL) and brine (20 mL). The organic layer was dried with anhydrous Na2SO4, then concentrated under vacuum. The product was purified by flash column chromatography on silica gel using hexane/EtOAc as eluent.

2.5 Scale-up Reaction

A dry 100 mL flask equipped with a teflon-coated magnetic stir bar was charged with 4-iodo-1,1'-biphenyl (5 mmol, 1 equiv., 1.4 g), NiCl2·dme (110 mg, 0.5 mmol, 10 mol%), 4,7-dimethoxy-1,10-phenanthroline (d-OMe-phen) (120 mg, 0.5 mmol, 10 mol%), and Mn (550 mg, 10 mmol, 2 equiv.) in
glovebox. Anhydrous and degassed DMA (50 mL), 1-iodo-2-methylpropyl acetate (3.6 g, 0.6 mmol, 3 equiv), were added via syringe. The reaction mixture was stirred for 16 h at room temperature. After the reaction is completed, the solution was diluted with H$_2$O (100 mL). The layers were separated, then the aqueous layer was extracted with EtOAc (3×200 mL). The combined organic layers were washed by water (3 ×100 mL) and concentrated with a rotary evaporator. The title compound was isolated in 94% (1.26 g) yield after flash chromatography on silica gel.

2.6 General procedure for the nickel catalyzed cross-coupling of α-oxy halides with aryl/acyl halide utilizing ball milling

A dry 1.5 mL stainless steel grinding jar equipped with a 0.5 g stainless steel ball was charged with aryl iodide (0.2 mmol, 1 equiv., if solid), NiCl$_2$·dme (4.4 mg, 0.02 mmol, 10 mol%), 4,7-dimethoxy-1,10-phenanthroline (d-OMe-phen) (4.8 mg, 0.02 mmol, 10 mol%), and Mn (22 mg, 0.4 mmol, 2 equiv.) in glovebox. Anhydrous and degassed DMA (55 μL), and α-oxy halides (0.6 mmol, 3 equiv) were added via syringe. The grinding jar was closed and placed on the ball mill. The reaction was milled for 5 min at 30 Hz. After the reaction is completed, the mixture was transferred to a 50 mL round bottom flask. Then H$_2$O (20 mL) was added and the mixture was extracted with EtOAc (20 mL) for three times. The combined organic layer was washed with H$_2$O (20 mL) and brine (20 mL). The organic layer was dried with anhydrous Na$_2$SO$_4$, then concentrated under vacuum. The product was purified by flash column chromatography on silica gel using hexane/EtOAc as eluent.

3. Sequential transformation reactions

1-(4’-methoxy-[1,1’-biphenyl]-4-yl)ethyl acetate (17)

A reaction tube (10 mL) equipped with a Teflon-coated magnetic stir bar (6mm*10mm) was charged with 16 (122.0 mg, 0.5 mmol, 1 equiv.), (4-methoxyphenyl)boronic acid (114.0 mg, 0.75 mmol, 1.5 equiv.), PdCl$_2$(PPh$_3$)$_4$ (35.1 mg, 0.05 mmol, 10 mol%), and K$_3$PO$_4$ (636.9 mg, 3.0 mmol, 6 equiv.) in glovebox. Toluene (1.5 mL) and H$_2$O (1.5 mL) were added via syringe. The reaction mixture was stirred at 90 °C for 12 h. After the reaction was completed, it was diluted with H$_2$O (30 mL), and extracted by
ethyl acetate (3×20 mL), and the combined organic layers were concentrated with a rotary evaporator. The product was purified by flash column chromatography on silica gel using hexane/EtOAc as eluent.

Yield: 87% (117.5 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.52 (t, $J = 8.9$ Hz, 4H), 7.41 (d, $J = 8.0$ Hz, 2H), 6.98 (d, $J = 8.4$ Hz, 2H), 5.92 (q, $J = 6.7$ Hz, 1H), 3.85 (s, 3H), 2.09 (s, 3H), 1.57 (d, $J = 6.6$ Hz, 3H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 170.4, 159.2, 140.5, 140.0, 133.3, 128.1, 126.8, 126.6, 114.2, 72.1, 55.3, 22.1, 21.4. HRMS (ESI) for C$_{17}$H$_{18}$O$_3$: calculated for [M+Na]$^+$ 293.11482, found 293.11523.

4-methoxy-4'-(pent-4-en-2-yl)-1,1'-biphenyl (18)

To a stirred solution of B(C$_6$F$_5$)$_3$ (5.1 mg, 0.01 mmol, 5 mol %) in anhydrous CH$_2$Cl$_2$ (1 mL) was added 17 (0.2 mmol, 54.0 mg, 1 equiv.), followed by the addition of allyltrimethylsilane (34.3 mg, 0.3 mmol, 1.5 equiv.). The mixture was stirred at room temperature for 12h. The product was purified by flash column chromatography on silica gel using hexane/EtOAc as eluent.$^{[2]}$

Yield: 84% (42.3 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.56 (dd, $J = 13.3$, 8.2 Hz, 4H), 7.30 (d, $J = 7.8$ Hz, 2H), 7.02 (d, $J = 8.4$ Hz, 2H), 5.91 – 5.71 (m, 1H), 5.15 – 4.99 (m, 2H), 3.89 (s, 3H), 2.89 (h, $J = 7.1$ Hz, 1H), 2.57 – 2.30 (m, 2H), 1.34 (d, $J = 6.9$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 158.9, 145.5, 138.4, 137.1, 133.6, 127.9, 127.3, 126.6, 115.9, 114.1, 55.3, 42.6, 39.4, 21.5. HRMS (ESI) for C$_{18}$H$_{20}$O: calculated for [M+Na]$^+$ 275.14064, found 275.14102.

4. Cyclic Voltammetry Measurements

All measurements were performed under anhydrous conditions in argon-filled glovebox. All supporting electrolytes were dried under dynamic vacuum (less than 0.1 mbar) over 24 h at 100 °C and stored inside the glovebox. The cell for the analysis was equipped with a glass vial (working volume is 10 mL) and Teflon cap, equipped with O-ring for tight sealing. Glassy carbon was used as working electrodes (circle, $d = 3$ mm), platinum wire as a counter electrode, and Ag/AgNO$_3$ (0.01 M in 0.1 M Bu$_4$NPF$_6$ in acetonitrile) as a reference. All measurements were conducted in 0.1 M solutions of Bu$_4$NPF$_6$ in CH$_3$CN. The potentials were given relative to the Fc/Fe$^+$ redox couple with ferrocene as internal standard. For
conversion to SCE as reference, it is known that SCE is 400 mV more negative than Fe/Fe+ in MeCN with NBu4PF6 as supporting electrolyte.\(^3\)

![Cyclic voltammetry measurement of 2a](attachment:image.png)

**Figure S1**: Cyclic voltammetry measurement of 2a

\[ E_{1/2}(\text{Fc/Fc}^+) = +0.092 \text{ V vs. Ag/AgNO}_3 \]
\[ E_{p/2}(2a) = -1.30 \text{ V vs. Ag/AgNO}_3 \]
\[ E_{p/2}(2a) = -1.39 \text{ V vs. Fe/Fe}^+ \]
\[ E_{p/2}(2a) = -0.99 \text{ V vs. SCE} \]

5. **Steady-State Stern-Volmer Quenching Experiments**

Steady-state Stern-Volmer quenching experiments were carried out using a 0.1 mM solution of photocatalyst 3CzClIPN and variable concentrations (0.4, 0.8, 1.2, 1.6, 2.0 mM) of HE, tributylamine, or α-acetoxy bromide 9 in anhydrous DMA. The samples were prepared in 2 mL quartz cuvettes, equipped with PTFE stoppers, and sealed with parafilm inside argon filled glove-box. The intensity of the emission peak at 540 nm (\(\lambda_{ex} = 457 \text{ nm}\)) for 3CzClIPN expressed as the ratio \(I_0/I\), where \(I_0\) is the emission intensity of 3CzClIPN at 540 nm in the absence of a quencher and \(I\) is the observed intensity, as a function of the quencher concentration was measured. Fluorescence emission spectra and Steady-state Stern-Volmer plots for each component are given in Figure below.
Figure S2: Emission spectra of 3CzClIPN (0.1 mM) at different concentrations of HE.

Figure S3: Emission spectra of 3CzClIPN (0.1 mM) at different concentrations of tributylamine.

Figure S4: Emission spectra of 3CzClIPN (0.1 mM) at different concentrations of α-acetoxy bromide 9.
6. Spectroscopic Data of the Products

1-phenylbutyl acetate (3a, 10a, 11a)

Yield: 95% (36.5 mg) for 3a, 85% (32.6 mg) for 10a, 72% (27.7 mg) for 11a. \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 7.39 – 7.34 (m, 4H), 7.31 (ddd, \(J = 8.7, 5.2, 3.2\) Hz, 1H), 5.78 (dd, \(J = 7.6, 6.3\) Hz, 1H), 2.09 (s, 3H), 1.97 – 1.89 (m, 1H), 1.81 – 1.74 (m, 1H), 1.43 – 1.26 (m, 2H), 0.95 (t, \(J = 7.4\) Hz, 3H). \(^13\)C NMR (126 MHz, CDCl\(_3\)) \(\delta\) 170.3, 166.7, 146.0, 129.7, 129.5, 126.3, 75.3, 52.1, 38.3, 21.1, 18.6, 13.7. HRMS (ESI) for C\(_{12}\)H\(_{16}\)O\(_2\): calculated for [M+Na]\(^+\) 215.10425, found 215.10423.

Methyl 4-(1-acetoxybutyl)benzoate (3b)

Yield: 76% (38.0 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.00 (d, \(J = 7.9\) Hz, 2H), 7.37 (d, \(J = 8.0\) Hz, 2H), 5.75 (t, \(J = 6.9\) Hz, 1H), 3.89 (s, 3H), 2.07 (s, 3H), 1.93 – 1.82 (m, 1H), 1.76 – 1.68 (m, 1H), 1.40 – 1.22 (m, 2H), 0.90 (t, \(J = 7.3\) Hz, 3H). \(^13\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.3, 166.7, 146.0, 129.7, 129.5, 126.3, 75.3, 52.1, 38.3, 21.1, 18.6, 13.7. HRMS (ESI) for C\(_{14}\)H\(_{18}\)O\(_3\): calculated for [M+Na]\(^+\) 273.10973, found 273.11006.
Methyl-3-(1-acetoxybutyl)benzoate (3c, 10d, 11b)

Yield: 96% (48.2 mg) for 3c, 69% (34.5 mg) for 10d, 74% (37.1 mg) for 11b. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.99 (s, 1H), 7.94 (d, $J = 7.2$ Hz, 1H), 7.50 (d, $J = 7.2$ Hz, 1H), 7.44 – 7.35 (m, 1H), 5.75 (t, $J = 7.0$ Hz, 1H), 3.90 (s, 3H), 2.06 (s, 3H), 1.93 – 1.85 (m, 1H), 1.76 – 1.68 (m, 1H), 1.39 – 1.21 (m, 2H), 0.90 (t, $J = 7.2$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.3, 166.8, 141.3, 131.1, 130.3, 129.0, 128.4, 127.5, 75.3, 52.1, 38.3, 21.2, 18.6, 13.7. HRMS (ESI) for C$_{14}$H$_{18}$O$_4$: calculated for [M+Na]$^+$ 273.10973, found 273.11030.

1-(4-cyanophenyl)butyl acetate (3d, 10b)

Yield: 79% (34.3 mg) for 3d, 79% (34.5 mg) for 10b. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.62 (d, $J = 8.1$ Hz, 2H), 7.41 (d, $J = 8.1$ Hz, 2H), 5.76 – 5.67 (m, 1H), 2.08 (s, 3H), 1.92 – 1.80 (m, 1H), 1.75 – 1.67 (m, 1H), 1.41 – 1.21 (m, 2H), 0.91 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.2, 146.2, 132.3, 127.0, 118.6, 111.5, 75.0, 38.2, 21.0, 18.5, 13.6. HRMS (ESI) for C$_{13}$H$_{15}$NO$_2$: calculated for [M+Na]$^+$ 240.09950, found 240.09906.

1-(3-cyanophenyl)butyl acetate (3e)

Yield: 79% (34.1 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.60 (s, 1H), 7.55 (t, $J = 8.5$ Hz, 2H), 7.43 (t, $J = 7.7$ Hz, 1H), 5.70 (t, $J = 6.9$ Hz, 1H), 2.08 (s, 3H), 1.92 – 1.81 (m, 1H), 1.74 – 1.68 (m, 1H), 1.40 – 1.31 (m, 1H), 1.28 – 1.20 (m, 1H), 0.91 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.2, 142.5, 131.4, 130.9, 129.9, 129.2, 118.6, 112.6, 74.7, 38.2, 21.1, 18.5, 13.6. HRMS (ESI) for C$_{13}$H$_{15}$NO$_2$: calculated for [M+Na]$^+$ 240.09950, found 240.09976.

1-(2-cyanophenyl)butyl acetate (3f, 10c, 11c)

Yield: 90% (39.2 mg) for 3f, 92% (39.9 mg) for 10c, 69% (30.1 mg) for 11c. $^1$H NMR (400 MHz,
CDCl$_3$ δ 7.63 (d, J = 7.7 Hz, 1H), 7.57 (t, J = 7.7 Hz, 1H), 7.45 (d, J = 7.9 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 5.98 – 5.92 (m, 1H), 2.10 (s, 3H), 1.98 – 1.89 (m, 1H), 1.84 – 1.76 (m, 1H), 1.49 – 1.38 (m, 1H), 1.34 – 1.26 (m, 1H), 0.93 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.0, 144.9, 133.1, 132.9, 128.0, 126.6, 117.2, 110.6, 73.8, 38.0, 20.9, 18.6, 13.6. HRMS (ESI) for C$_{13}$H$_{15}$NO$_2$: calculated for [M+Na]$^+$ 240.09950, found 240.09975.

1-(4-acetylphenyl)butyl acetate (3g)

Yield: 88% (41.2 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.92 (d, J = 7.7 Hz, 2H), 7.39 (d, J = 7.8 Hz, 2H), 5.74 (t, J = 6.9 Hz, 1H), 2.57 (s, 3H), 2.07 (s, 3H), 1.93 – 1.82 (m, 1H), 1.80 – 1.66 (m, 1H), 1.44 – 1.16 (m, 2H), 0.90 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 197.6, 170.2, 146.2, 136.5, 128.5, 126.4, 75.3, 38.2, 26.6, 21.1, 18.6, 13.7. HRMS (ESI) for C$_{14}$H$_{18}$O$_3$: calculated for [M+Na]$^+$ 257.11482, found 257.11551.

1-(3-(trifluoromethyl)phenyl)butyl acetate (3h)

Yield: 80% (41.6 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.60 – 7.40 (m, 4H), 5.81 – 5.73 (m, 1H), 2.09 (s, 3H), 1.96 – 1.84 (m, 1H), 1.79 – 1.67 (m, 1H), 1.42 – 1.21 (m, 2H), 0.93 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.3, 162.2, 136.6, 128.3, 115.2, 124.87 – 122.92, 124.02 (d, J = 272.4 Hz), 123.86 (dd, J = 154.4, 3.9 Hz), 75.1, 38.4, 21.1, 18.7, 13.7. $^{19}$F NMR (377 MHz, CDCl$_3$) δ -62.6. HRMS (ESI) for C$_{13}$H$_{15}$F$_3$O$_2$: calculated for [M+Na]$^+$ 283.09164, found 283.09249.

1-(4-fluorophenyl)butyl acetate (3i)

Yield: 91% (38.2 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.30 (dd, J = 8.4, 5.4 Hz, 2H), 7.01 (t, J = 8.6 Hz, 2H), 5.70 (t, J = 7.1 Hz, 1H), 2.05 (s, 3H), 1.92 – 1.83 (m, 1H), 1.76 – 1.66 (m, 1H), 1.39 – 1.20 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.3, 162.2 (d, J = 246.1 Hz), 136.6, 128.3 (d, J = 3.1 Hz), 115.2 (d, J = 21.4 Hz), 75.2, 38.3, 21.2, 18.7, 13.7. $^{19}$F NMR (377 MHz, CDCl$_3$) δ -114.5. HRMS (ESI) for C$_{12}$H$_{15}$FO$_2$: calculated for [M+Na]$^+$ 233.09483, found 233.09476.
1-(3-fluorophenyl)butyl acetate (3j)

Yield: 90% (37.8 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.32 (dd, $J = 14.4$, 8.3 Hz, 1H), 7.11 (d, $J = 7.7$ Hz, 1H), 7.05 (d, $J = 9.7$ Hz, 1H), 7.02 – 6.95 (m, 1H), 5.74 (t, $J = 6.9$ Hz, 1H), 2.10 (s, 3H), 1.94 – 1.84 (m, 1H), 1.79 – 1.69 (m, 1H), 1.42 – 1.25 (m, 2H), 0.94 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 162.8 (d, $J = 246.0$ Hz), 143.5 (d, $J = 7.0$ Hz), 129.9 (d, $J = 8.2$ Hz), 122.1 (d, $J = 2.8$ Hz), 114.6 (d, $J = 21.1$ Hz), 113.3 (d, $J = 21.9$ Hz), 75.1, 38.3, 21.2, 18.6, 13.7. $^{19}$F NMR (377 MHz, CDCl$_3$) $\delta$ -112.9. HRMS (ESI) for C$_{12}$H$_{15}$FO$_2$: calculated for [M+Na]$^+$ 233.09483, found 233.09435.

1-(2-fluorophenyl)butyl acetate (3k)

Yield: 60% (25.2 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.37 (t, $J = 7.4$ Hz, 1H), 7.27 (q, $J = 7.0$ Hz, 1H), 7.14 (t, $J = 9.3$ Hz, 1H), 6.06 (t, $J = 6.8$ Hz, 1H), 2.11 (s, 3H), 1.99 – 1.87 (m, 1H), 1.85 – 1.74 (m, 1H), 1.43 – 1.28 (m, 2H), 0.95 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.1, 159.8 (d, $J = 247.1$ Hz), 129.2 (d, $J = 8.2$ Hz), 128.1 (d, $J = 13.7$ Hz), 127.5 (d, $J = 4.2$ Hz), 124.1 (d, $J = 3.5$ Hz), 115.4 (d, $J = 21.9$ Hz), 69.9 (d, $J = 2.4$ Hz), 37.5, 21.1, 18.6, 13.7. $^{19}$F NMR (377 MHz, CDCl$_3$) $\delta$ -118.2. HRMS (ESI) for C$_{12}$H$_{15}$FO$_2$: calculated for [M+Na]$^+$ 233.09483, found 233.09458.

1-(4-chlorophenyl)butyl acetate (3l)

Yield: 82% (37.1 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.43 – 7.19 (m, 4H), 5.71 (t, $J = 7.0$ Hz, 1H), 2.08 (s, 3H), 1.96 – 1.83 (m, 1H), 1.78 – 1.66 (m, 1H), 1.43 – 1.21 (m, 2H), 0.94 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 139.3, 133.5, 128.5, 127.9, 75.1, 38.2, 21.2, 18.7, 13.7. HRMS (ESI) for C$_{12}$H$_{15}$ClO$_2$: calculated for [M+Na]$^+$ 249.06528, found 249.06543.

1-(4-bromophenyl)butyl acetate (3m, 10g)

Yield: 75% (40.5 mg) for 3m, 50% (27.2 mg) for 10g. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.46 (d, $J = 7.6$ Hz, 2H), 7.20 (d, $J = 7.7$ Hz, 2H), 5.67 (t, $J = 7.0$ Hz, 1H), 2.06 (s, 3H), 1.91 – 1.82 (m, 1H), 1.75 – 1.65
(m, 1H), 1.39 – 1.19 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.3, 139.9, 131.5, 128.2, 121.6, 75.2, 38.2, 21.2, 18.6, 13.7. HRMS (ESI) for C$_{12}$H$_{18}$BrO$_2$: calculated for [M+Na]$^+$ 293.01476, found 293.01459.

**1-(2-bromophenyl)butyl acetate (3n)**

![Structure](image)

Yield: 80% (43.2 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.52 (d, J = 8.0 Hz, 1H), 7.37 (dd, J = 7.8, 1.6 Hz, 1H), 6.13 – 6.07 (m, 1H), 2.10 (s, 3H), 1.82 – 1.75 (m, 2H), 1.47 – 1.33 (m, 2H), 0.94 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.0, 140.6, 132.8, 128.9, 127.5, 127.0, 122.1, 74.6, 37.6, 21.1, 18.7, 13.7. HRMS (ESI) for C$_{12}$H$_{15}$BrO$_2$: calculated for [M+Na]$^+$ 293.01476, found 293.01484.

**1-(4-formylphenyl)butyl acetate (3o, 10f)**

![Structure](image)

Yield: 67% (29.5 mg) for 3o, 89% (39.1 mg) for 10f. $^1$H NMR (400 MHz, CDCl$_3$) δ 9.99 (s, 1H), 7.85 (d, J = 7.8 Hz, 2H), 7.47 (d, J = 7.9 Hz, 2H), 5.79 – 5.74 (m, 1H), 2.09 (s, 3H), 1.94 – 1.85 (m, 1H), 1.77 – 1.69 (m, 1H), 1.43 – 1.33 (m, 1H), 1.31 – 1.22 (m, 1H), 0.92 (t, J = 7.3 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 191.8, 170.3, 147.7, 135.8, 129.9, 126.9, 75.3, 38.3, 21.1, 18.6, 13.7. HRMS (ESI) for C$_{13}$H$_{16}$O$_3$: calculated for [M+Na]$^+$ 243.09917, found 243.09925.

**1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)butyl acetate (3p, 10e, 11d)**

![Structure](image)

Yield: 90% (57.2 mg) for 3p, 75% (47.7 mg) for 10e, 84% (53.4 mg) for 11d. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.78 (d, J = 7.8 Hz, 2H), 7.32 (d, J = 7.9 Hz, 2H), 5.73 (t, J = 6.9 Hz, 1H), 2.06 (s, 3H), 1.92 – 1.82 (m, 1H), 1.77 – 1.69 (m, 1H), 1.42 – 1.35 (m, 1H), 1.33 (s, 12H), 1.28 – 1.22 (m, 1H), 0.90 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.3, 143.9, 134.8, 125.7, 83.7, 75.8, 38.3, 24.8, 21.2, 18.7, 13.7. HRMS (ESI) for C$_{19}$H$_{27}$BO$_4$: calculated for [M+Na]$^+$ 341.18946, found 341.18954.
1-(4-(pentafluoro-16-sulfaneyl)phenyl)butyl acetate (3q)

Yield: 74% (47.1 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.72 (d, $J = 8.7$ Hz, 2H), 7.40 (d, $J = 8.3$ Hz, 2H), 5.77 – 5.70 (m, 1H), 2.08 (s, 3H), 1.93 – 1.83 (m, 1H), 1.77 – 1.66 (m, 1H), 1.40 – 1.22 (m, 2H), 0.92 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.2, 153.1 (p, $J = 17.1$ Hz), 144.8, 126.1 (p, $J = 4.6$ Hz), 74.8, 38.3, 21.1, 18.6, 13.7. $^{19}$F NMR (377 MHz, CDCl$_3$) $\delta$ 84.5 (p, $J = 150.6$, 149.3 Hz), 63.1, 62.7. HRMS (ESI) for C$_{12}$H$_{15}$F$_5$O$_2$: calculated for [M+Na]$^+$ 341.06051, found 341.06064.

1-(4-((trimethylsilyl)ethynyl)phenyl)butyl acetate (3r)

Yield: 84% (48.4 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.45 (d, $J = 8.1$ Hz, 2H), 7.27 (d, $J = 8.2$ Hz, 2H), 5.73 (t, $J = 6.9$ Hz, 1H), 2.08 (s, 3H), 1.94 – 1.82 (m, 1H), 1.78 – 1.66 (m, 1H), 1.41 – 1.19 (m, 2H), 0.93 (t, $J = 7.4$ Hz, 3H), 0.26 (s, 9H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.2, 141.2, 132.0, 126.3, 122.6, 104.7, 94.3, 75.4, 38.2, 21.2, 18.6, 13.7, -0.1. HRMS (ESI) for C$_{17}$H$_{24}$O$_2$Si: calculated for [M+Na]$^+$ 311.14378, found 311.14362.

1-(p-tolyl)butyl acetate (3s)

Yield: 90% (37.1 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.23 (d, $J = 7.8$ Hz, 2H), 7.15 (d, $J = 7.8$ Hz, 2H), 5.72 (t, $J = 7.0$ Hz, 1H), 2.34 (s, 3H), 2.06 (s, 3H), 1.96 – 1.85 (m, 1H), 1.79 – 1.69 (m, 1H), 1.40 – 1.20 (m, 2H), 0.92 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.4, 137.8, 137.5, 129.0, 126.5, 75.8, 38.3, 21.3, 21.1, 18.8, 13.8. HRMS (ESI) for C$_{13}$H$_{18}$O$_2$: calculated for [M+Na]$^+$ 229.11990, found 229.11990.

1-(o-tolyl)butyl acetate (3t)

Yield: 64% (26.4 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.34 (dd, $J = 7.1$, 2.0 Hz, 1H), 7.23 – 7.11 (m, 3H), 5.98 (dd, $J = 8.2$, 5.5 Hz, 1H), 2.41 (s, 3H), 2.07 (s, 3H), 1.93 – 1.82 (m, 1H), 1.76 – 1.65 (m, 1H), 1.50
– 1.37 (m, 1H), 1.36 – 1.24 (m, 1H), 0.94 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.4, 139.5, 135.0, 130.3, 127.4, 126.1, 125.6, 72.5, 38.0, 21.2, 19.2, 18.8, 13.8. HRMS (ESI) for C$_{13}$H$_{18}$O$_2$: calculated for [M+Na]$^+$ 229.11990, found 229.11985.

1-(4-(tert-butyl)phenyl)butyl acetate (3u)

Yield: 62% (30.8 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.38 (d, J = 7.4 Hz, 2H), 7.29 (d, J = 7.3 Hz, 2H), 5.77 (t, J = 6.9 Hz, 1H), 2.09 (s, 3H), 1.98 – 1.86 (m, 1H), 1.81 – 1.71 (m, 1H), 1.44 – 1.36 (m, 1H), 1.34 (s, 9H), 1.32 – 1.22 (m, 1H), 0.94 (t, J = 7.3 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.5, 150.6, 137.7, 126.2, 125.2, 75.7, 38.3, 34.5, 31.3, 21.3, 18.8, 13.8. HRMS (ESI) for C$_{16}$H$_{24}$O$_2$: calculated for [M+Na]$^+$ 271.16685, found 271.16673.

1-(4-methoxyphenyl)butyl acetate (3v)

Yield: 63% (27.9 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.29 (d, J = 8.1 Hz, 2H), 6.89 (d, J = 8.3 Hz, 2H), 5.72 (t, J = 7.1 Hz, 1H), 3.82 (s, 3H), 2.06 (s, 3H), 1.97 – 1.86 (m, 1H), 1.80 – 1.69 (m, 1H), 1.39 – 1.22 (m, 2H), 0.93 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.4, 159.1, 132.9, 127.9, 113.7, 75.6, 55.2, 38.1, 21.3, 18.8, 13.7. HRMS (ESI) for C$_{16}$H$_{24}$O$_2$: calculated for [M+Na]$^+$ 245.11482, found 245.11468.

1-(3-methoxyphenyl)butyl acetate (3w, 10i)

Yield: 86% (37.8 mg) for 3w, 71% (31.5 mg) for 10i. $^1$H NMR (400 MHz, CDCl$_3$) δ 7.25 (t, J = 7.9 Hz, 1H), 6.91 (d, J = 7.6 Hz, 1H), 6.87 (s, 1H), 6.82 (dd, J = 8.2, 2.4 Hz, 1H), 5.71 (t, J = 6.9 Hz, 1H), 3.81 (s, 3H), 2.07 (s, 3H), 1.93 – 1.83 (m, 1H), 1.78 – 1.69 (m, 1H), 1.40 – 1.23 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.3, 159.5, 142.5, 129.4, 118.8, 112.9, 112.2, 75.7, 55.1, 38.4, 21.2, 18.7, 13.7. HRMS (ESI) for C$_{15}$H$_{18}$O$_3$: calculated for [M+Na]$^+$ 245.11482, found 245.11486.
1-(2-methoxyphenyl)butyl acetate (3x)

Yield: 80% (35.5 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.33 (d, $J = 7.6$ Hz, 1H), 7.26 (t, $J = 8.0$ Hz, 1H), 6.97 (t, $J = 7.5$ Hz, 1H), 6.89 (d, $J = 8.2$ Hz, 1H), 6.21 (t, $J = 6.5$ Hz, 1H), 3.86 (s, 3H), 2.11 (s, 3H), 1.86 – 1.74 (m, 2H), 1.44 – 1.30 (m, 2H), 0.94 (t, $J = 7.4$ Hz, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 156.1, 129.7, 128.4, 126.1, 120.4, 110.5, 70.3, 55.4, 37.6, 21.2, 18.7, 13.8. HRMS (ESI) for C$_{13}$H$_{18}$O$_3$: calculated for [M+Na]$^+$ 245.11482, found 245.11498.

1-(4-(methylthio)phenyl)butyl acetate (3y, 10j)

Yield: 81% (38.6 mg) for 3y, 82% (39.1 mg) for 10j. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.26 (q, $J = 8.3$ Hz, 4H), 5.71 (t, $J = 7.0$ Hz, 1H), 2.49 (s, 3H), 2.07 (s, 3H), 1.96 – 1.85 (m, 1H), 1.79 – 1.66 (m, 1H), 1.41 – 1.33 (m, 1H), 1.30 – 1.22 (m, 1H), 0.93 (t, $J = 7.4$ Hz, 3H).

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 138.0, 137.6, 127.1, 126.4, 75.5, 38.1, 21.2, 18.7, 15.7, 13.7. HRMS (ESI) for C$_{13}$H$_{18}$O$_2$: calculated for [M+Na]$^+$ 261.09197, found 261.09214.

4-(1-acetoxy-2-methylpropyl)phenyl 11-bromoundecanoate (3z)

Yield: 57% (51.8 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.29 (d, $J = 7.8$ Hz, 2H), 7.04 (d, $J = 7.5$ Hz, 2H), 5.46 (d, $J = 7.7$ Hz, 1H), 3.40 (t, $J = 6.8$ Hz, 1H), 3.18 (t, $J = 7.0$ Hz, 1H), 2.53 (t, $J = 7.4$ Hz, 2H), 2.13 – 2.00 (m, 5H), 1.92 – 1.80 (m, 2H), 1.78 – 1.69 (m, 2H), 1.48 – 1.23 (m, 13H), 0.96 (d, $J = 6.5$ Hz, 3H), 0.79 (d, $J = 6.7$ Hz, 3H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 172.1, 170.2, 150.1, 137.1, 128.1, 121.2, 80.3, 34.3, 34.0, 33.5, 33.4, 32.8, 30.4, 29.3, 29.3, 29.1, 29.0, 28.7, 28.4, 28.1, 24.8, 21.1, 18.6, 18.4, 7.2. HRMS (ESI) for C$_{23}$H$_{35}$BrO$_4$: calculated for [M+Na]$^+$ 477.16109, found 477.16107.

1-(3,5-bis(trifluoromethyl)phenyl)butyl acetate (3aa)

Yield: 71% (46.8 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.80 (s, 1H), 7.76 (s, 2H), 5.81 (dd, $J = 7.9$, 5.9 Hz, 1H), 5.60 (d, $J = 8.0$ Hz, 1H), 5.11 (d, $J = 6.5$ Hz, 1H), 3.86 (s, 3H), 2.11 (s, 3H), 1.86 – 1.74 (m, 2H), 1.44 – 1.30 (m, 2H), 0.94 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 156.1, 129.7, 128.4, 126.1, 120.4, 110.5, 70.3, 55.4, 37.6, 21.2, 18.7, 13.8. HRMS (ESI) for C$_{13}$H$_{18}$O$_2$: calculated for [M+Na]$^+$ 261.09197, found 261.09214.
Hz, 1H), 2.11 (s, 3H), 1.97 – 1.87 (m, 1H), 1.79 – 1.69 (m, 1H), 1.44 – 1.24 (m, 2H), 0.94 (t, \(J = 7.4\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta 170.2, 143.6, 131.80 \) (q, \(J = 33.4\) Hz), 126.6 (d, \(J = 3.9\) Hz), 124.5, 121.9 – 121.7 (m), 74.5, 38.4, 21.0, 18.6, 13.6. \(^{19}\)F NMR (377 MHz, CDCl\(_3\)) \(\delta -62.9\). HRMS (ESI) for C\(_{14}\)H\(_{14}\)F\(_6\)O\(_2\): calculated for [M+Na]\(^+\) 351.07902, found 351.07917.

1-(2,4-difluorophenyl)butyl acetate (3ab)

Yield: 45% (20.5 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 7.31 \) (q, \(J = 8.0\) Hz, 1H), 6.86 (td, \(J = 8.3, 2.3\) Hz, 1H), 6.78 (td, \(J = 9.8, 2.5\) Hz, 1H), 5.97 (t, \(J = 7.0\) Hz, 1H), 2.07 (s, 3H), 1.94 – 1.83 (m, 1H), 1.79 – 1.69 (m, 1H), 1.40 – 1.33 (m, 1H), 1.30 – 1.23 (m, 1H), 0.92 (t, \(J = 7.4\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta 170.1, 161.1 \) (t, \(J = 11.3\) Hz), 161.1 (dd, \(J = 488.0, 11.9\) Hz), 128.6 (dd, \(J = 9.7, 5.8\) Hz), 124.2 (d, \(J = 10.0\) Hz), 111.3 (dd, \(J = 21.3, 3.7\) Hz), 103.8 (t, \(J = 25.6\) Hz), 69.5, 37.4, 21.1, 18.6, 13.7. \(^{19}\)F NMR (377 MHz, CDCl\(_3\)) \(\delta -111.0 \) (dd, \(J = 16.2, 6.4\) Hz), -113.9 – -114.0 (m). HRMS (ESI) for C\(_{12}\)H\(_{16}\)F\(_2\)O\(_2\): calculated for [M+Na]\(^+\) 251.08541, found 251.08519.

1-(2-methyl-4-(trifluoromethoxy)phenyl)butyl acetate (3ac)

Yield: 77% (44.6 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 7.34 \) (d, \(J = 8.5\) Hz, 1H), 7.03 (d, \(J = 8.6\) Hz, 1H), 6.98 (s, 1H), 5.95 – 5.88 (m, 1H), 2.41 (s, 3H), 2.07 (s, 3H), 1.90 – 1.79 (m, 1H), 1.72 – 1.63 (m, 1H), 1.47 – 1.23 (m, 2H), 0.93 (t, \(J = 7.3\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta 170.3, 148.2, 138.3, 137.2, 127.1, 122.4, 120.4 \) (q, \(J = 256.9\) Hz), 118.4, 71.9, 38.0, 21.1, 19.2, 18.8, 13.8. \(^{19}\)F NMR (377 MHz, CDCl\(_3\)) \(\delta -57.7\). HRMS (ESI) for C\(_{14}\)H\(_{17}\)F\(_3\)O\(_3\): calculated for [M+Na]\(^+\) 313.10220, found 313.10206.

1-(benzo[d][1,3]dioxol-5-yl)butyl acetate (3ad)

Yield: 72% (34.1 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 6.85 – 6.72 \) (m, 3H), 5.94 (d, \(J = 1.2\) Hz, 2H), 5.63 (t, \(J = 7.1\) Hz, 1H), 2.04 (s, 3H), 1.90 – 1.81 (m, 1H), 1.73 – 1.64 (m, 1H), 1.36 – 1.20 (m, 2H), 0.92 – 0.88 (m, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta 170.3, 147.6, 147.1, 134.7, 120.3, 108.0, 106.9, 101.0, 75.7, 38.3, 21.3, 18.8, 13.7. HRMS (ESI) for C\(_{15}\)H\(_{16}\)O\(_4\): calculated for [M+Na]\(^+\) 259.09408, found 259.09402.
1-[(1,1'-biphenyl)-4-yl]butyl acetate (3ae, 10h)

Yield: 87% (46.6 mg) for 3ae, 82% (44.0 mg) for 10h. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.64 – 7.56 (m, 4H), 7.45 (q, \(J = 7.6\) Hz, 4H), 7.39 – 7.31 (m, 1H), 5.82 (t, \(J = 7.0\) Hz, 1H), 2.11 (s, 3H), 2.02 – 1.91 (m, 1H), 1.86 – 1.76 (m, 1H), 1.46 – 1.28 (m, 2H), 0.97 (t, \(J = 7.4\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.4, 140.7, 139.8, 128.7, 127.3, 127.1, 127.0, 126.9, 75.6, 38.3, 21.3, 18.8, 13.8. HRMS (ESI) for C\(_{18}\)H\(_{20}\)O\(_2\): calculated for [M+Na\(^+\)] 291.13555, found 291.13510.

1-[(1,1'-biphenyl)-2-yl]butyl acetate (3af)

Yield: 40% (21.5 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.49 – 7.29 (m, 8H), 7.20 (d, \(J = 7.4\) Hz, 1H), 5.85 (dd, \(J = 8.4, 5.1\) Hz, 1H), 2.05 (s, 3H), 1.80 – 1.69 (m, 1H), 1.57 – 1.49 (m, 1H), 1.25 – 1.06 (m, 2H), 0.70 (t, \(J = 7.4\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.3, 140.8, 140.7, 139.1, 130.0, 129.3, 128.1, 127.6, 127.2, 127.1, 125.5, 72.9, 38.8, 21.2, 18.7, 13.5. HRMS (ESI) for C\(_{18}\)H\(_{20}\)O\(_2\): calculated for [M+Na\(^+\)] 291.13555, found 291.13544.

1-(naphthalen-2-yl)butyl acetate (3ag)

Yield: 91% (44.0 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.88 – 7.79 (m, 4H), 7.48 (dt, \(J = 6.6, 1.7\) Hz, 3H), 5.94 (t, \(J = 7.0\) Hz, 1H), 2.11 (s, 3H), 2.06 – 1.95 (m, 1H), 1.92 – 1.81 (m, 1H), 1.46 – 1.26 (m, 2H), 0.95 (t, \(J = 7.4\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.4, 138.1, 133.1, 133.0, 128.2, 128.0, 127.6, 126.1, 126.0, 124.3, 76.0, 38.2, 21.3, 18.8, 13.8. HRMS (ESI) for C\(_{18}\)H\(_{18}\)O\(_2\): calculated for [M+Na\(^+\)] 265.11990, found 265.11978.

1-(naphthalen-1-yl)butyl acetate (3ah)

Yield: 83% (40.1 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.19 (d, \(J = 8.4\) Hz, 1H), 7.88 – 7.79 (m, 4H), 7.48 (dt, \(J = 6.6, 1.7\) Hz, 3H), 5.94 (t, \(J = 7.0\) Hz, 1H), 2.11 (s, 3H), 2.06 – 1.95 (m, 1H), 1.92 – 1.81 (m, 1H), 1.46 – 1.26 (m, 2H), 0.95 (t, \(J = 7.4\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.4, 136.8,
133.8, 130.4, 128.8, 128.2, 126.1, 125.6, 125.2, 123.7, 123.3, 73.1, 38.2, 21.2, 19.1, 13.8. HRMS (ESI) for C_{16}H_{18}O_{2}: calculated for [M+Na]^+ 265.11990, found 265.11990.

1-((phenanthren-9-yl)butyl acetate (3ai)

Yield: 95% (55.5 mg). \(^{1}\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.80 – 8.74 (m, 1H), 8.68 (d, \(J = 8.1\) Hz, 1H), 8.28 – 8.21 (m, 1H), 7.96 – 7.87 (m, 1H), 7.83 (s, 1H), 7.73 – 7.57 (m, 4H), 6.60 (t, \(J = 6.6\) Hz, 1H), 2.20 (s, 3H), 2.12 – 2.05 (m, 2H), 1.57 – 1.42 (m, 2H), 0.99 (t, \(J = 7.4\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.4, 135.0, 131.2, 130.7, 130.1, 129.4, 128.7, 126.7, 126.7, 126.7, 126.3, 124.6, 124.0, 123.3, 122.4, 73.3, 37.8, 21.3, 19.2, 13.8. HRMS (ESI) for C\(_{20}\)H\(_{20}\)O\(_2\): calculated for [M+Na]^+ 315.13555, found 315.13549.

1-((4-((1,3-dioisoindolin-2-yl)methyl)phenyl)-2-methylpropyl acetate (3aj)

Yield: 54% (37.9 mg). \(^{1}\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.83 (dd, \(J = 5.4, 3.1\) Hz, 2H), 7.69 (dd, \(J = 5.5, 3.1\) Hz, 2H), 7.39 (d, \(J = 7.9\) Hz, 2H), 7.23 (d, \(J = 7.9\) Hz, 2H), 5.41 (d, \(J = 7.6\) Hz, 1H), 4.82 (s, 2H), 2.03 (s, 4H), 0.93 (d, \(J = 6.6\) Hz, 3H), 0.76 (d, \(J = 6.8\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.3, 168.0, 139.4, 135.7, 133.9, 132.1, 128.5, 127.3, 123.3, 80.6, 41.2, 33.4, 21.1, 18.6, 18.4. HRMS (ESI) for C\(_{21}\)H\(_{21}\)NO\(_4\): calculated for [M+Na]^+ 374.13628, found 374.13616.

4-(1-acetoxy-2-methylpropyl)phenyl furan-2-carboxylate (3ak)

Yield: 77% (46.5 mg). \(^{1}\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.66 (s, 1H), 7.40 – 7.29 (m, 3H), 7.18 (d, \(J = 8.2\) Hz, 2H), 6.61 – 6.55 (m, 1H), 5.48 (d, \(J = 7.6\) Hz, 1H), 2.07 (s, 4H), 0.97 (d, \(J = 6.6\) Hz, 3H), 0.81 (d, \(J = 6.8\) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta\) 170.2, 156.7, 149.5, 147.1, 143.9, 137.5, 128.2, 121.2, 119.4, 112.1, 80.2, 33.4, 21.1, 18.6, 18.4. HRMS (ESI) for C\(_{17}\)H\(_{18}\)O\(_5\): calculated for [M+Na]^+ 325.10464, found 325.10458.
4-(1-acetoxy-2-methylpropyl)phenyl thiophene-2-carboxylate (3al)

Yield: 77% (49.0 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 7.97 \) (d, \(J = 3.7 \) Hz, 1H), 7.66 (d, \(J = 4.9 \) Hz, 1H), 7.34 (d, \(J = 8.4 \) Hz, 2H), 7.23 – 7.14 (m, 3H), 5.49 (d, \(J = 7.7 \) Hz, 1H), 2.08 (s, 4H), 0.98 (d, \(J = 6.7 \) Hz, 3H), 0.82 (d, \(J = 6.7 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta 170.2, 160.4, 149.9, 137.4, 134.7, 133.5, 132.8, 128.1, 128.0, 121.3, 80.3, 33.4, 21.1, 18.6, 18.4. HRMS (ESI) for C\(_{17}\)H\(_{16}\)O\(_4\)S: calculated for [M+Na]\(^+\) 341.08180, found 341.08160.

1-(quinolin-6-yl)butyl acetate (3am, 10k)

Yield: 50% (24.3 mg) for 3am, 40% (19.5 mg) for 10k. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 8.89 \) (dd, \(J = 4.4, 1.7 \) Hz, 1H), 8.18 – 8.12 (m, 1H), 8.09 (d, \(J = 8.7 \) Hz, 1H), 7.75 (d, \(J = 1.9 \) Hz, 1H), 7.69 (dd, \(J = 8.7, 2.0 \) Hz, 1H), 7.39 (dd, \(J = 8.3, 4.2 \) Hz, 1H), 5.91 (t, \(J = 7.0 \) Hz, 1H), 2.09 (s, 3H), 2.02 – 1.92 (m, 1H), 1.87 – 1.77 (m, 1H), 1.43 – 1.23 (m, 2H), 0.93 (t, \(J = 7.4 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta 170.4, 150.5, 147.9, 139.0, 136.1, 129.8, 127.9, 127.8, 125.5, 121.3, 75.6, 38.2, 21.2, 18.7, 13.7. HRMS (ESI) for C\(_{15}\)H\(_{17}\)NO\(_2\): calculated for [M+Na]\(^+\) 266.11515, found 266.11538.

1-(pyridin-2-yl)butyl acetate (3an, 10l)

Yield: 52% (20.1 mg) for 3an, 48% (18.6 mg) for 10l. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta 8.60 \) (d, \(J = 4.8 \) Hz, 1H), 7.68 (t, \(J = 7.7 \) Hz, 1H), 7.31 (d, \(J = 7.8 \) Hz, 1H), 7.24 – 7.15 (m, 1H), 5.80 (t, \(J = 6.7 \) Hz, 1H), 2.14 (s, 3H), 1.99 – 1.87 (m, 2H), 1.46 – 1.28 (m, 2H), 0.94 (t, \(J = 7.3 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \(\delta 170.5, 159.7, 149.3, 136.6, 122.6, 120.9, 76.4, 36.9, 21.1, 18.6, 13.8. HRMS (ESI) for C\(_{11}\)H\(_{15}\)NO\(_2\): calculated for [M+Na]\(^+\) 216.09950, found 216.09955.
1-(thiophen-3-yl)butyl acetate (3ao, 10m, 11e)

![Chemical structure](image)

Yield: 66% (26.1 mg) for 3ao, 66% (26.3 mg) for 10m, 50% (19.8 mg) for 11e. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.34 – 7.27 (m, 1H), 7.27 – 7.22 (m, 1H), 7.09 (d, $J = 4.8$ Hz, 1H), 5.91 (t, $J = 7.0$ Hz, 1H), 2.08 (s, 3H), 2.00 – 1.88 (m, 1H), 1.87 – 1.75 (m, 1H), 1.44 – 1.23 (m, 2H), 0.95 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.4, 141.7, 126.0, 125.8, 122.3, 71.6, 37.6, 21.3, 18.7, 13.7. HRMS (ESI) for C$_{10}$H$_{14}$O$_2$S: calculated for [M+Na]$^+$ 221.06067, found 221.06082.

1-(thiophen-2-yl)butyl acetate (3ap, 10n)

![Chemical structure](image)

Yield: 60% (23.8 mg) for 3ap, 35% (14.0 mg) for 10n. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.28 (d, $J = 4.9$ Hz, 1H), 7.07 (d, $J = 3.5$ Hz, 1H), 7.01 – 6.94 (m, 1H), 6.07 (t, $J = 7.1$ Hz, 1H), 2.08 (s, 3H), 2.04 – 1.96 (m, 1H), 1.93 – 1.83 (m, 1H), 1.46 – 1.30 (m, 2H), 0.96 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 143.6, 126.5, 125.8, 125.1, 70.9, 38.4, 21.2, 18.9, 13.6. HRMS (ESI) for C$_{10}$H$_{14}$O$_2$S: calculated for [M+Na]$^+$ 221.06067, found 221.06084.

1-(dibenzo[b,d]thiophen-4-yl)butyl acetate (3aq)

![Chemical structure](image)

Yield: 73% (43.5 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.19 – 8.06 (m, 2H), 7.92 – 7.83 (m, 1H), 7.52 – 7.41 (m, 4H), 6.05 (dd, $J = 7.8$, 6.1 Hz, 1H), 2.16 (s, 3H), 2.14 – 1.93 (m, 2H), 1.53 – 1.29 (m, 2H), 0.96 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.2, 139.4, 136.7, 136.4, 135.4, 135.4, 126.8, 124.5, 124.5, 124.3, 122.5, 121.5, 120.9, 75.4, 36.5, 21.0, 18.9, 13.7. HRMS (ESI) for C$_{18}$H$_{18}$O$_2$S: calculated for [M+Na]$^+$ 321.09197, found 321.09189.

1-(benzo[b]thiophen-3-yl)butyl acetate (3ar)

![Chemical structure](image)

Yield: 57% (28.3 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.96 – 7.82 (m, 2H), 7.45 – 7.33 (m, 3H), 6.22 (t, $J = 6.9$ Hz, 1H), 2.09 (s, 3H), 2.07 – 1.93 (m, 2H), 1.45 – 1.31 (m, 2H), 0.95 (t, $J = 7.4$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.4, 140.7, 137.2, 135.6, 124.4, 124.1, 123.6, 122.9, 122.4, 71.0, 36.9,
21.2, 18.9, 13.7. HRMS (ESI) for C_{14}H_{16}O_{2}S: calculated for [M+Na]^+ 271.07632, found 271.07629.

1,4-phenylenebis(butane-1,1-diyl) diacetate (3as)

![Chemical structure of 3as]

Yield: 96% (58.8 mg). \(^1^H\text{NMR} (400 \text{MHz, CDCl}_3) \delta 7.28 (s, 4H), 5.75 – 5.69 (m, 2H), 2.05 (s, 6H), 1.92 – 1.82 (m, 2H), 1.76 – 1.68 (m, 2H), 1.42 – 1.31 (m, 2H), 1.28 – 1.19 (m, 2H), 0.90 (t, J = 7.4 Hz, 6H). \(^{13}C\text{NMR} (101 \text{MHz, CDCl}_3) \delta 170.4, 140.3, 126.6, 126.5, 75.6, 75.6, 38.3, 21.3, 18.7, 13.7. HRMS (ESI) for C_{18}H_{26}O_{4}: calculated for [M+Na]^+ 329.17233, found 329.17211.

4-(1-acetoxy-2-methylpropyl)phenyl bicyclo[2.2.1]hept-5-ene-2-carboxylate (3at)

![Chemical structure of 3at]

Yield: 60% (39.4 mg). \(^1^H\text{NMR} (400 \text{MHz, CDCl}_3) \delta 7.30 (d, J = 8.4 \text{ Hz, 2H}), 7.02 (d, J = 8.2 \text{ Hz, 2H}), 6.28 (dd, J = 5.8, 3.1 \text{ Hz, 1H}), 6.09 (dd, J = 6.0, 2.7 \text{ Hz, 1H}), 5.47 (d, J = 7.7 \text{ Hz, 1H}), 3.39 (s, 1H), 3.23 (dt, J = 8.4, 3.7 \text{ Hz, 1H}), 2.99 (s, 1H), 2.13 – 2.06 (m, 4H), 2.06 – 1.99 (m, 1H), 1.59 – 1.51 (m, 2H), 1.38 (d, J = 8.2 \text{ Hz, 1H}), 0.98 (d, J = 6.5 \text{ Hz, 3H}), 0.81 (d, J = 6.8 \text{ Hz, 3H}). \(^{13}C\text{NMR} (101 \text{MHz, CDCl}_3) \delta 173.1, 170.2, 150.3, 138.1, 137.0, 132.1, 128.0, 121.2, 80.3, 49.7, 45.9, 43.6, 42.6, 33.4, 29.3, 21.1, 18.6, 18.5. HRMS (ESI) for C_{20}H_{24}O_{4}: calculated for [M+Na]^+ 351.15668, found 351.15665.

4-(1-acetoxybutyl)phenyl (3r,5r,7r)-adamantane-1-carboxylate (3au, 10o, 11f)

![Chemical structure of 3au, 10o, 11f]

Yield: 92% (68.1 mg) for 3au, 80% (59.2 mg) for 10o, 78% (57.7 mg) for 11f. \(^1^H\text{NMR} (400 \text{MHz, CDCl}_3) \delta 7.32 (d, J = 7.6 \text{ Hz, 2H}), 7.01 (d, J = 7.5 \text{ Hz, 2H}), 5.73 (t, J = 6.9 \text{ Hz, 1H}), 2.08 – 2.01 (m, 12H), 1.93 – 1.83 (m, 1H), 1.78 – 1.68 (m, 7H), 1.37 – 1.20 (m, 2H), 0.90 (t, J = 7.3 \text{ Hz, 3H}). \(^{13}C\text{NMR} (101 \text{MHz, CDCl}_3) \delta 176.0, 170.2, 150.5, 138.0, 127.6, 121.4, 75.2, 40.9, 38.6, 38.2, 36.4, 27.8, 21.2, 18.7, 13.7. HRMS (ESI) for C_{23}H_{30}O_{4}: calculated for [M+Na]^+ 393.20363, found 393.20358.
4-(1-acetoxybutyl)phenyl 4-(N,N-dipropylsulfamoyl)benzoate (3av)

Yield: 77% (73.2 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.30 (d, $J$ = 7.7 Hz, 2H), 7.93 (d, $J$ = 7.7 Hz, 2H), 7.40 (d, $J$ = 7.9 Hz, 2H), 7.19 (d, $J$ = 7.7 Hz, 2H), 5.76 (t, $J$ = 6.9 Hz, 1H), 3.15 – 3.07 (m, 4H), 2.06 (s, 3H), 1.95 – 1.84 (m, 1H), 1.79 – 1.68 (m, 1H), 1.60 – 1.50 (m, 4H), 1.42 – 1.22 (m, 2H), 0.94 – 0.85 (m, 9H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 163.7, 150.0, 144.8, 138.8, 132.7, 130.7, 127.8, 127.1, 121.3, 75.1, 49.8, 38.3, 21.9, 21.2, 18.7, 13.7, 11.1. HRMS (ESI) for C$_{25}$H$_{33}$N$_2$O$_6$S: calculated for [M+Na]$^+$ 498.19208, found 498.19198.

4-(1-acetoxy-2-methylpropyl)phenyl 2-(6-methoxynaphthalen-2-yl)propanoate (3aw)

Yield: 78% (65.5 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.84 – 7.72 (m, 3H), 7.53 (d, $J$ = 8.4 Hz, 1H), 7.28 (d, $J$ = 8.3 Hz, 2H), 7.24 – 7.14 (m, 2H), 7.00 (d, $J$ = 8.3 Hz, 2H), 5.48 (d, $J$ = 7.7 Hz, 1H), 4.12 (q, $J$ = 7.1 Hz, 3H), 3.95 (s, 3H), 2.08 (s, 4H), 1.72 (d, $J$ = 7.1 Hz, 3H), 1.05 – 0.96 (m, 3H), 0.80 (d, $J$ = 6.8 Hz, 3H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 173.0, 170.2, 157.7, 150.2, 137.2, 135.0, 133.8, 129.3, 128.9, 128.0, 127.3, 126.1, 126.0, 121.0, 119.1, 105.5, 80.2, 80.2, 55.2, 45.5, 33.4, 21.1, 18.5, 18.4, 18.4. HRMS (ESI) for C$_{26}$H$_{28}$O$_5$: calculated for [M+Na]$^+$ 443.18290, found 443.18259.

4-(1-acetoxy-2-methylpropyl)phenyl 2-(4-isobutylphenyl)propanoate (3ax)

Yield: 78% (61.8 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.31 (dd, $J$ = 17.6, 7.5 Hz, 4H), 7.17 (d, $J$ = 7.5 Hz, 2H), 7.00 (d, $J$ = 8.3 Hz, 2H), 5.50 – 5.41 (m, 1H), 3.96 (q, $J$ = 7.2 Hz, 1H), 2.56 – 2.47 (m, 2H), 2.08 (d, $J$ = 1.8 Hz, 4H), 1.95 – 1.85 (m, 1H), 1.63 (d, $J$ = 7.1 Hz, 3H), 0.98 (d, $J$ = 6.6 Hz, 3H), 0.94 (d, $J$ = 6.6 Hz, 6H), 0.80 (d, $J$ = 6.8 Hz, 3H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 173.1, 170.2, 150.2, 140.8, 137.1, 137.1, 129.4, 128.0, 127.1, 121.0, 80.3, 45.2, 45.0, 33.4, 30.1, 22.3, 21.1, 18.6, 18.4, 18.4. HRMS (ESI) for C$_{25}$H$_{32}$O$_4$: calculated for [M+Na]$^+$ 419.21928, found 419.21905.
4-(1-acetoxy-2-methylpropyl)phenyl (E)-3,7-dimethylocta-2,6-dienoate (3ay)

Yield: 65% (46.5 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.32 (d, $J = 8.5$ Hz, 2H), 7.09 (d, $J = 8.5$ Hz, 2H), 5.92 (s, 1H), 5.49 (d, $J = 7.8$ Hz, 1H), 5.18 – 5.09 (m, 1H), 2.30 – 2.05 (m, 1H), 1.73 (s, 3H), 1.66 (s, 3H), 0.99 (d, $J = 6.6$ Hz, 3H), 0.82 (d, $J = 6.8$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 165.0, 163.5, 150.1, 136.9, 132.8, 128.1, 122.8, 121.5, 114.6, 80.4, 41.2, 33.5, 26.1, 25.7, 21.2, 19.2, 18.7, 18.5, 17.8.

1-((1,1’-biphenyl)-4-yl)propyl acetate (4a)

Yield: 70% (41.5 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.62 – 7.56 (m, 4H), 7.44 (q, $J = 7.8$ Hz, 4H), 7.36 (t, $J = 7.3$ Hz, 1H), 5.79 (t, $J = 7.0$ Hz, 1H), 2.10 (s, 3H), 2.01 – 1.91 (m, 1H), 1.87 – 1.76 (m, 1H), 1.38 – 1.27 (m, 6H), 0.89 (t, $J = 6.0$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.4, 140.7, 140.7, 139.8, 128.7, 127.3, 127.1, 127.0, 75.9, 36.2, 31.5, 25.2, 21.3, 14.0. HRMS (ESI) for C$_{20}$H$_{24}$O$_2$: calculated for [M+Na]$^+$ 319.16685, found 319.16675.

1-((1,1’-biphenyl)-4-yl)ethyl acetate (4b, 11g)

Yield: 76% (36.5 mg) for 4b, 65% (31.2 mg) for 11g. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.60 (t, $J = 6.6$ Hz, 4H), 7.46 (t, $J = 6.4$ Hz, 4H), 7.37 (t, $J = 7.3$ Hz, 1H), 5.96 (q, $J = 6.5$ Hz, 1H), 2.11 (s, 3H), 1.60 (d, $J = 6.6$ Hz, 3H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 170.3, 140.8, 140.7, 140.6, 128.7, 127.3, 127.2, 127.1, 126.5, 72.1, 22.1, 21.3. HRMS (ESI) for C$_{16}$H$_{16}$O$_2$: calculated for [M+Na]$^+$ 263.10425, found 263.10427.

1-((1,1’-biphenyl)-4-yl)-3-methylbutyl acetate (4c, 11h)

Yield: 90% (50.8 mg) for 4c, 62% (35.0 mg) for 11h. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.59 (t, $J = 6.6$ Hz, 4H), 7.45 (t, $J = 8.5$ Hz, 4H), 7.36 (t, $J = 7.3$ Hz, 1H), 5.90 (dd, $J = 8.1, 5.4$ Hz, 1H), 2.10 (s, 3H), 1.97 – 1.89 (m, 1H), 1.69 – 1.62 (m, 2H), 0.99 (dd, $J = 11.1, 5.9$ Hz, 6H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$
170.4, 140.7, 140.1, 128.7, 127.3, 127.2, 127.1, 127.0, 74.3, 45.3, 24.7, 22.7, 22.4, 21.3. HRMS (ESI) for C_{19}H_{22}O_{2}: calculated for [M+Na]^+ 305.15120, found 305.15118.

**1-((1,1'-biphenyl)-4-yl)-2-methylpropyl acetate (4d, 11i)**

![Chemical structure](image)

Yield: 88% (47.2 mg) for 4d, 65% (34.8 mg) for 11i. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.62 – 7.55 (m, 4H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.36 (dd, $J = 15.3$, 7.6 Hz, 3H), 5.54 (d, $J = 7.6$ Hz, 1H), 2.21 – 2.12 (m, 1H), 2.11 (s, 3H), 1.03 (d, $J = 6.6$ Hz, 3H), 0.86 (d, $J = 6.8$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.4, 140.8, 140.5, 138.7, 128.7, 127.4, 127.2, 127.0, 126.9, 80.7, 33.4, 21.2, 18.7, 18.5. HRMS (ESI) for C$_{18}$H$_{20}$O$_2$: calculated for [M+Na]$^+$ 291.13555, found 291.13568.

**1-((1,1'-biphenyl)-4-yl)-2-ethylhexyl acetate (4e)**

![Chemical structure](image)

Yield: 98% (63.5 mg). $dr = 1:1$. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.60 (dd, $J = 13.3$, 8.2 Hz, 4H), 7.46 (t, $J = 7.6$ Hz, 2H), 7.41 – 7.33 (m, 3H), 5.79 (dd, $J = 7.2$, 2.7 Hz, 1H), 2.12 (s, 3H), 1.83 (dq, $J = 12.6$, 6.9, 5.8 Hz, 1H), 1.53 – 1.21 (m, 8H), 0.95 – 0.85 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.4, 140.8, 140.4, 139.1, 128.8, 127.4, 127.3, 127.1, 126.9, 44.4, 44.2, 28.9, 28.8, 28.4, 28.2, 23.1, 22.9, 22.1, 21.5, 21.3, 14.1, 14.0, 11.0, 10.9. HRMS (ESI) for C$_{22}$H$_{28}$O$_2$: calculated for [M+Na]$^+$ 347.19815, found 347.19833.

**1-((1,1'-biphenyl)-4-yl)-2-methylbutyl acetate (4f)**

![Chemical structure](image)

Yield: 96% (54.1 mg). $dr = 1.7:1$. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.58 (t, $J = 9.2$ Hz, 4H), 7.44 (t, $J = 7.4$ Hz, 2H), 7.41 – 7.32 (m, 3H), 5.65 (dd, $J = 32.5$, 7.2 Hz, 1H), 2.16 – 2.09 (m, 3H), 2.00 – 1.84 (m, 1H), 1.48 – 1.35 (m, 1H), 1.22 – 1.08 (m, 1H), 0.99 – 0.90 (m, 6H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 140.7, 140.4, 139.0, 128.7, 127.6, 127.2, 127.0, 126.9, 126.8, 79.6, 79.1, 40.2, 39.6, 25.5, 25.0, 21.2, 21.1, 14.9, 14.5, 11.4, 11.2. HRMS (ESI) for C$_{19}$H$_{22}$O$_2$: calculated for [M+Na]$^+$ 305.15120, found 305.15155.
1-[(1,1'-biphenyl)-4-yl]-2,2-dimethylpropyl acetate (4g)

Yield: 63% (35.5 mg). $^1$H NMR (500 MHz, CDCl$_3$) δ 7.57 (dd, $J = 25.2$, 7.3 Hz, 4H), 7.44 (t, $J = 7.1$ Hz, 2H), 7.35 (d, $J = 7.4$ Hz, 3H), 5.55 (s, 1H), 2.13 (s, 3H), 0.98 (s, 9H). $^{13}$C NMR (126 MHz, CDCl$_3$) δ 170.3, 140.8, 140.3, 137.5, 128.7, 128.1, 127.2, 127.0, 126.3, 82.6, 35.1, 26.0, 21.2. HRMS (ESI) for C$_{18}$H$_{22}$O$_2$: calculated for [M+Na]$^+$ 305.15120, found 305.15146.

[1,1'-biphenyl]-4-yl(cyclohexyl)methyl acetate (4h)

Yield: 88% (54.2 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.62–7.55 (m, 4H), 7.45–7.40 (m, 4H), 7.35 (t,$J = 7.3$ Hz, 1H), 5.61 (dd, $J = 7.7$, 6.0 Hz, 1H), 2.49–2.37 (m, 2H), 2.09 (s, 3H), 1.91–1.82 (m, 1H), 1.74–1.54 (m, 4H), 1.52–1.42 (m, 2H), 1.26–1.16 (m, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.4, 140.7, 140.5, 138.7, 128.7, 127.5, 127.2, 127.0, 126.9, 80.0, 42.8, 28.9, 26.2, 25.8, 25.8, 21.2. HRMS (ESI) for C$_{21}$H$_{24}$O$_2$: calculated for [M+Na]$^+$ 331.16685, found 331.16696.

[1,1'-biphenyl]-4-yl(cyclopentyl)methyl acetate (4i)

Yield: 94% (55.3 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.62–7.55 (m, 4H), 7.47–7.40 (m, 4H), 7.35 (t, $J = 7.3$ Hz, 1H), 5.61 (d, $J = 9.1$ Hz, 1H), 2.49–2.37 (m, 1H), 2.09 (s, 3H), 1.91–1.82 (m, 1H), 1.74–1.54 (m, 4H), 1.52–1.42 (m, 2H), 1.26–1.16 (m, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) δ 170.4, 140.7, 140.6, 139.6, 128.7, 127.4, 127.2, 127.0, 127.0, 79.7, 45.4, 29.6, 29.2, 25.2, 25.2, 21.2. HRMS (ESI) for C$_{20}$H$_{22}$O$_2$: calculated for [M+Na]$^+$ 317.15120, found 317.15127.

1-[(1,1'-biphenyl)-4-yl]-3-phenylpropyl acetate (4j)

Yield: 91% (60.1 mg). $^1$H NMR (400 MHz, CDCl$_3$) δ 7.62 (dd, $J = 8.0$, 1.7 Hz, 4H), 7.52–7.43 (m, 4H), 7.39 (t, $J = 7.3$ Hz, 1H), 7.33 (t, $J = 7.3$ Hz, 2H), 7.26–7.20 (m, 3H), 5.85 (dd, $J = 7.7$, 6.0 Hz, 1H), 2.78–2.63 (m, 2H), 2.35 (td, $J = 13.9$, 8.7 Hz, 1H), 2.24–2.15 (m, 1H), 2.13 (s, 3H). $^{13}$C NMR
(101 MHz, CDCl$_3$) $\delta$ 170.5, 141.2, 141.0, 140.8, 139.5, 128.8, 128.5, 128.4, 127.4, 127.3, 127.2, 127.1, 126.1, 75.4, 37.8, 31.9, 21.3. HRMS (ESI) for C$_{23}$H$_{22}$O$_2$: calculated for [M+Na]$^+$ 353.15120, found 353.15124.

1-((1,1'-biphenyl)-4-yl)-3-(benzo[d][1,3]dioxol-5-yl)-2-methylpropyl acetate (4k)

Yield: 77% (59.8 mg). $dr = 1.7:1$, $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.60 (t, $J = 7.1$ Hz, 4H), 7.51 – 7.29 (m, 5H), 6.74 (t, $J = 7.3$ Hz, 1H), 6.68 – 6.56 (m, 2H), 5.93 (d, $J = 3.9$ Hz, 2H), 5.73 (d, $J = 5.1$ Hz, 0.63H), 5.68 (d, $J = 6.3$ Hz, 0.37H), 2.74 – 2.51 (m, 1H), 2.34 – 2.19 (m, 2H), 2.14 (d, $J = 12.8$ Hz, 3H), 1.87 – 1.78 (m, 1H), 1.42 – 1.29 (m, 12H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 147.6, 145.8, 140.8, 138.7, 134.1, 128.8, 127.6, 127.4, 127.2, 127.1, 127.1, 122.0, 122.0, 109.5, 109.3, 108.1, 108.1, 100.8, 79.7, 78.7, 41.2, 40.4, 39.2, 38.7, 21.3, 21.2, 15.4, 14.7. HRMS (ESI) for C$_{25}$H$_{24}$O$_4$: calculated for [M+Na]$^+$ 411.15668, found 411.15695.

1-((1,1'-biphenyl)-4-yl)-2-(benzyloxy)ethyl acetate (4l)

Yield: 41% (28.5 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.59 (d, $J = 8.0$ Hz, 4H), 7.51 – 7.42 (m, 4H), 7.41 – 7.36 (m, 3H), 7.35 – 7.31 (m, 3H), 6.07 (dd, $J = 7.9$, 4.0 Hz, 1H), 4.63 – 4.59 (m, 2H), 3.85 (dd, $J = 10.8$, 7.9 Hz, 1H), 3.72 (dd, $J = 10.9$, 4.1 Hz, 1H), 2.17 (s, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.3, 141.3, 140.7, 137.9, 136.6, 128.8, 128.4, 127.7, 127.4, 127.3, 127.2, 127.2, 74.3, 73.2, 72.6, 21.3. HRMS (ESI) for C$_{23}$H$_{22}$O$_2$: calculated for [M+Na]$^+$ 369.14612, found 369.14605.

1-((1,1'-biphenyl)-4-yl)undec-10-en-1-yl acetate (4m)

Yield: 75% (54.6 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.63 – 7.57 (m, 4H), 7.49 – 7.41 (m, 4H), 7.37 (t, $J = 7.3$ Hz, 1H), 5.95 – 5.72 (m, 2H), 5.07 – 4.91 (m, 2H), 2.12 (s, 3H), 2.08 – 2.03 (m, 2H), 2.00 – 1.92 (m, 1H), 1.87 – 1.78 (m, 1H), 1.42 – 1.29 (m, 12H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.5, 140.8, 140.8, 139.9, 139.2, 128.8, 127.3, 127.2, 127.1, 127.0, 114.2, 76.0, 36.3, 33.8, 29.4, 29.4, 29.3, 29.1, 28.9, 25.6, 21.4. HRMS (ESI) for C$_{23}$H$_{32}$O$_2$: calculated for [M+Na]$^+$ 387.22945, found 387.22940.
1-([1,1'-biphenyl]-4-yl)-2-methylpropyl pivalate (4n, 11j)

Yield: 76% (47.1 mg) for 4n, 70% (43.4 mg) for 11j. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.57 (dd, $J = 14.0$, 7.9 Hz, 4H), 7.44 (t, $J = 7.5$ Hz, 2H), 7.35 (d, $J = 7.7$ Hz, 3H), 5.50 (d, $J = 7.0$ Hz, 1H), 2.18–2.09 (m, 1H), 1.25 (s, 9H), 1.01 (d, $J = 6.7$ Hz, 3H), 0.88 (d, $J = 6.9$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 177.5, 140.8, 140.3, 139.1, 128.7, 127.2, 127.1, 127.0, 126.8, 80.2, 38.9, 33.8, 27.2, 18.9, 18.2. HRMS (ESI) for C$_{21}$H$_{26}$O$_2$: calculated for [M+Na]$^+$ 333.18250, found 333.18258.

1-([1,1'-biphenyl]-4-yl)-2-methylpropyl benzoate (4o)

Yield: 52% (34.3 mg). $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 8.13 (d, $J = 7.4$ Hz, 2H), 7.63–7.54 (m, 5H), 7.49–7.41 (m, 6H), 7.34 (t, $J = 7.2$ Hz, 1H), 5.79 (d, $J = 6.9$ Hz, 1H), 2.37–2.23 (m, 1H), 1.11 (d, $J = 6.0$ Hz, 3H), 0.96 (d, $J = 6.1$ Hz, 3H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 165.9, 140.8, 140.6, 138.8, 133.0, 130.6, 129.7, 128.8, 128.4, 127.4, 127.3, 127.1, 127.0, 81.3, 33.9, 18.9, 18.5. HRMS (ESI) for C$_{23}$H$_{22}$O$_2$: calculated for [M+Na]$^+$ 353.15120, found 353.15130.

1-phenylpentan-1-ol (4p)

Yield: 81% (26.5 mg). $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.41–7.34 (m, 4H), 7.34–7.28 (m, 1H), 4.68 (dd, $J = 7.4$, 6.0 Hz, 1H), 1.94 (s, 1H), 1.88–1.68 (m, 2H), 1.46–1.23 (m, 4H), 0.92 (t, $J = 7.1$ Hz, 3H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 145.0, 128.4, 127.5, 125.9, 74.7, 38.8, 28.0, 22.6, 14.0.

(E)-4-methyl-1-phenylpent-1-en-3-yl acetate (8a)

Yield: 70% (30.5 mg). $E:Z = 5:1, ^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.37 (dt, $J = 22.8$, 7.5 Hz, 4H), 7.30–7.25 (m, 1H), 6.62 (d, $J = 16.0$ Hz, 1H), 6.14 (dd, $J = 15.9$, 7.6 Hz, 0.84H), 5.65–5.56 (m, 0.29H), 5.23 (t, $J = 7.0$ Hz, 0.84H), 2.12 (s, 2.53H), 2.07 (s, 0.43H), 0.99 (t, $J = 6.6$ Hz, 5H), 0.92 (dd, $J = 6.8$, 2.3 Hz, 1H). $^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 170.5, 136.5, 133.3, 128.6, 127.9, 126.6, 126.1, 79.4, 32.3,
21.3, 18.3, 18.2. HRMS (ESI) for C\textsubscript{14}H\textsubscript{18}O\textsubscript{2}: calculated for [M+Na]\textsuperscript{+} 241.11990, found 241.11991.

**(E)-4-methyl-1-(4-(trifluoromethyl)phenyl)pent-1-en-3-yl acetate (8b)**

Yield: 63% (36.0 mg). \(E:Z = 5:1\). \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta 7.60 (d, J = 8.0 \text{ Hz}, 2H), 7.48 (d, J = 8.0 \text{ Hz}, 2H), 6.63 (d, J = 11.9 \text{ Hz}, 1H), 5.67 (dd, J = 11.8, 9.7 \text{ Hz}, 1H), 5.46 (dd, J = 9.6, 6.5 \text{ Hz}, 1H), 2.04 (s, 3H), 1.94 – 1.83 (m, 1H), 0.88 (t, J = 6.4 \text{ Hz}, 6H). \(^{13}\)C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta 170.4, 140.2, 131.2, 130.7, 128.8, 125.3, 125.3, 125.2, 75.1, 32.6, 21.1, 18.0, 17.9.\) HRMS (ESI) for C\textsubscript{15}H\textsubscript{17}F\textsubscript{3}O\textsubscript{2}: calculated for [M+Na]\textsuperscript{+} 309.10729, found 309.10730.

**1-(1H-inden-2-yl)-2-methylpropyl acetate (8c)**

Yield: 52% (23.9 mg). \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta 7.45 (d, J = 7.3 \text{ Hz}, 1H), 7.37 (d, J = 7.5 \text{ Hz}, 1H), 7.28 (t, J = 7.4 \text{ Hz}, 1H), 7.20 (t, J = 7.4 \text{ Hz}, 1H), 6.78 (s, 1H), 5.54 (d, J = 7.3 \text{ Hz}, 1H), 3.42 (s, 2H), 2.12 (s, 4H), 1.02 (d, J = 6.7 \text{ Hz}, 3H), 0.95 (d, J = 6.8 \text{ Hz}, 3H). \(^{13}\)C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta 170.4, 146.5, 144.2, 142.9, 129.6, 126.4, 124.6, 123.6, 121.0, 77.7, 38.3, 32.1, 21.1, 18.9, 18.2.\) HRMS (ESI) for C\textsubscript{15}H\textsubscript{18}O\textsubscript{2}: calculated for [M+Na]\textsuperscript{+} 253.11990, found 253.12041.

**(E)-4-methyl-1-(thiophen-2-yl)pent-1-en-3-yl acetate (8d)**

Yield: 45% (20.2 mg). \(E:Z = 4:1\). \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta 7.16 (d, J = 4.6 \text{ Hz}, 1H), 6.96 (d, J = 4.7 \text{ Hz}, 2H), 6.72 (d, J = 15.7 \text{ Hz}, 1H), 5.94 (dd, J = 15.7, 7.6 \text{ Hz}, 1H), 5.15 (t, J = 7.1 \text{ Hz}, 1H), 2.08 (s, 3H), 1.97 – 1.88 (m, 1H), 0.95 (t, J = 6.3 \text{ Hz}, 6H). \(^{13}\)C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta 170.4, 141.5, 127.4, 126.5, 126.3, 125.7, 124.5, 79.1, 32.2, 21.2, 18.2, 18.1.\) HRMS (ESI) for C\textsubscript{12}H\textsubscript{16}O\textsubscript{2}S: calculated for [M+Na]\textsuperscript{+} 247.07632, found 247.07675.

**(E)-4-methyl-1-(trimethylsilyl)pent-1-en-3-yl acetate (8e)**

Yield: 50% (21.6 mg). \(^1\)H NMR (400 MHz, CDCl\textsubscript{3}) \(\delta 5.98 – 5.75 (m, 2H), 5.05 (t, J = 5.5 \text{ Hz}, 1H), 2.08 (s, 3H), 1.91 – 1.80 (m, 1H), 0.89 (d, J = 6.8 \text{ Hz}, 6H), 0.66 (s, 9H). \(^{13}\)C NMR (101 MHz, CDCl\textsubscript{3}) \(\delta 170.4, 24.0, 23.5, 22.1, 18.9, 18.2.\) HRMS (ESI) for C\textsubscript{12}H\textsubscript{16}O\textsubscript{2}S: calculated for [M+Na]\textsuperscript{+} 255.11990, found 255.12041.
HRMS (ESI) for \( \text{C}_{11}\text{H}_{22}\text{O}_{2}\text{Si} \): calculated for \([\text{M+Na}]^+\) 237.12813, found 237.12819.

4-methyl-1-(triisopropylsilyl)pent-1-yn-3-yl acetate (8f)

Yield: 46% (27.2 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 5.25 (d, \( J = 5.5 \) Hz, 1H), 2.07 (s, 3H), 2.03 – 1.94 (m, 1H), 1.06 (s, 21H), 1.03 (d, \( J = 6.6 \) Hz, 3H), 1.00 (d, \( J = 6.8 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 169.9, 103.3, 87.0, 69.4, 32.4, 21.0, 18.5, 18.3, 17.4, 11.1.

HRMS (ESI) for \( \text{C}_{17}\text{H}_{32}\text{O}_{2}\text{Si} \): calculated for \([\text{M+Na}]^+\) 319.20638, found 319.20620.

5-methyl-1-(triisopropylsilyl)hex-1-yn-3-yl acetate (8g)

Yield: 53% (32.9 mg). \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 5.43 (t, \( J = 7.2 \) Hz, 1H), 2.06 (s, 3H), 1.86 – 1.78 (m, 1H), 1.68 – 1.61 (m, 2H), 1.05 (s, 18H), 0.94 (d, \( J = 6.6 \) Hz, 6H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 169.9, 105.0, 86.4, 63.4, 43.7, 24.9, 22.6, 22.3, 18.5, 11.1. HRMS (ESI) for \( \text{C}_{18}\text{H}_{34}\text{O}_{2}\text{Si} \): calculated for \([\text{M+Na}]^+\) 333.22203, found 333.22192.

2-methyl-4-oxo-6-phenylhexan-3-yl acetate (8h, 11k)

Yield: 50% (24.9 mg) for 8h, 45% (22.3 mg) for 11k. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 7.34 – 7.27 (m, 2H), 7.21 (t, \( J = 6.6 \) Hz, 3H), 4.90 (d, \( J = 4.3 \) Hz, 1H), 2.98 – 2.66 (m, 4H), 2.26 – 2.18 (m, 1H), 2.17 (s, 3H), 0.98 (d, \( J = 6.9 \) Hz, 3H), 0.88 (d, \( J = 6.8 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \) 206.45, 170.76, 140.85, 128.45, 128.35, 126.13, 82.55, 41.26, 29.52, 29.04, 28.93, 20.58, 19.20, 19.13, 17.61, 16.76. HRMS (ESI) for \( \text{C}_{15}\text{H}_{20}\text{O}_{3} \): calculated for \([\text{M+Na}]^+\) 271.13047, found 271.13055.

1-cyclohexyl-3-methyl-1-oxobut-2-yl acetate (8i, 11l)

Yield: 50% (22.8 mg) for 8i, 43% (19.5 mg) for 11l. \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 5.04 (d, \( J = 3.5 \) Hz, 1H), 2.57 – 2.43 (m, 1H), 2.31 – 2.20 (m, 1H), 2.13 (s, 3H), 1.81 – 1.74 (m, 2H), 1.67 – 1.62 (m, 2H), 1.32 – 1.19 (m, 6H), 1.01 (d, \( J = 6.9 \) Hz, 3H), 0.87 (d, \( J = 6.8 \) Hz, 3H). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)) \( \delta \)
209.7, 170.6, 81.4, 47.4, 29.3, 29.0, 27.6, 25.8, 25.7, 25.3, 20.6, 19.6, 16.6. HRMS (ESI) for C_{13}H_{22}O_{3}: calculated for [M+Na]^+ 249.14612, found 249.14613.

3-methyl-1-oxo-1-(p-tolyl)butan-2-yl acetate (8j)

Yield: 61% (28.5 mg). ^1^H NMR (400 MHz, CDCl$_3$) $\delta$ 7.87 (d, $J$ = 7.9 Hz, 2H), 7.28 (d, $J$ = 7.9 Hz, 2H), 5.74 (d, $J$ = 4.7 Hz, 1H), 2.43 (s, 3H), 2.36 – 2.23 (m, 1H), 2.18 (s, 3H), 1.05 (d, $J$ = 6.9 Hz, 3H), 0.94 (d, $J$ = 6.8 Hz, 3H). ^1^C NMR (101 MHz, CDCl$_3$) $\delta$ 196.2, 170.8, 144.3, 133.0, 129.4, 128.5, 79.2, 30.2, 21.6, 20.6, 19.5, 16.9. HRMS (ESI) for C$_{14}$H$_{18}$O$_{3}$: calculated for [M+Na]$^+$ 257.11482, found 257.11490.

1-(4-methoxyphenyl)-3-methyl-1-oxobutan-2-yl acetate (8k)

Yield: 64% (32.3 mg). ^1^H NMR (400 MHz, CDCl$_3$) $\delta$ 7.94 (d, $J$ = 8.6 Hz, 2H), 6.93 (d, $J$ = 8.6 Hz, 2H), 5.69 (d, $J$ = 4.9 Hz, 1H), 3.86 (s, 3H), 2.32 – 2.22 (m, 1H), 2.15 (s, 3H), 1.01 (d, $J$ = 6.9 Hz, 3H), 0.93 (d, $J$ = 6.8 Hz, 3H). ^1^C NMR (101 MHz, CDCl$_3$) $\delta$ 195.0, 170.8, 143.3, 133.0, 129.4, 128.5, 79.0, 55.4, 30.3, 20.6, 19.4, 17.0. HRMS (ESI) for C$_{14}$H$_{18}$O$_{4}$: calculated for [M+Na]$^+$ 273.10973, found 273.10961.

1-(4-bromophenyl)ethyl acetate (16)

Yield: 73% (2 mmol scale, 351.9 mg). ^1^H NMR (400 MHz, CDCl$_3$) $\delta$ 7.50 (d, $J$ = 8.1 Hz, 2H), 7.25 (d, $J$ = 8.1 Hz, 2H), 5.84 (q, $J$ = 6.6 Hz, 1H), 2.09 (s, 3H), 1.53 (d, $J$ = 6.6 Hz, 3H). ^1^C NMR (101 MHz, CDCl$_3$) $\delta$ 170.2, 140.7, 131.7, 127.9, 121.8, 71.7, 22.1, 21.3. HRMS (ESI) for C$_{10}$H$_{11}$BrO$_{2}$: calculated for [M+Na]$^+$ 264.98346, found 264.98361.
7. **Computational Methods and Details**

7.1 **Computational Methods**

All DFT-calculations were performed using Gaussian 16, Revision B.01. The geometry optimization and frequency analysis were performed using meta-hybrid-GGA DFT functional oB97xD.[5] The triple-ζ basis set Def2-TZVP was used for Ni, Mn, and I atoms and the split-valence plus one polarization function Def2-SVP basis set was used for other atoms.[6] In all cases, the default integral grid (Ultrafine Grid) was employed. Frequency calculations were performed in order to obtain thermal corrections (298 K) and to confirm the nature of the stationary points (minima with no imaginary frequency or transition states with one imaginary frequency). All transition states were optimized using the default Berny algorithm implemented in the Gaussian 16 code.[4] For transition state structures, IRC calculations were undertaken to confirm that the transition states were connected to the correct minima. For further validation of energetics, single-point calculations were performed on the oB97xD/Def2-SVP optimized geometries using meta-hybrid GGA functional M06[7] employing a valence triple-ζ-type of basis set Def2-TZVPP[6] for all atoms. The solvent effects (n,n-DiMethylAcetamide (DMA): \( \varepsilon = 37.781 \)) were evaluated implicitly by a self-consistent reaction field (SCRF) approach for all the intermediates and transition states, using the SMD continuum solvation model.[8] Unless specified otherwise, \( \Delta G \) was used throughout the text. The \( \Delta G \) value was obtained by augmenting the \( E_{el} \) energy terms at M06(SMD-DMA)/Def2-TZVPP with the respective free energy corrections at the oB97xD/Def2-TZVP(Ni, Mn, I)/Def2-SVP(other atoms) level in gas phase. The geometries were realized using CYLview20, Build 0001.[9] The wavefunction analysis were performed using Multiwfn 3.7.[10] VMD was used to visualize the spin density.[11]
8. References


9. Cartesian Coordinates and Energies of Calculated Structures (in Hartree)

SA1 (iodobenzene):

\[ E_{el} = -529.316715 \]

Zero-point correction = 0.091121
Thermal correction to Energy = 0.096911
Thermal correction to Enthalpy = 0.097856
Thermal correction to Gibbs Free Energy = 0.059462

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SB1 (1-iodoethyl acetate):

$E_{el} = -604.812517$

Zero-point correction = 0.108745
Thermal correction to Energy = 0.116996
Thermal correction to Enthalpy = 0.117940
Thermal correction to Gibbs Free Energy = 0.073881

SB2:

$E_{el} = -306.978888$

Zero-point correction = 0.104460
Thermal correction to Energy = 0.111845
Thermal correction to Enthalpy = 0.112789
Thermal correction to Gibbs Free Energy = 0.072352
H     2.89908600  -0.77152800  -0.76549100  
O     0.24197400  -0.52443700  -0.02146000  
C     -1.08461100  -0.22181100   0.00458600  
O     -1.87455900  -1.11815100  -0.02114600  
C     -1.45135900   1.23877300   0.07748700  
H     -2.53104600  1.31196200   0.24531500  
H     -0.90351100  1.74606500   0.88463400  
H     -1.20244500  1.74823500  -0.86593700  

Mn:

\( E_{el} = -1150.787453 \)  
Zero-point correction = 0.000000  
Thermal correction to Energy = 0.001416  
Thermal correction to Enthalpy = 0.002360  
Thermal correction to Gibbs Free Energy = -0.016317  

Mn    0.00000000  0.00000000  0.00000000  

MnI₂:

\( E_{el} = -1746.485439 \)  
Zero-point correction = 0.001210  
Thermal correction to Energy = 0.005928  
Thermal correction to Enthalpy = 0.006872  
Thermal correction to Gibbs Free Energy = -0.031796  

Mn    0.00000000  0.00000000  0.28100300  
I     0.00000000  2.40311100  -0.06627400  
I     0.00000000 -2.40311100  -0.06627400  

1-phenylethyl acetate:

\( E_{el} = -538.599126 \)  
Zero-point correction = 0.200846  
Thermal correction to Energy = 0.212257  
Thermal correction to Enthalpy = 0.213201  
Thermal correction to Gibbs Free Energy = 0.162580  

C     -0.68023700   1.14646000  -0.16302200  
H     -0.91608000   1.29129200  -1.23124300  
C     -0.62890800   2.51009900   0.51049300  
H     -1.59681900   3.02088600   0.40938100  
H     -0.40162400   2.39311600   1.57967300  
H     0.15499500   3.12924600   0.05252300
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\[ E_d = -2606.613728 \]
Zero-point correction = 0.242514
Thermal correction to Energy = 0.260565
Thermal correction to Enthalpy = 0.261509
Thermal correction to Gibbs Free Energy = 0.192262
H  4.57922800  1.24291200  -0.00078500  
C  3.64484400  -0.67912200  -0.00059400  
H  4.58092500  -1.23765300  -0.00075200  
I  -4.01218900  -0.00125000  0.00063500  
O  3.51001400  3.48450700  -0.00062100  
O  3.51480700  -3.48070400  -0.00056400  
C  3.52279300  4.89362500  -0.00066100  
H  4.57633800  5.19417500  -0.00083900  
H  3.03026400  5.29746000  -0.90021900  
H  3.03055200  5.29750500  -0.89903400  
C  3.52952800  -4.88980300  -0.00077700  
H  4.58348600  -5.18890000  -0.00078100  
H  3.03765900  -5.29444500  -0.89877900  
H  3.03773800  -5.29423000  -0.90047300  

A-BTS:

\[ E_a = -3135.927023 \]

Zero-point correction = 0.333634
Thermal correction to Energy = 0.358741
Thermal correction to Enthalpy = 0.359685
Thermal correction to Gibbs Free Energy = 0.274223

C  1.81070600  -0.58081000  -0.29266200  
C  3.04880400  -1.23029800  -0.17846600  
C  3.02610500  -2.65373400  -0.07998800  
C  1.80236400  -3.30532200  -0.11587100  
C  0.62915200  -2.54439000  -0.24750300  
N  0.62912100  -1.23161200  -0.32902400  
H  1.72125000  -4.38893100  -0.05188200  
H  -0.35013700  -3.02926700  -0.29789900  
C  1.76634100  0.85726200  -0.38928700  
C  2.96718000  1.58339300  -0.39629500  
N  0.54206500  1.43499300  -0.46675600  
C  2.87020800  3.00149200  -0.52108200  
C  0.48030800  2.74646800  -0.58609500  
C  1.61147100  3.57608000  -0.62503300  
H  -0.52089700  3.18181300  -0.64228400  
H  1.47128600  4.65069200  -0.72758700  
Ni  -1.04136700  0.04687700  -0.32636900  
C  4.21939700  0.89456300  -0.28259900  
H  5.13685600  1.48286300  -0.28694800  
C  4.25819500  -0.46198400  -0.17200800  
H  5.20805600  -0.98934500  -0.08359000  
I  -2.72768400  1.58356100  0.98749800
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**B:**

\[ E_{a1} = -3135.933141 \]

Zero-point correction = 0.334625
Thermal correction to Energy = 0.360268
Thermal correction to Enthalpy = 0.361212
Thermal correction to Gibbs Free Energy = 0.274310

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C    3.87384500   1.53894600   0.25865600
H    4.65622900   2.28910900   0.37276600
C    4.18495200   0.22279500   0.09721200
H    5.22308700  -0.10864500   0.07905200
I    -3.37459500   0.52711600   0.36365600
I    -1.15130300  -0.36911900  -2.75307100
C    -1.16349600  -0.93112100   1.70594400
C    -0.59930800  -0.24621400   2.77930500
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H    -1.77337900  -3.92252800   3.21244200
H    -0.72760300  -2.71759800   5.12875300
O     4.69784100  -2.50626000  -0.27379800
O     3.10148900   4.21772200   0.55150800
C     5.03886800  -3.85926400  -0.47798800
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Cl:

E_{el} = -2838.147971
Zero-point correction = 0.334522
Thermal correction to Energy = 0.357581
Thermal correction to Enthalpy = 0.358526
Thermal correction to Gibbs Free Energy = 0.279805

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C    -2.46949900   1.97992100  -0.00005300
C    -2.05341800   3.34430600  -0.00014300
C    -0.69421500   3.61866700  -0.00015900
C     0.22521700   2.55885000  -0.00007800
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C2:

\[ E_d = -2904.417796 \]
Zero-point correction = 0.244501
Thermal correction to Energy = 0.264231
Thermal correction to Enthalpy = 0.265175
Thermal correction to Gibbs Free Energy = 0.192350
D:

\[ E_{el} = -2540.306198 \]
\[ \text{Zero-point correction} = 0.331926 \]
\[ \text{Thermal correction to Energy} = 0.353424 \]
\[ \text{Thermal correction to Enthalpy} = 0.354368 \]
\[ \text{Thermal correction to Gibbs Free Energy} = 0.278848 \]

\[
\begin{align*}
C & \quad -1.43053500 \quad -0.50254500 \quad -0.00370600 \\
C & \quad -2.83052500 \quad -0.58417900 \quad 0.02601700
\end{align*}
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**D-CTS:**

\[ E_d = -3145.119905 \]

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Thermal correction to Enthalpy = 0.472595
Thermal correction to Gibbs Free Energy = 0.373408

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**D-CTS2:**

E<sub>d</sub> = -3145.108344

Zero-point correction = 0.440124

Thermal correction to Energy = 0.471621

Thermal correction to Enthalpy = 0.472565

Thermal correction to Gibbs Free Energy = 0.372626
D-CTS3:

$E_{el} = -3145.094295$

Zero-point correction = 0.439769

Thermal correction to Energy = 0.471179

Thermal correction to Enthalpy = 0.472123

Thermal correction to Gibbs Free Energy = 0.372372

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C  -2.33832600  2.25270400  1.01160600
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$E_{el} = -3145.094295$

Zero-point correction = 0.439769

Thermal correction to Energy = 0.471179

Thermal correction to Enthalpy = 0.472123

Thermal correction to Gibbs Free Energy = 0.372372
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Thermal correction to Enthalpy = 0.472778

Thermal correction to Gibbs Free Energy = 0.376878
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E:

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Thermal correction to Enthalpy = 0.475005
Thermal correction to Gibbs Free Energy = 0.378613

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N  -0.69744700  -1.36723000   0.05658100
C   -3.37742100  -2.17036100   0.15706200
C  -1.01959300  -2.62821500   0.36116200
C   -2.52748900  -4.14282700   0.48170400
Ni   1.15132800  -0.51458600   0.18518700
H  -5.09022800  -0.06932200  -0.24263000
C   -3.67167500   1.49124900  -0.57952400
H   -4.42024800   2.26350300  -0.75448000
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C   2.93207600   0.14787100   0.56513100
C   3.17558000   1.45757700   0.99759500
C   4.03822500  -0.70368200   0.42795700
C   4.47060000   1.91826200   1.24751600
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C   5.33193200  -0.25589900   0.69770900
H   3.89885000  -1.73081000   0.08324300
C   5.55722400   1.06028800  -0.09944800
H   4.62565900   2.95071800   1.57201300
H   6.17355400  -0.94301500   0.57870800
H   6.57180800   1.41218500   1.29941000
O  -4.67412000  -2.46700600   0.20480300
O  -2.78218100   4.06643900  -1.23093100
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H  -1.85098700   5.38527300  -2.54210100
C   0.94231600  -0.39029500   2.16685400
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E-ATS:

$E_d = -3145.141752$

Zero-point correction = 0.442461
Thermal correction to Energy = 0.473012
Thermal correction to Enthalpy = 0.473956
Thermal correction to Gibbs Free Energy = 0.377983

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C  1.77803300  -3.32719200  0.78315800
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N  0.67689700  -1.36776300  -0.04446800
H  1.66513500  -4.36401300  1.09497500
H  -0.33599200  -3.11095100  0.31351600
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C  3.07279700  1.36944400  -0.47200500
N  0.66583200  1.20896900  -0.79490400
C  3.02797300  2.73463500  -0.88294800
C  0.65618400  2.47691400  -1.16326400
C  1.80310900  3.28119300  -1.23088300
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C  4.29008300  0.72474900  -0.07680100
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C  -1.70294700  0.19845200  1.18237600
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10. Copies of NMR Spectra
8d. E/Z = 4:1

[Chemical structure image]

[Graphical representation of chemical spectra]

[Chemical structure image]