

Supporting Information

Visible-Light-Promoted Photoredox Syntheses of α,β -Epoxy Ketones from Styrenes and Benzaldehydes under Alkaline Condition

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Table of Contents

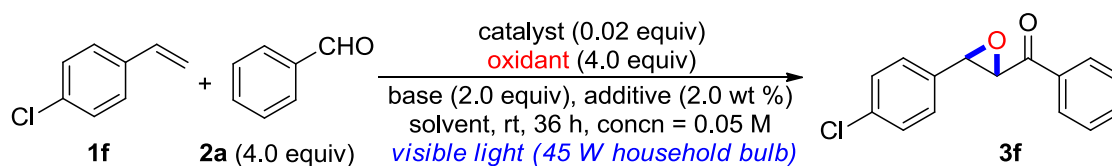
(53 Pages)

Materials and methods	S2
Table 1. Identification of the optimal reaction conditions	S3
General procedure for visible-light-promoted photoredox reactions	S4
Examinations of other alkenes and aldehydes under standard conditions	S5
Experimental probes on reaction mechanism	S6
^1H NMR and ^{13}C NMR spectra data of the products	S8
Copies of ^1H NMR and ^{13}C NMR spectra	S19

Materials and methods

All reactions were carried out under a nitrogen atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. All the chemicals were purchased commercially, and used without further purification. Anhydrous THF and toluene were distilled from sodium-benzophenone. Dichloromethane and acetonitrile were distilled from calcium hydride. Thin-layer chromatography (TLC) was conducted with 0.25 mm Tsingdao silica gel plates (60F-254) and visualized by exposure to UV light (254 nm) or stained with potassium permanganate. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040–0.063 mm). Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. ^1H NMR spectra were recorded on Bruker spectrometers (at 300, 400 or 500 MHz) and are reported relative to deuterated solvent signals. Data for ^1H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. ^{13}C NMR spectra were recorded on Bruker Spectrometers (at 75, 100 or 125 MHz). Data for ^{13}C NMR spectra are reported in terms of chemical shift. Mass spectrometric data were obtained using Bruker Apex IV RTMS. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad.

Table 1. Identification of the optimal reaction conditions



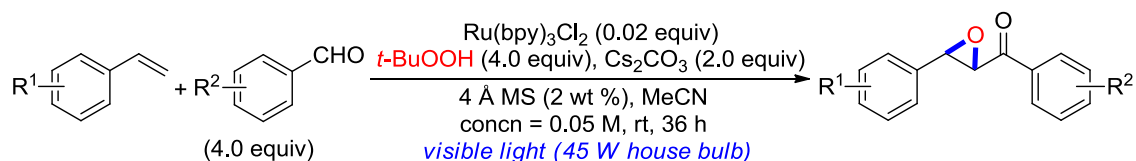
entry	catalyst	base	additive	solvent	oxidant ^f	yield ^g (%)
1	Ru(bpy) ₃ Cl ₂	K ₂ CO ₃	-	MeCN	<i>t</i> -BuOOH	39
2	Ru(bpy) ₃ Cl ₂	Et ₃ N	-	MeCN	<i>t</i> -BuOOH	trace
3	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	-	MeCN	<i>t</i> -BuOOH	61
4 ^a	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	-	MeCN	<i>t</i> -BuOOH	46
5 ^b	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	Mg(ClO ₄) ₂	MeCN	<i>t</i> -BuOOH	trace
6	Ru(bpy)₃Cl₂	Cs₂CO₃	4 Å MS	MeCN	<i>t</i>-BuOOH	82
7	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	DMSO	<i>t</i> -BuOOH	trace
8	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	DMF	<i>t</i> -BuOOH	37
9	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	toluene	<i>t</i> -BuOOH	trace
10	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	CH ₂ Cl ₂	<i>t</i> -BuOOH	trace
11	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	Et ₂ O	<i>t</i> -BuOOH	21
12	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeOH	<i>t</i> -BuOOH	trace
13	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	THF	<i>t</i> -BuOOH	35
14	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	(BzO) ₂	0
15	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	(<i>t</i> -BuO) ₂	0
16	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	K ₂ S ₂ O ₈	0
17	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	H ₂ O ₂	0
18	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	<i>m</i> -CPBA	0
19	Ir(ppy) ₃	Cs ₂ CO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	trace
20	Eosin Y	Cs ₂ CO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	0
21 ^c	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	0
22	-	Cs ₂ CO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	0
23	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	-	0
24	Ru(bpy) ₃ Cl ₂	DBU	4 Å MS	MeCN	<i>t</i> -BuOOH	trace
25	Ru(bpy) ₃ Cl ₂	pyridine	4 Å MS	MeCN	<i>t</i> -BuOOH	0
26	Ru(bpy) ₃ Cl ₂	NaH	4 Å MS	MeCN	<i>t</i> -BuOOH	0
27	Ru(bpy) ₃ Cl ₂	NaHCO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	trace
28	Ru(bpy) ₃ Cl ₂	Na ₂ CO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	32
29	Ru(bpy) ₃ Cl ₂	CsF	4 Å MS	MeCN	<i>t</i> -BuOOH	52
30	Ru(bpy) ₃ Cl ₂	LiOH	4 Å MS	MeCN	<i>t</i> -BuOOH	54
31	Ru(bpy) ₃ Cl ₂	NaOH	4 Å MS	MeCN	<i>t</i> -BuOOH	51
32	Ru(bpy) ₃ Cl ₂	KOH	4 Å MS	MeCN	<i>t</i> -BuOOH	21
33	Ru(bpy) ₃ Cl ₂	LiOt-Bu	4 Å MS	MeCN	<i>t</i> -BuOOH	36
34	Ru(bpy) ₃ Cl ₂	NaOt-Bu	4 Å MS	MeCN	<i>t</i> -BuOOH	0
35	Ru(bpy) ₃ Cl ₂	KOt-Bu	4 Å MS	MeCN	<i>t</i> -BuOOH	0
36 ^d	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	64
37 ^e	Ru(bpy) ₃ Cl ₂	Cs ₂ CO ₃	4 Å MS	MeCN	<i>t</i> -BuOOH	61

^aCs₂CO₃ (0.5 equiv) was used. ^bMg(ClO₄)₂ (1.0 equiv) was used.

^cNo light. ^d**2a** (2.0 equiv) was used. ^e*t*-BuOOH 70% in water.

^f*t*-BuOOH 5.5 M in decane. ^gYield was determined by ¹H NMR.

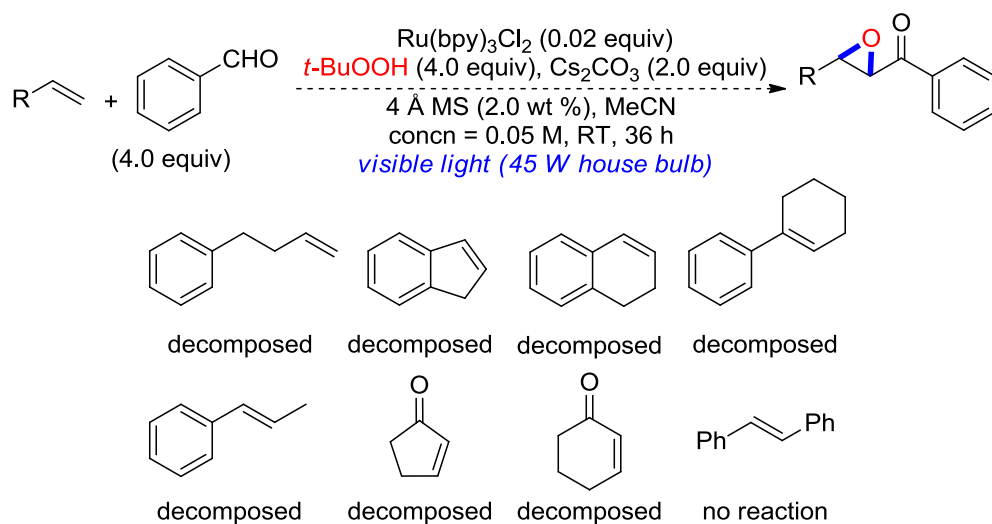
General procedure for visible-light-promoted photoredox reactions



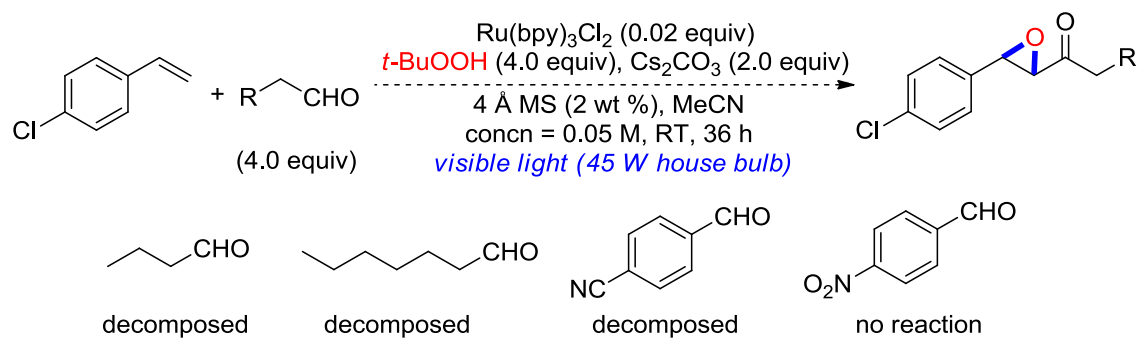
To a solution of alkenes compounds (0.2 mmol, 1.0 equiv), aldehydes compounds (0.8 mmol, 4.0 equiv), $Ru(bpy)_3Cl_2$ (0.004 mmol, 0.02 equiv), 4 Å MS (80 mg, 2 wt %), Cs_2CO_3 (0.4 mmol, 2.0 equiv) in a solvent of MeCN (4.0 mL) was added $t-BuOOH$ (5.5 M in decane) (0.8 mmol, 4.0 equiv). Then the reaction was irradiated by a household bulb (45 W) under a balloon-argon atmosphere at room temperature. The reaction was monitored by TLC to establish the consumption of starting material. After the reaction was complete, the reaction mixture was filtrated through celite and washed with ether. Then the filtrate was concentrated under reduced pressure, and the crude product was purified by flash column chromatography on silica gel (n -Hexane/Ethyl Acetate = 20/1) to afford desired pure products in 51–86% isolated yields.^{1–4}

Examinations of other alkenes and aldehydes under standard conditions

1. Examinations of other alkenes



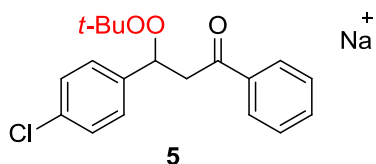
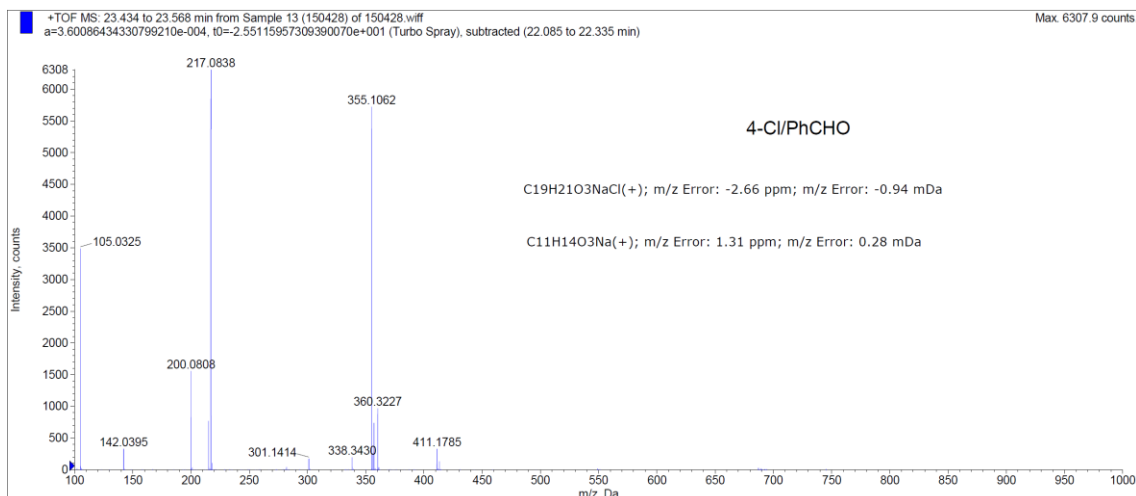
2. Examinations of other aldehydes



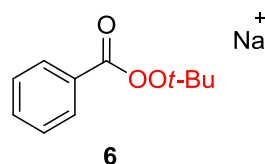
Other alkenes and aldehydes had been examined. However, we did not obtain desired products under standard conditions.

Experimental probes on reaction mechanism

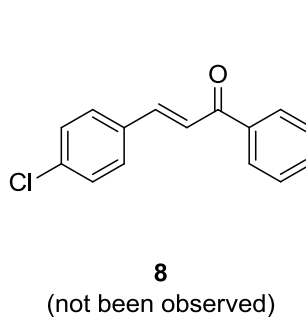
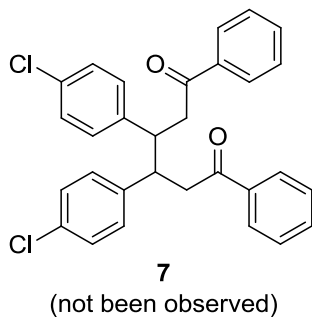
High resolution mass spectrum of 5 and 6



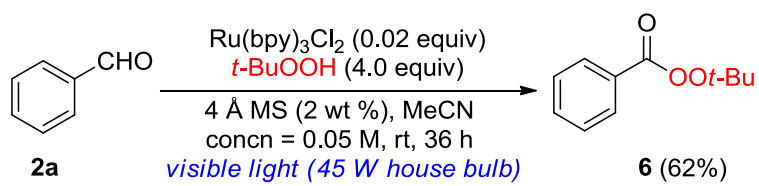
Chemical Formula: $C_{19}H_{21}ClNaO_3^+$
Exact Mass: 355.1071



Chemical Formula: $C_{11}H_{14}NaO_3^+$
Exact Mass: 217.0835

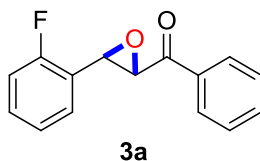


Both structures **5** and **6** were detected by high-resolution mass spectrum (HRMS) analysis of the reaction mixture when the base Cs_2CO_3 was absent. Structure **5** was inseparable and labile. Furthermore, structures **7** and **8** were not detected by HRMS and NMR under standard conditions.

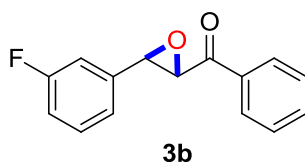


Structure **6** was isolated in 62% yield under the above condition.

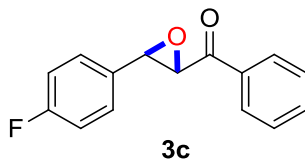
¹H NMR and ¹³C NMR spectra data of products



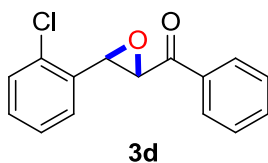
3-(2-fluorophenyl)oxiran-2-yl(phenyl)methanone (3a): ¹H NMR (400 MHz, CDCl₃) δ 8.02 (d, *J* = 7.5 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.34 (dd, *J* = 13.6, 7.0 Hz, 2H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.11 – 7.04 (m, 1H), 4.33 (s, 1H), 4.30 (d, *J* = 1.7 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 192.8, 162.6, 160.2, 135.2, 134.0, 130.3, 128.8, 128.2, 126.3, 124.5, 122.9, 115.5, 115.3, 59.8, 54.1; HRMS calculated for C₁₅H₁₁FO₂Na (M + Na⁺): 265.0635, found: 265.0635. (Pale yellow oil, 30.5 mg, 63% isolated yield).



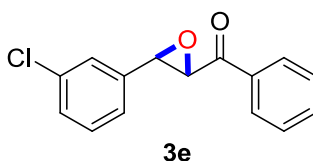
3-(3-fluorophenyl)oxiran-2-yl(phenyl)methanone (3b): ¹H NMR (400 MHz, CDCl₃) δ 8.06 – 7.94 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.37 (ddd, *J* = 8.8, 7.9, 5.7 Hz, 1H), 7.17 (d, *J* = 7.7 Hz, 1H), 7.12 – 7.01 (m, 2H), 4.26 (d, *J* = 1.8 Hz, 1H), 4.08 (d, *J* = 1.5 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 192.6, 164.2, 161.8, 138.1, 135.2, 134.0, 130.4, 128.8, 128.3, 121.5, 116.1, 115.8, 112.6, 112.3, 60.7, 58.5; HRMS calculated for C₁₅H₁₁FO₂Na (M + Na⁺): 265.0635, found: 265.0636. (White solid, 29.6 mg, 61% isolated yield).



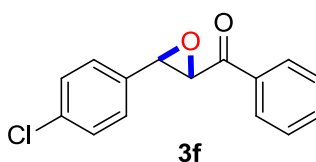
3-(4-fluorophenyl)oxiran-2-yl(phenyl)methanone (3c): ¹H NMR (400 MHz, CDCl₃) δ 8.03 – 7.96 (m, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.37 – 7.31 (m, 2H), 7.08 (dd, *J* = 12.0, 5.3 Hz, 2H), 4.26 (d, *J* = 1.8 Hz, 1H), 4.06 (d, *J* = 1.7 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 192.8, 164.3, 161.8, 135.3, 134.0, 131.2, 128.8, 128.2, 127.5, 115.8, 115.6, 60.8, 58.7; HRMS calculated for C₁₅H₁₁FO₂Na (M + Na⁺): 265.0635, found: 265.0633. (Pale yellow oil, 30.5 mg, 63% isolated yield).



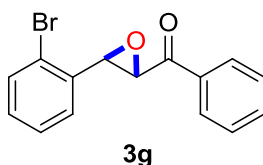
3-(2-chlorophenyl)oxiran-2-yl(phenyl)methanone (3d): ^1H NMR (300 MHz, CDCl_3) δ 8.09 – 7.99 (m, 2H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.49 (t, $J = 7.6$ Hz, 2H), 7.39 (tt, $J = 5.7$, 3.0 Hz, 2H), 7.31 (dt, $J = 4.7$, 3.6 Hz, 2H), 4.40 (d, $J = 1.7$ Hz, 1H), 4.17 (d, $J = 1.8$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 192.8, 135.3, 134.1, 133.7, 133.3, 129.8, 129.3, 128.9, 128.4, 127.3, 126.1, 60.0, 57.1; HRMS calculated for $\text{C}_{15}\text{H}_{11}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 281.0340, found: 281.0338. (Pale yellow oil, 32.1 mg, 62% isolated yield).



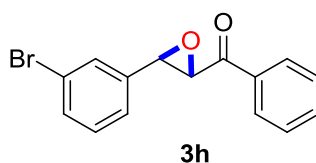
3-(3-chlorophenyl)oxiran-2-yl(phenyl)methanone (3e): ^1H NMR (400 MHz, CDCl_3) δ 8.04 – 7.95 (m, 2H), 7.62 (dd, $J = 10.6$, 4.3 Hz, 1H), 7.49 (t, $J = 7.7$ Hz, 2H), 7.37 – 7.23 (m, 4H), 4.26 (d, $J = 1.8$ Hz, 1H), 4.05 (d, $J = 1.7$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.5, 137.5, 135.2, 134.8, 134.0, 130.0, 129.1, 128.8, 128.3, 125.6, 124.0, 60.7, 58.4; HRMS calculated for $\text{C}_{15}\text{H}_{11}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 281.0340, found: 281.0338. (Pale yellow oil, 35.2 mg, 68% isolated yield).



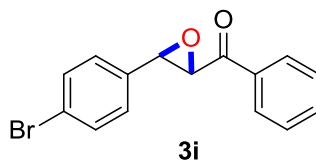
3-(4-chlorophenyl)oxiran-2-yl(phenyl)methanone (3f): ^1H NMR (400 MHz, CDCl_3) δ 8.05 – 7.94 (m, 2H), 7.63 (t, $J = 7.4$ Hz, 1H), 7.49 (t, $J = 7.7$ Hz, 2H), 7.38 (dd, $J = 6.2$, 4.6 Hz, 2H), 7.30 (d, $J = 8.5$ Hz, 2H), 4.25 (d, $J = 1.8$ Hz, 1H), 4.06 (d, $J = 1.7$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.6, 135.3, 134.8, 134.0, 133.9, 128.9, 128.8, 128.2, 127.0, 60.8, 58.6; HRMS calculated for $\text{C}_{15}\text{H}_{11}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 281.0340, found: 281.0341. (Pale yellow oil, 37.2 mg, 72% isolated yield).



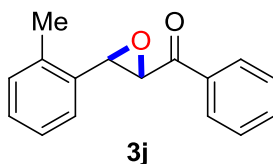
3-(2-bromophenyl)oxiran-2-yl(phenyl)methanone (3g): ^1H NMR (500 MHz, CDCl_3) δ 8.08 – 8.00 (m, 2H), 7.61 (t, $J = 7.4$ Hz, 1H), 7.54 (d, $J = 7.9$ Hz, 1H), 7.48 (t, $J = 7.8$ Hz, 2H), 7.40 – 7.31 (m, 2H), 7.22 (td, $J = 8.0, 2.1$ Hz, 1H), 4.32 (d, $J = 1.7$ Hz, 1H), 4.15 (d, $J = 1.9$ Hz, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 192.7, 135.4, 135.3, 134.0, 132.5, 130.1, 128.8, 128.4, 127.8, 126.4, 122.5, 60.0, 59.3; HRMS calculated for $\text{C}_{15}\text{H}_{11}\text{BrO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 324.9835, found: 324.9835. (Pale yellow oil, 44.9 mg, 74% isolated yield).



3-(3-bromophenyl)oxiran-2-yl(phenyl)methanone (3h): ^1H NMR (400 MHz, CDCl_3) δ 8.04 – 7.91 (m, 2H), 7.61 (t, $J = 7.4$ Hz, 1H), 7.47 (dd, $J = 9.1, 4.3$ Hz, 4H), 7.26 (dt, $J = 14.5, 7.8$ Hz, 2H), 4.25 (d, $J = 1.8$ Hz, 1H), 4.02 (d, $J = 1.6$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.5, 137.8, 135.2, 134.0, 132.0, 130.3, 128.8, 128.5, 128.3, 124.5, 122.9, 60.7, 58.3; HRMS calculated for $\text{C}_{15}\text{H}_{11}\text{BrO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 324.9835, found: 324.9834. (Pale yellow oil, 44.3 mg, 73% isolated yield).

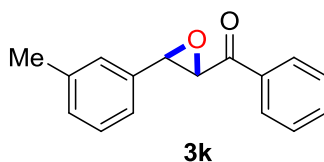


3-(4-bromophenyl)oxiran-2-yl(phenyl)methanone (3i): ^1H NMR (400 MHz, CDCl_3) δ 7.99 (d, $J = 7.5$ Hz, 2H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.55 – 7.43 (m, 4H), 7.25 (t, $J = 6.2$ Hz, 2H), 4.25 (d, $J = 1.8$ Hz, 1H), 4.04 (d, $J = 1.4$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.6, 135.2, 134.5, 134.0, 131.9, 128.8, 128.2, 127.3, 123.0, 60.8, 58.6; HRMS calculated for $\text{C}_{15}\text{H}_{11}\text{BrO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 324.9835, found: 324.9833. (Pale yellow oil, 50.3 mg, 83% isolated yield).

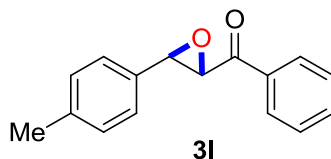


phenyl(3-(o-tolyl)oxiran-2-yl)methanone (3j): ^1H NMR (500 MHz, CDCl_3) δ 8.09 – 8.01 (m, 2H), 7.64 (t, $J = 7.4$ Hz, 1H), 7.51 (t, $J = 7.8$ Hz, 2H), 7.34 (dd, $J = 6.9, 2.1$ Hz, 1H), 7.29 – 7.23 (m, 2H), 7.21 – 7.17 (m, 1H), 4.23 (d, $J = 1.7$ Hz, 1H), 4.21 (d, $J = 1.9$

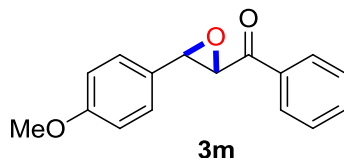
Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 193.3, 136.3, 135.4, 134.0, 133.9, 130.1, 128.9, 128.5, 128.3, 126.3, 124.2, 60.1, 57.7, 18.8; HRMS calculated for $\text{C}_{16}\text{H}_{14}\text{O}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 261.0886, found: 261.0884. (Pale yellow oil, 40.5 mg, 85% isolated yield).



phenyl(3-(*m*-tolyl)oxiran-2-yl)methanone (3k): ^1H NMR (400 MHz, CDCl_3) δ 8.05 – 7.97 (m, 2H), 7.67 – 7.56 (m, 1H), 7.48 (t, $J = 7.7$ Hz, 2H), 7.33 – 7.26 (m, 1H), 7.19 (t, $J = 6.5$ Hz, 3H), 4.30 (d, $J = 1.9$ Hz, 1H), 4.04 (d, $J = 1.8$ Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 193.0, 138.5, 135.4, 135.3, 133.9, 129.7, 128.8, 128.6, 128.2, 126.2, 122.9, 60.9, 59.4, 21.3; HRMS calculated for $\text{C}_{16}\text{H}_{14}\text{O}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 261.0886, found: 261.0888. (White solid, 32.4 mg, 68% isolated yield).

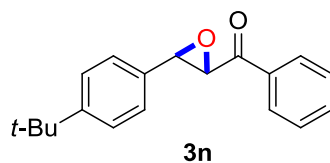


phenyl(3-(*p*-tolyl)oxiran-2-yl)methanone (3l): ^1H NMR (400 MHz, CDCl_3) δ 8.01 (dd, $J = 8.3, 1.1$ Hz, 2H), 7.64 – 7.58 (m, 1H), 7.48 (dd, $J = 10.7, 4.7$ Hz, 2H), 7.24 (dd, $J = 21.9, 8.0$ Hz, 4H), 4.30 (d, $J = 1.9$ Hz, 1H), 4.04 (d, $J = 1.8$ Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 193.1, 139.0, 135.4, 133.8, 132.4, 129.4, 128.8, 128.2, 125.7, 61.0, 59.3, 21.2; HRMS calculated for $\text{C}_{16}\text{H}_{14}\text{O}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 261.0886, found: 261.0883. (Pale yellow oil, 36.2 mg, 76% isolated yield).

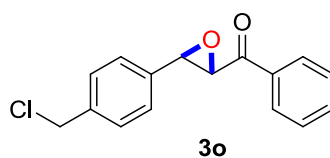


(3-(4-methoxyphenyl)oxiran-2-yl)(phenyl)methanone (3m): ^1H NMR (400 MHz, CDCl_3) δ 8.05 – 7.96 (m, 2H), 7.61 (dd, $J = 10.6, 4.3$ Hz, 1H), 7.49 (t, $J = 7.7$ Hz, 2H), 7.34 – 7.27 (m, 2H), 6.97 – 6.90 (m, 2H), 4.29 (d, $J = 1.9$ Hz, 1H), 4.03 (d, $J = 1.8$ Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 193.2, 160.2, 135.4, 133.8, 128.7, 128.2, 127.2, 127.1, 114.1, 61.0, 59.3, 55.3; HRMS calculated for $\text{C}_{16}\text{H}_{14}\text{O}_3\text{Na}$ ($\text{M} +$

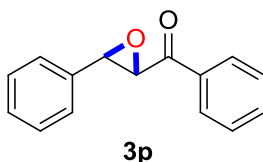
Na⁺): 277.0835, found: 277.0837. (Pale yellow oil, 38.6 mg, 76% isolated yield).



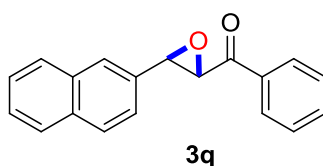
(3-(4-(*tert*-butyl)phenyl)oxiran-2-yl)(phenyl)methanone (3n): ¹H NMR (500 MHz, CDCl₃) δ 8.01 (d, *J* = 8.0 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.41 (m, 4H), 7.32 (d, *J* = 8.2 Hz, 2H), 4.33 (s, 1H), 4.06 (s, 1H), 1.34 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 193.2, 152.3, 135.5, 133.9, 132.5, 128.8, 128.3, 125.7, 125.6, 60.9, 59.4, 34.7, 31.3; HRMS calculated for C₁₉H₂₀O₂Na (M + Na⁺): 303.1356, found: 303.1356. (Pale yellow oil, 35.9 mg, 64% isolated yield).



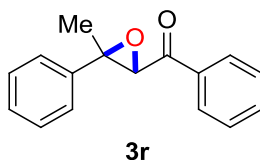
(3-(4-(chloromethyl)phenyl)oxiran-2-yl)(phenyl)methanone (3o): ¹H NMR (300 MHz, CDCl₃) δ 8.07 – 7.94 (m, 2H), 7.63 (dd, *J* = 10.5, 4.3 Hz, 1H), 7.56 – 7.32 (m, 6H), 4.61 (s, 2H), 4.29 (d, *J* = 1.8 Hz, 1H), 4.08 (d, *J* = 1.7 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 192.8, 138.4, 135.8, 135.3, 134.1, 129.0, 128.9, 128.3, 126.2, 61.0, 59.0, 45.7; HRMS calculated for C₁₆H₁₃ClO₂Na (M + Na⁺): 295.0496, found: 295.0499. (Pale yellow oil, 33.3 mg, 61% isolated yield).



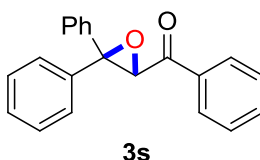
phenyl(3-phenyloxiran-2-yl)methanone (3p): ¹H NMR (500 MHz, CDCl₃) δ 8.07 – 7.95 (m, 2H), 7.62 (dd, *J* = 10.6, 4.3 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.43 – 7.34 (m, 5H), 4.30 (d, *J* = 1.9 Hz, 1H), 4.08 (d, *J* = 1.7 Hz, 1H); ¹³C NMR (126 MHz, CDCl₃) δ 193.1, 135.5, 134.0, 129.0, 128.9, 128.8, 128.3, 125.8, 61.0, 59.4; HRMS calculated for C₁₅H₁₂O₂Na (M + Na⁺): 247.0730, found: 247.0730. (White solid, 29.6 mg, 66% isolated yield).



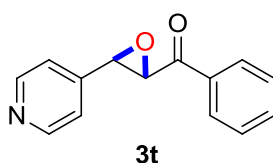
(3-(naphthalen-2-yl)oxiran-2-yl)(phenyl)methanone (3q): ^1H NMR (400 MHz, CDCl_3) δ 8.07 – 7.98 (m, 2H), 7.93 – 7.82 (m, 4H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.55 – 7.39 (m, 5H), 4.40 (d, $J = 1.8$ Hz, 1H), 4.25 (d, $J = 1.6$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.9, 135.4, 133.9, 133.6, 133.0, 132.8, 128.8, 128.7, 128.3, 127.8, 127.7, 126.6, 126.5, 125.8, 122.3, 61.1, 59.5; HRMS calculated for $\text{C}_{19}\text{H}_{15}\text{O}_2$ ($\text{M} + \text{H}^+$): 275.1067, found: 275.1067. (Pale yellow oil, 31.8 mg, 58% isolated yield).



(3-methyl-3-phenyloxiran-2-yl)(phenyl)methanone (3r): ^1H NMR (500 MHz, CDCl_3) δ 8.01 – 7.91 (m, 2H), 7.61 (d, $J = 7.4$ Hz, 1H), 7.52 – 7.46 (m, 4H), 7.43 (t, $J = 7.5$ Hz, 2H), 7.38 (d, $J = 7.2$ Hz, 1H), 4.16 (s, 1H), 1.64 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 193.0, 140.4, 135.6, 133.9, 128.9, 128.7, 128.2, 125.1, 66.8, 62.8, 17.0; ^1H NMR (500 MHz, CDCl_3) δ 7.86 – 7.78 (m, 2H), 7.53 (t, $J = 7.4$ Hz, 1H), 7.41 (t, $J = 7.7$ Hz, 2H), 7.34 – 7.29 (m, 2H), 7.22 – 7.12 (m, 3H), 4.34 (s, 1H), 1.93 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 192.5, 136.7, 135.5, 133.5, 128.6, 128.1, 128.0, 127.8, 126.2, 66.1, 64.5, 24.4; HRMS calculated for $\text{C}_{16}\text{H}_{14}\text{O}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 261.0886, found: 261.0890. (Pale yellow oil, 30.0 mg, 63% isolated yield, dr = 1:1).

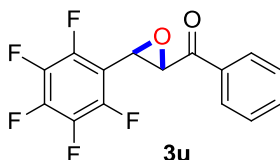


(3,3-diphenyloxiran-2-yl)(phenyl)methanone (3s): ^1H NMR (400 MHz, CDCl_3) δ 7.94 (d, $J = 7.4$ Hz, 2H), 7.58 (t, $J = 7.4$ Hz, 1H), 7.49 – 7.30 (m, 9H), 7.24 – 7.19 (m, 3H), 4.68 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 191.8, 139.0, 135.6, 134.8, 133.6, 128.7, 128.6, 128.5, 128.2, 128.0, 127.9, 126.8, 67.6, 66.7; HRMS calculated for $\text{C}_{21}\text{H}_{16}\text{O}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 323.1043, found: 323.1045. (White solid, 38.4 mg, 64% isolated yield).

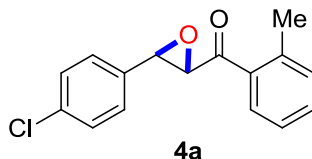


phenyl(3-(pyridin-4-yl)oxiran-2-yl)methanone (3t): ^1H NMR (500 MHz, CDCl_3) δ

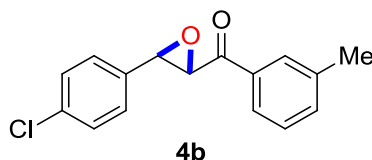
8.59 (d, $J = 5.3$ Hz, 2H), 7.95 (d, $J = 7.6$ Hz, 2H), 7.58 (d, $J = 7.4$ Hz, 1H), 7.45 (t, $J = 7.7$ Hz, 2H), 7.26 (d, $J = 5.2$ Hz, 2H), 4.23 (d, $J = 1.1$ Hz, 1H), 4.04 (s, 1H); ^{13}C NMR (126 MHz, CDCl_3) δ 192.1, 150.1, 144.6, 135.2, 134.2, 128.9, 128.3, 120.5, 60.5, 57.5; HRMS calculated for $\text{C}_{14}\text{H}_{11}\text{NO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 248.0682, found: 248.0683. (Yellow solid, 28.4 mg, 63% isolated yield).



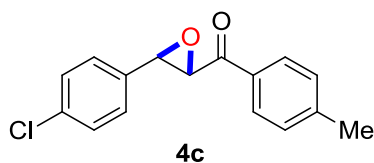
(3-(perfluorophenyl)oxiran-2-yl)(phenyl)methanone (3u): ^1H NMR (400 MHz, CDCl_3) δ 8.22 – 7.95 (m, 2H), 7.67 (t, $J = 7.4$ Hz, 1H), 7.54 (t, $J = 7.7$ Hz, 2H), 4.79 (d, $J = 2.0$ Hz, 1H), 4.25 (d, $J = 1.8$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.3, 135.0, 134.3, 128.9, 128.3, 55.6, 55.5, 50.4; HRMS calculated for $\text{C}_{15}\text{H}_7\text{F}_5\text{O}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 337.0258, found: 337.0258. (Pale yellow oil, 32.0 mg, 51% isolated yield).



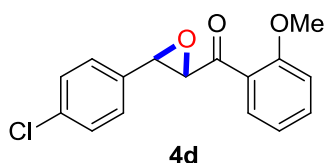
(3-(4-chlorophenyl)oxiran-2-yl)(o-tolyl)methanone (4a): ^1H NMR (400 MHz, CDCl_3) δ 7.82 – 7.75 (m, 2H), 7.43 (d, $J = 7.6$ Hz, 1H), 7.40 – 7.34 (m, 3H), 7.33 – 7.28 (m, 2H), 4.25 (d, $J = 1.9$ Hz, 1H), 4.05 (d, $J = 1.8$ Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.8, 138.8, 135.3, 134.8, 134.0, 128.9, 128.7, 128.6, 127.0, 125.5, 60.7, 58.6, 21.2; HRMS calculated for $\text{C}_{16}\text{H}_{13}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 295.0496, found: 295.0494. (Pale yellow oil, 35.4 mg, 65% isolated yield).



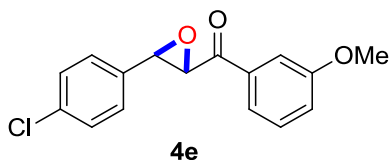
(3-(4-chlorophenyl)oxiran-2-yl)(m-tolyl)methanone (4b): ^1H NMR (400 MHz, CDCl_3) δ 7.79 (d, $J = 11.5$ Hz, 2H), 7.43 (d, $J = 7.6$ Hz, 1H), 7.37 (dt, $J = 7.1, 3.2$ Hz, 3H), 7.30 (d, $J = 8.5$ Hz, 2H), 4.24 (d, $J = 1.8$ Hz, 1H), 4.05 (d, $J = 1.7$ Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.8, 138.8, 135.3, 134.9, 134.8, 134.0, 128.9, 128.7, 128.6, 127.0, 125.5, 60.7, 58.6, 21.2; HRMS calculated for $\text{C}_{16}\text{H}_{13}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 295.0496, found: 295.0494. (Pale yellow oil, 36.5 mg, 67% isolated yield).



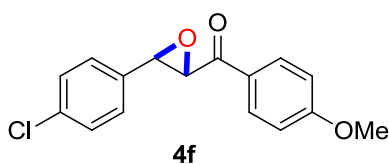
(3-(4-chlorophenyl)oxiran-2-yl)(p-tolyl)methanone (4c): ^1H NMR (500 MHz, CDCl_3) δ 7.90 (d, $J = 8.2$ Hz, 2H), 7.37 (d, $J = 8.4$ Hz, 2H), 7.32 – 7.26 (m, 4H), 4.23 (d, $J = 1.7$ Hz, 1H), 4.04 (d, $J = 1.5$ Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 192.2, 145.2, 134.8, 134.2, 132.9, 129.6, 129.0, 128.4, 127.1, 60.8, 58.6, 21.8; HRMS calculated for $\text{C}_{16}\text{H}_{13}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 295.0496, found: 295.0495. (White solid, 37.1 mg, 68% isolated yield).



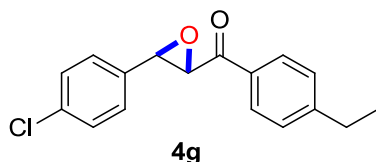
3-(4-chlorophenyl)oxiran-2-yl(2-methoxyphenyl)methanone (4d): ^1H NMR (400 MHz, CDCl_3) δ 7.81 (dd, $J = 7.7, 1.6$ Hz, 1H), 7.59 – 7.46 (m, 1H), 7.34 (dd, $J = 22.8, 8.5$ Hz, 4H), 7.04 (t, $J = 7.5$ Hz, 1H), 6.93 (d, $J = 8.4$ Hz, 1H), 4.26 (d, $J = 1.8$ Hz, 1H), 3.97 (d, $J = 1.5$ Hz, 1H), 3.62 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 194.3, 159.4, 135.0, 134.9, 134.4, 130.6, 128.7, 127.0, 125.7, 121.0, 111.5, 64.3, 58.9, 55.6; HRMS calculated for $\text{C}_{16}\text{H}_{13}\text{ClO}_3\text{Na}$ ($\text{M} + \text{Na}^+$): 311.0445, found: 311.0447. (White solid, 35.8mg, 62% isolated yield).



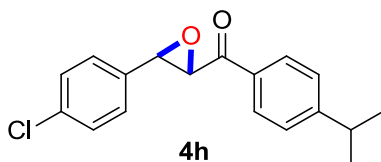
3-(4-chlorophenyl)oxiran-2-yl(3-methoxyphenyl)methanone (4e): ^1H NMR (500 MHz, CDCl_3) δ 7.59 – 7.48 (m, 2H), 7.41 – 7.33 (m, 3H), 7.29 (d, $J = 8.5$ Hz, 2H), 7.18 – 7.13 (m, 1H), 4.23 (d, $J = 1.8$ Hz, 1H), 4.04 (d, $J = 1.7$ Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 192.5, 160.0, 136.6, 134.9, 134.0, 129.9, 129.0, 127.1, 120.9, 120.6, 112.4, 60.9, 58.7, 55.5; HRMS calculated for $\text{C}_{16}\text{H}_{13}\text{ClO}_3\text{Na}$ ($\text{M} + \text{Na}^+$): 311.0445, found: 311.0445. (White solid, 47.4 mg, 82% isolated yield).



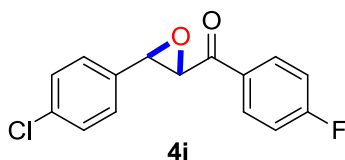
3-(4-chlorophenyl)oxiran-2-yl(4-methoxyphenyl)methanone (4f): ^1H NMR (500 MHz, CDCl_3) δ 8.02 – 7.96 (m, 2H), 7.39 – 7.34 (m, 2H), 7.29 (d, J = 8.5 Hz, 2H), 6.98 – 6.92 (m, 2H), 4.20 (d, J = 1.8 Hz, 1H), 4.04 (d, J = 1.7 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 190.9, 164.3, 134.8, 134.3, 130.7, 129.0, 128.5, 127.1, 114.1, 60.8, 58.4, 55.5; HRMS calculated for $\text{C}_{16}\text{H}_{13}\text{ClO}_3\text{Na}$ ($\text{M} + \text{Na}^+$): 311.0445, found: 311.0445. (White solid, 41.6 mg, 72% isolated yield).



3-(4-chlorophenyl)oxiran-2-yl(4-ethylphenyl)methanone (4g): ^1H NMR (500 MHz, CDCl_3) δ 7.96 – 7.89 (m, 2H), 7.40 – 7.34 (m, 2H), 7.34 – 7.28 (m, 4H), 4.24 (d, J = 1.9 Hz, 1H), 4.05 (d, J = 1.8 Hz, 1H), 2.72 (q, J = 7.6 Hz, 2H), 1.25 (t, J = 7.6 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 192.2, 151.3, 134.9, 134.2, 133.1, 129.0, 128.6, 128.4, 127.1, 60.9, 58.6, 29.0, 15.1; HRMS calculated for $\text{C}_{17}\text{H}_{15}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 309.0653, found: 309.0652. (Pale yellow oil, 38.9 mg, 68% isolated yield).

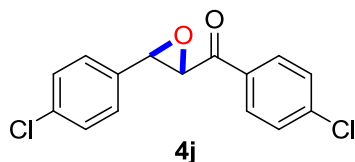


(3-(4-chlorophenyl)oxiran-2-yl)(4-isopropylphenyl)methanone (4h): ^1H NMR (400 MHz, CDCl_3) δ 7.97 – 7.91 (m, 2H), 7.41 – 7.27 (m, 6H), 4.24 (d, J = 1.9 Hz, 1H), 4.04 (d, J = 1.8 Hz, 1H), 2.97 (dt, J = 13.8, 6.9 Hz, 1H), 1.26 (d, J = 6.9 Hz, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 192.1, 155.8, 134.8, 134.1, 133.2, 128.9, 128.5, 127.0, 126.9, 60.8, 58.5, 34.3, 23.5; HRMS calculated for $\text{C}_{18}\text{H}_{17}\text{ClO}_2\text{Na}$ ($\text{M} + \text{Na}^+$): 323.0809, found: 323.0804. (Pale yellow oil, 36.7 mg, 61% isolated yield).

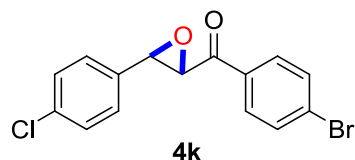


3-(4-chlorophenyl)oxiran-2-yl(4-fluorophenyl)methanone (4i): ^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, J = 8.7, 5.4 Hz, 2H), 7.37 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 8.4 Hz, 2H), 7.16 (t, J = 8.6 Hz, 2H), 4.19 (d, J = 1.6 Hz, 1H), 4.05 (d, J = 1.2 Hz, 1H); ^{13}C

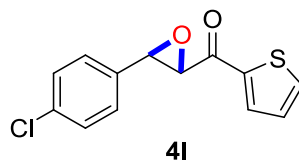
NMR (101 MHz, CDCl₃) δ 191.1, 167.5, 164.9, 134.9, 133.8, 131.7, 131.6, 131.1, 131.0, 128.9, 127.0, 116.2, 116.0, 60.8, 58.5; HRMS calculated for C₁₅H₁₀ClFO₂Na (M + Na⁺): 299.0246, found: 299.0244. (Pale yellow oil, 39.3 mg, 71% isolated yield).



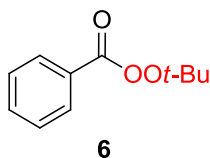
(4-chlorophenyl)(3-(4-chlorophenyl)oxiran-2-yl)methanone (4j): ¹H NMR (400 MHz, CDCl₃) δ 7.96 (d, *J* = 8.6 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.38 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 4.18 (d, *J* = 1.8 Hz, 1H), 4.05 (d, *J* = 1.6 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 191.1, 140.6, 135.0, 133.7, 133.5, 129.7, 129.2, 129.0, 127.0, 60.9, 58.6; HRMS calculated for C₁₅H₁₀Cl₂O₂Na (M + Na⁺): 314.9950, found: 314.9950. (Pale yellow oil, 36.3 mg, 62% isolated yield).



(4-bromophenyl)(3-(4-chlorophenyl)oxiran-2-yl)methanone (4k): ¹H NMR (400 MHz, CDCl₃) δ 7.87 (d, *J* = 8.6 Hz, 2H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.33 (dd, *J* = 34.6, 8.5 Hz, 4H), 4.18 (d, *J* = 1.8 Hz, 1H), 4.05 (d, *J* = 1.6 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 191.8, 135.0, 133.9, 133.7, 132.2, 129.7, 129.4, 129.0, 127.0, 60.8, 58.6; HRMS calculated for C₁₅H₁₀ClBrO₂Na (M + Na⁺): 358.9445, found: 358.9443. (White solid, 52.6 mg, 78% isolated yield).



(4-chlorophenyl)oxiran-2-yl(thiophen-2-yl)methanone (4l): ¹H NMR (500 MHz, CDCl₃) δ 7.99 (dd, *J* = 3.9, 1.0 Hz, 1H), 7.75 (dd, *J* = 4.9, 1.0 Hz, 1H), 7.39 – 7.33 (m, 2H), 7.30 – 7.25 (m, 2H), 7.18 (dd, *J* = 4.9, 3.9 Hz, 1H), 4.14 (d, *J* = 1.6 Hz, 1H), 4.03 (d, *J* = 1.8 Hz, 1H); ¹³C NMR (126 MHz, CDCl₃) δ 186.1, 140.8, 135.4, 134.9, 133.8, 133.7, 129.0, 128.5, 127.1, 61.9, 58.7; HRMS calculated for C₁₃H₉ClSO₂Na (M + Na⁺): 286.9904, found: 286.9909. (White solid, 43.9 mg, 83% isolated yield).



tert-butyl benzoperoxoate (6): ^1H NMR (400 MHz, CDCl_3) δ 8.00 – 7.88 (m, 2H), 7.61 – 7.54 (m, 1H), 7.48 – 7.41 (m, 2H), 1.41 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 164.3, 133.2, 129.0, 128., 127.6, 83.8, 26.16 (s); HRMS calculated for $\text{C}_{11}\text{H}_{13}\text{O}_3\text{Na}$ ($\text{M} + \text{Na}^+$): 217.0835, found: 217.0837. (Pale yellow oil, 38.8 mg, 62% isolated yield).

References:

- (1) Liu, W.; Li, Y.; Liu, K.; Li, Z. *J. Am. Chem. Soc.* **2011**, *133*, 10756.
- (2) Wei, W. T; Yang, X. H.; Li, H. B.; Li, J. H. *Adv. Synth. Catal.* **2015**, *357*, 59.
- (3) Ke, Q.; Zhang, B.; Hu, B.; Jin, Y.; Lu, G. *Chem. Commun.* **2015**, *51*, 1012.
- (4) Xiang, M.; Ni, X.; Yi, X.; Zheng, A.; Wang, W.; He, M.; Xiong, J.; Liu, T.; Ma, Y.; Zhu, P.; Zheng, X.; Tang, T. *ChemCatChem* **2015**, *7*, 521.

Copies of ^1H NMR and ^{13}C NMR spectra

