Electron Transfer Reduction of Unactivated Esters using SmI$_2$-H$_2$O

Michal Szostak, Malcolm Spain and David J. Procter*

School of Chemistry, University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

david.j.procter@manchester.ac.uk

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Corresponding Author:

Professor David J. Procter
School of Chemistry
University of Manchester
Oxford Road
Manchester, M13 9PL
United Kingdom
### Additional Optimization Data

**Table ESI-1.** Optimization of reduction of hydrocinnamic methyl ester with SmI$_2$.\(^a\)

<table>
<thead>
<tr>
<th>entry</th>
<th>amine</th>
<th>proton source</th>
<th>equiv (amine)</th>
<th>equiv (proton source)</th>
<th>time(^b)</th>
<th>conversion(^c) [%]</th>
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<td>Et$_3$N</td>
<td>H$_2$O</td>
<td>12</td>
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<td>5 min</td>
<td>96</td>
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<tr>
<td>2</td>
<td>(i)-Pr$_2$NH</td>
<td>H$_2$O</td>
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<td>24 h</td>
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<td>8</td>
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<td>24 h</td>
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<td>-</td>
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<td>24 h</td>
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<td>800</td>
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\(^a\)All reactions carried out using standard Schlenk techniques for handling air-sensitive reagents.

\(^b\)Quenched by bubbling air through reaction mixtures. Determined by GC or $^1$H NMR.
Table ESI-2. Optimization of reduction of hydrocinnamic acid tert-butyl ester with SmI₂-H₂O.ᵃ

<table>
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<th>SmI₂ (equiv)</th>
<th>H₂O (equiv)</th>
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<th>timeᵇ</th>
<th>conversionᶜ [%]</th>
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ᵃᵇᶜ See, Table ESI-1.

Table ESI-3. Optimization of reduction of methyl adamantane-1-carboxylate with SmI₂-H₂O.ᵃ

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<th>SmI₂ (equiv)</th>
<th>H₂O (equiv)</th>
<th>amine (equiv)</th>
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ᵃᵇᶜ See, Table ESI-1.

ESI-3
Figure ESI-1. Influence of concentration of water on reduction of hydrocinnamic acid methyl ester.

Interestingly, we have determined that the rate of reduction of hydrocinnamic acid methyl ester with SmI$_2$-H$_2$O-Et$_3$N does not exhibit a linear dependence on concentration of water (Figure ESI-1). Detailed studies on the mechanism and kinetic profile of the reduction of unactivated esters with SmI$_2$ are in progress and will be disclosed in a full account of this work.
List of Known Compounds

All compounds used in this study have been described in literature or are commercially available. Esters were purchased from commercial suppliers or prepared by standard methods.\textsuperscript{1-9} Samarium(II) iodide was prepared by standard methods and titrated prior to use.\textsuperscript{10-13} Tetrahydrofuran (THF) was purchased from Fisher Scientific and purified by passing through activated alumina columns.

Experimental Procedures and Characterization Data

General procedure for the reduction of esters with SmI\textsubscript{2}-H\textsubscript{2}O. To ester (neat or dissolved in 1.0 mL of THF), samarium(II) iodide (THF solution, typically 6 or 8 equiv) was added, followed by amine (typically 18 or 24 equiv) and water (typically 18 or 24 equiv) under inert atmosphere at room temperature and stirred vigorously. After the specified time (typically 2-6 h), the excess of SmI\textsubscript{2} was oxidized by bubbling air through the reaction mixture. The reaction mixture was diluted with EtOAc (20 mL) and HCl (10 mL, 1.0 M). The aqueous layer was extracted with EtOAc (3 x 20 mL), organic layers were combined, washed with brine (1 x 10 mL), dried over Na\textsubscript{2}SO\textsubscript{4}, filtered and concentrated. The crude product was purified by flash chromatography using a short plug of silica gel. All yields refer to isolated yields unless stated otherwise.

Note: we have noticed very small differences in reactivity between systems employing SmI\textsubscript{2}-H\textsubscript{2}O-amine in 6-18-12 ratio and SmI\textsubscript{2}-H\textsubscript{2}O-amine in 6-18-18 ratio. Due to a slightly higher reactivity the latter system has been typically preferred. For the reduction of more sterically-demanding esters systems employing SmI\textsubscript{2}-H\textsubscript{2}O-amine in 8-24-24 ratio have been typically preferred over the systems employing 6 equivalents of SmI\textsubscript{2}, however conversions higher than 95\% have been routinely observed even with the limiting number of equivalents of the reductant. As shown in Tables ESI-2 and ESI-3, in the case of very demanding substrates the increase of reactivity could be typically achieved by employing larger number of equivalents of the reducing agent. The amount of samarium(II) iodide used (typically, 6-8 equiv) is consistent with the proposed four-electron mechanism: a 1.5-2-fold excess of the reagent was used to ensure that the reactions were complete.

3-Phenylpropan-1-ol (Table 1, entry 1)

\[
\begin{align*}
\text{CO}_2\text{Me} \quad \overset{\text{SmI}_2\text{-H}_2\text{O-Et}_3\text{N}}{\text{THF, rt}} \quad \text{OH} \\
\text{1} & \quad \text{2}
\end{align*}
\]

According to the general procedure, the reaction of methyl 3-phenylpropanoate (0.25 mmol), samarium(II) iodide (1.5 mmol), water (4.5 mmol) and triethylamine (4.5 mmol) for 2 h at rt, afforded after chromatography (1/4-1/1 EtOAc/hexanes) the title compound in 97\% yield. Oil (R_f
= 0.20, 1/4 EtOAc/hexanes). $^1$H NMR (500 MHz, CDCl$_3$) δ 1.27 (br, 1H), 1.80-1.86 (m, 2H), 2.64 (t, $J = 7.5$ Hz, 2H), 3.61 (t, $J = 6.5$ Hz, 2H), 7.10-7.24 (m, 5H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 32.1, 34.3, 62.3, 125.9, 128.4, 128.5, 141.8.

3-Phenylpropan-1-ol (Table 1, entry 2)

According to the general procedure, the reaction of ethyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.6 mmol), water (1.8 mmol) and triethylamine (1.8 mmol) for 2 h at rt, afforded after chromatography (1/4-1/1 EtOAc/hexanes) the title compound in 99% yield. Oil ($R_f$ = 0.20, 1/4 EtOAc/hexanes). Spectroscopic properties matched those previously described.

3-Phenylpropan-1-ol (Table 1, entry 3)

According to the general procedure, the reaction of isopropyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (2.4 mmol) for 5 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 88% yield. Oil ($R_f$ = 0.20, 1/4 EtOAc/hexanes). Spectroscopic properties matched those previously described.

3-Phenylpropan-1-ol (Table 1, entry 4)

According to the general procedure, the reaction of tert-butyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (1.2 mmol), water (3.6 mmol) and pyrrolidine (3.6 mmol) for 5 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 83% yield. Oil ($R_f$ = 0.20, 1/4 EtOAc/hexanes). Spectroscopic properties matched those previously described.

3-Phenylpropan-1-ol (Table 1, entry 5)

ESI-6
According to the general procedure, the reaction of phenyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.6 mmol), water (1.8 mmol) and triethylamine (1.8 mmol) for 2 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 94% yield. Oil (R_f = 0.20, 1/4 EtOAc/hexanes). Spectroscopic properties matched those previously described.

**3-Phenylpropan-1-ol** (Table 1, entry 6)

![Chemical Structure](image)

According to the general procedure, the reaction of benzyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (1.0 mmol), water (3.0 mmol) and triethylamine (3.0 mmol) for 2 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 97% yield. Oil (R_f = 0.20, 1/4 EtOAc/hexanes). Spectroscopic properties matched those previously described.

**Decan-1-ol** (Table 2, entry 1)

![Chemical Structure](image)

According to the general procedure, the reaction of methyl decanoate (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (1.8 mmol) for 15 h at rt, afforded after chromatography (1/1 EtOAc/hexanes-EtOAc) the title compound in 95% yield. Oil (R_f = 0.24, 1/4 EtOAc/hexanes). ^1^H NMR (500 MHz, CDCl_3) δ 0.81 (t, J = 6.9 Hz, 3H), 1.15-1.33 (m, 15H), 1.47-1.52 (m, 2H), 3.57 (t, J = 5.8 Hz, 2H); ^1^C NMR (125 MHz, CDCl_3) δ 14.1, 22.7, 25.7, 29.3, 29.4, 29.6, 31.9, 32.8, 63.1.

**Cycloheptylmethanol** (Table 2, entry 2)

![Chemical Structure](image)

According to the general procedure, the reaction of methyl cycloheptanecarboxylate (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (2.4 mmol) for 3 h at rt, afforded after chromatography (CH_2Cl_2-1/4 Et_2O/CH_2Cl_2) the title compound in 98% yield. Note: work-up with CH_2Cl_2 (3 x 20 mL) and 1.0 M HCl (1 x 10 mL). Oil (R_f = 0.39, 1/4 Et_2O/CH_2Cl_2). ^1^H NMR (500 MHz, CDCl_3) δ 1.08-1.15 (m, 2H), 1.30 (br, 1H), 1.34-1.46 (m,
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According to the general procedure, the reaction of methyl trans-4-pentylcyclohexanecarboxylate (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (2.4 mmol) for 6 h at rt, afforded after chromatography (1/10-1/4 EtOAc/hexanes) the title compound in 87% yield. Oil (R$_f$ = 0.43, 1/4 EtOAc/hexanes). $^1$H NMR (300 MHz, CDCl$_3$) δ 0.77-0.92 (m, 7H), 1.06-1.28 (m, 10H), 1.35 (br, 1H), 1.71 (d, $J$ = 8.7 Hz, 4H), 3.37 (d, $J$ = 6.4 Hz, 2H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 14.1, 22.7, 26.6, 29.5, 32.2, 32.7, 37.4, 37.8, 40.7, 68.8.

1-Adamantanemethanol (Table 2, entry 4)

According to the general procedure, the reaction of methyl adamantane-1-carboxylate (0.10 mmol), samarium(II) iodide (1.0 mmol), water (3.0 mmol) and triethylamine (3.0 mmol) for 20 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 80% yield. Solid (R$_f$ = 0.57, 1/4 EtOAc/hexanes). $^1$H NMR (500 MHz, CDCl$_3$) δ 1.23 (br, 1H), 1.44 (m, 6H), 1.57 (m, 1H), 1.59 (m, 2H), 1.65 (m, 2H), 1.68 (m, 1H), 1.92 (m, 3H), 3.13 (s, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 28.2, 34.5, 37.2, 39.0, 73.9.

3-(4-Methoxyphenyl)propan-1-ol (Table 2, entry 5)

According to the general procedure, the reaction of methyl 3-(4-methoxyphenyl)propanoate (0.25 mmol), samarium(II) iodide (1.5 mmol), water (4.5 mmol) and triethylamine (4.5 mmol) for 2 h at rt, afforded after chromatography (1/4-1/1 EtOAc/hexanes) the title compound in 99% yield. Oil (R$_f$ = 0.62, 1/1 EtOAc/hexanes). $^1$H NMR (500 MHz, CDCl$_3$) δ 1.55 (br, 1H), 1.75-
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1.81 (m, 2H), 2.57 (t, $J = 7.5$ Hz, 2H), 3.58 (t, $J = 6.5$ Hz, 2H), 3.71 (s, 3H), 6.75 (d, $J = 8.5$ Hz, 2H), 7.03 (d, $J = 8.5$ Hz, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 31.2, 34.5, 55.3, 62.2, 113.8, 129.3, 133.9, 157.8.

3-(p-Tolyl)propan-1-ol (Table 2, entry 6)

According to the general procedure, the reaction of methyl 3-(p-tolyl)propanoate (0.10 mmol), samarium(II) iodide (0.6 mmol), water (1.8 mmol) and triethylamine (1.8 mmol) for 3 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 97% yield. Oil ($R_f$ = 0.63, 1/1 EtOAc/hexanes). $^1$H NMR (300 MHz, CDCl$_3$) δ 1.24 (br, 1H), 1.76-1.85 (m, 2H), 2.25 (s, 3H), 2.60 (t, $J = 7.5$ Hz, 2H), 3.60 (t, $J = 6.6$ Hz, 2H), 7.02 (s, 4H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 21.0, 31.6, 34.4, 62.4, 128.3, 129.1, 135.3, 138.7.

2-Phenylpropan-1-ol (Table 2, entry 7)

According to the general procedure, the reaction of methyl 2-phenylpropanoate (0.25 mmol), samarium(II) iodide (1.5 mmol), water (4.5 mmol) and triethylamine (4.5 mmol) for 24 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 95% yield. Oil ($R_f$ = 0.56, 1/1 EtOAc/hexanes). $^1$H NMR (500 MHz, CDCl$_3$) δ 1.21 (d, $J = 7.0$ Hz, 3H), 1.33 (br, 1H), 2.84-2.91 (m, 1H), 3.63 (d, $J = 7.0$ Hz, 2H), 7.14-7.18 (m, 3H), 7.24-7.28 (m, 2H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 17.6, 42.5, 68.7, 126.7, 127.5, 128.7, 143.7.

2-Methyl-3-phenylpropan-1-ol (Table 2, entry 8)

According to the general procedure, the reaction of methyl 2-methyl-3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (2.4 mmol) for 20 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 85% yield. Oil ($R_f$ = 0.66, 1/1 EtOAc/hexanes). $^1$H NMR (500 MHz, CDCl$_3$) δ 0.85 (d, $J = 6.5$ Hz, 3H), 1.35 ESI-9
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(br, 1H), 1.83-1.92 (m, 1H), 2.36 (dd, J = 8.5, 13.5 Hz, 1H), 2.69 (dd, J = 6.5, 13.5 Hz, 1H), 3.38-3.49 (m, 2H), 7.09-7.14 (m, 3H), 7.19-7.23 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 16.5, 37.8, 39.7, 67.7, 125.9, 128.3, 129.2, 140.6.

2-(4-Isobutylphenyl)propan-1-ol (Table 2, entry 9)

According to the general procedure, the reaction of methyl 2-(4-isobutylphenyl)propanoate (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (2.4 mmol) for 20 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 88% yield. Oil (Rf = 0.79, 1/1 EtOAc/hexanes). ¹H NMR (500 MHz, CDCl₃) δ 0.83 (d, J = 7.0 Hz, 6H), 1.19 (d, J = 7.0 Hz, 3H), 1.54 (br, 1H), 1.73-1.82 (m, 1H), 2.38 (d, J = 7.0 Hz, 2H), 2.81-2.89 (m, 1H), 3.61 (d, J = 6.5 Hz, 2H), 7.02-7.09 (m, 4H); ¹³C NMR (125 MHz, CDCl₃) δ 17.6, 22.4, 30.3, 42.0, 45.0, 68.8, 127.2, 129.4, 140.1, 140.7.

Heptane-1,7-diol (Table 2, entry 10)

According to the general procedure, the reaction of diethyl heptanedioate (0.10 mmol), samarium(II) iodide (1.2 mmol), water (3.6 mmol) and triethylamine (3.6 mmol) for 20 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 87% yield. Oil (Rf = 0.35, EtOAc). ¹H NMR (500 MHz, CDCl₃) δ 1.25 (br, 2H), 1.28-1.33 (m, 6H), 1.47-1.54 (m, 4H), 3.58 (t, J = 6.6 Hz, 4H); ¹³C NMR (125 MHz, CDCl₃) δ 25.7, 29.2, 32.7, 63.0.

2,2-Dibutylpropane-1,3-diol (Table 2, entry 11)

According to the general procedure, the reaction of diethyl 2,2-dibutylmalonate (0.10 mmol), samarium(II) iodide (1.6 mmol), water (4.8 mmol) and triethylamine (4.8 mmol) for 18 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes-EtOAc) the title compound in 76% yield. Oil (Rf = 0.64, EtOAc). ¹H NMR (300 MHz, CDCl₃) δ 0.84 (t, J = 6.9 Hz, 6H), 1.05-1.31
Electron Transfer Reduction of Unactivated Esters using SmI$_2$-$\text{H}_2\text{O}$

**Szostak, Spain and Procter**

(m, 12H), 2.36 (br, 2H), 3.50 (s, 4H); $^{13}\text{C}$ NMR (75 MHz, CDCl$_3$) $\delta$ 14.1, 23.6, 25.1, 30.6, 40.9, 69.5.

**Decane-1,5-diol** (Table 2, entry 12)

\[
\begin{align*}
\text{O} & \quad \text{Smi}_2\text{-H}_2\text{O-Et}_3\text{N} \\
n\text{-C}_3\text{H}_1 & \quad \text{THF, rt} \\
19 & \rightarrow 19a \\
n\text{-C}_5\text{H}_1
\end{align*}
\]

According to the general procedure, the reaction of 6-pentyltetrahydro-2H-pyran-2-one (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (1.6 mmol) for 2 h at rt, afforded after chromatography (EtOAc) the title compound in 97% yield. Oil (R$_f$ = 0.50, EtOAc). $^1\text{H}$ NMR (500 MHz, CDCl$_3$) $\delta$ 0.82 (t, $J$ = 6.9 Hz, 3H), 1.19-1.28 (m, 5H), 1.32-1.58 (m, 7H), 1.48-1.58 (m, 2H), 1.61 (br, 2H), 3.51-3.56 (m, 1H), 3.59 (t, $J$ = 6.0 Hz, 2H); $^{13}\text{C}$ NMR (125 MHz, CDCl$_3$) $\delta$ 14.0, 21.8, 22.6, 25.3, 31.9, 32.6, 37.0, 37.5, 62.7, 71.9.

**2-(3-Hydroxypropyl)phenol** (Table 2, entry 13)

\[
\begin{align*}
\text{O} & \quad \text{Smi}_2\text{-H}_2\text{O-Et}_3\text{N} \\
20 & \rightarrow 20a \\
\end{align*}
\]

According to the general procedure, the reaction of chroman-2-one (0.10 mmol), samarium(II) iodide (0.6 mmol), water (1.8 mmol) and triethylamine (1.8 mmol) for 2 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 92% yield. Oil (R$_f$ = 0.50, EtOAc). $^1\text{H}$ NMR (500 MHz, CDCl$_3$) $\delta$ 1.78-1.84 (m, 2H), 2.51 (br, 1H), 2.71 (t, $J$ = 6.8 Hz, 2H), 3.57 (t, $J$ = 5.8 Hz, 2H), 6.76-6.82 (m, 2H), 7.02-7.05 (m, 2H), 7.06 (br, 1H); $^{13}\text{C}$ NMR (125 MHz, CDCl$_3$) $\delta$ 25.1, 32.2, 60.8, 116.1, 120.8, 127.2, 127.6, 130.7, 154.6.

**4-Methoxyphenyl)methanol** (Table 2, entry 14)

\[
\begin{align*}
\text{CO}_2\text{Me} & \quad \text{Smi}_2\text{-H}_2\text{O-Et}_3\text{N} \\
21 & \rightarrow 21a \\
\end{align*}
\]

According to the general procedure, the reaction of methyl 4-methoxybenzoate (0.10 mmol), samarium(II) iodide (0.6 mmol), water (1.8 mmol) and triethylamine (1.8 mmol) for 1 h at rt, afforded after chromatography (4/1 EtOAc/hexanes) the title compound in 90% yield. Oil (R$_f$ = 0.54, 4/1 EtOAc/hexanes). $^1\text{H}$ NMR (300 MHz, CDCl$_3$) $\delta$ 1.57 (br, 1H), 3.74 (s, 3H), 4.54 (s,
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2H), 6.82 (d, $J = 8.7$ Hz, 2H), 7.22 (d, $J = 8.7$ Hz, 2H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 55.3, 65.1, 114.0, 128.7, 133.2, 159.3.

2-(1H-Indol-3-yl)ethanol (Table 2, entry 15)

According to the general procedure, the reaction of ethyl 2-(1H-indol-3-yl)acetate (0.10 mmol), samarium(II) iodide (0.8 mmol), water (2.4 mmol) and triethylamine (2.4 mmol) for 20 h at rt, afforded after chromatography (1/10-1/1 EtOAc/hexanes) the title compound in 81% yield. Oil ($R_f = 0.33$, 1/1 EtOAc/hexanes). $^1$H NMR (500 MHz, CDCl$_3$) δ 1.47 (br, 1H), 2.97 (t, $J = 6.3$ Hz, 2H), 3.84 (t, $J = 6.3$ Hz, 2H), 7.01 (d, $J = 1.5$ Hz, 1H), 7.06 (t, $J = 7.0$ Hz, 1H), 7.14 (t, $J = 7.5$ Hz, 1H), 7.30 (d, $J = 8.2$ Hz, 1H), 7.56 (d, $J = 7.9$ Hz, 1H), 7.99 (br, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 28.8, 62.6, 111.3, 112.3, 118.9, 119.5, 122.3, 122.5, 127.4, 136.5.
Mechanistic Studies

A) Deuterium incorporation

According to the general procedure, the reaction of methyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.6 mmol), deuterium oxide (1.8 mmol) and triethylamine (1.2 mmol) for 3 h at rt, afforded 1,1-D,D-3-phenylpropan-1-ol with >97% deuterium incorporation. Yield 88% (\(^1\)H NMR vs. internal standard). Purification by chromatography (1/4-1/1 EtOAc/hexanes) afforded the title product (R\(_f\) = 0.20, 1/4 EtOAc/hexanes). \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 1.50 (br, 1H), 1.82 (t, \(J = 7.7\) Hz, 2H), 2.64 (t, \(J = 7.5\) Hz, 2H), 7.10-7.24 (m, 5H); \(^13\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 32.0, 34.0, 61.6 (t, \(J = 21.3\) Hz), 125.9, 128.4, 128.4, 141.8.

B) Determination of primary kinetic isotope effect

Method 1. According to the general procedure, the reaction of isopropyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.6 mmol), deuterium oxide/water (1:1, 1.8 mmol) and triethylamine (1.2 mmol) for 5 min at rt, afforded 1,1-D,D-3-phenylpropan-1-ol and 3-phenylpropan-1-ol (45% conversion). The amount of each species was determined by \(^1\)H NMR (500 MHz, CDCl\(_3\)). Kinetic isotope effect, \(k_H/k_D = 1.4\).

Method 2. According to the general procedure, the reaction of isopropyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.6 mmol), water (1.8 mmol) and triethylamine (1.2 mmol) and the reaction of isopropyl 3-phenylpropanoate (0.10 mmol), samarium(II) iodide (0.6 mmol), deuterium oxide (1.8 mmol) and triethylamine (1.2 mmol) were followed by GC with undecane as the internal standard. Initial rates were determined from the slopes at low conversion. Kinetic isotope effect, \(k_H/k_D = 1.5\).
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