Divergent Synthesis of Flavones and Flavanones from 2′-Hydroxydihydrochalcones via Palladium-Catalyzed Oxidative Cyclization

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Abstract: Divergent and versatile synthetic routes to flavones and flavanones via efficient Pd(II) catalysis are disclosed. These Pd(II) catalysis expediently provide a variety of flavones and flavanones from 2′-hydroxydihydrochalcones as common intermediates, depending on oxidants and additives, via discriminate oxidative cyclization sequences involving dehydrogenation, respectively, in highly atom-economic manner.

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1. General Information

Unless stated otherwise, all reagents were purchased from commercial suppliers (Sigma Aldrich, TCI, Alfa Aesar and Strem chemicals) and used as received without further purification. If necessary, solvents were dried following the standard procedures. All reactions were performed in oven-dried reaction flasks with rubber septum under argon atmosphere. $^1$H NMR was measured and obtained using a Bruker 400 and $^{13}$C NMR spectra was measured on a Varian VNMR S500 spectrometer. $^1$H and $^{13}$C NMR chemical shifts were determined relative to the signal of the residual solvent peak used as an internal reference. Signals are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad). Coupling constants (J) were reported in Hertz (Hz). High-resolution mass spectrometry (HRMS) data were recorded using Jeol AccuTOF (JMS-T100TD) equipped with a DART (direct analysis in real time) ion source from ionsens, (Tokyo, Japan) in the EI or ESI mode. Flash column chromatography was performed using silica gel 60 (230-400 mesh) and analytical thin layer chromatography (TLC) was performed using Merck TLC Silica gel 60 F 254 plates. Visualization of the TLC were performed under UV light (254nm or 365 nm) or by TLC staining (Hanessian's stain or p-anisaldehyde stain).

2. Experimental Procedures

2.1 Synthesis of flavone derivatives (3a-3z, 3aa-3ac, 5a, and 5c)

2.1.1 General procedure for the synthesis of flavones from 2'-hydroxydihydrochalcones 1

A mixture of 2'-hydroxydihydrochalcones 1 (50 mg, 0.221 mmol), Pd(TFA)$_2$ (7.3 mg, 0.022 mmol), 5-nitro-1,10-phenanthroline (10 mg, 0.044 mmol) in anhydrous DMSO (0.3 M, 0.7 mL) was stirred in a 10-mL round-bottomed flask. Under an O$_2$ atmosphere, the reaction mixture was heated at 100 °C in oil bath until complete of the reaction on TLC. After cooling, water was added and the mixture was extracted with EtOAc. The combined organic layers were dried with MgSO$_4$, filtered, and concentrated in vacuo. The residue was purified by chromatography on silica gel column.

2-phenyl-4H-chromen-4-one 3a

![3a](image)

White solid (47 mg, 81%).

$^1$H NMR (400 MHz, Chloroform-d) δ 8.23 (dd, J = 7.9, 1.7 Hz, 1H), 7.92 (dd, J = 7.5, 2.2 Hz, 2H), 7.70 (ddd, J = 8.6, 7.1, 1.7 Hz, 1H), 7.56 (dd, J = 8.4 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.44 – 7.38 (m, 1H), 6.82 (s, 1H).

$^{13}$C NMR (126 MHz, Chloroform-d) δ 178.56, 163.49, 156.35, 133.89, 131.85, 131.72, 129.15, 126.38, 125.79, 125.33, 124.04, 118.20, 107.67.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{11}$O$_2$ 223.0759; Found 223.0772.

The characterization of the compound matched up with the data previously reported.$^1$

7-fluoro-2-phenyl-4H-chromen-4-one 3b

![3b](image)

White solid (34.6 mg, 70%).

$^1$H NMR (400 MHz, Chloroform-d) δ 8.25 (dd, J = 8.8, 6.3 Hz, 1H), 7.96 – 7.85 (m, 2H), 7.59 – 7.51 (m, 3H), 7.27 (dd, J = 9.0, 2.4 Hz, 1H), 7.16 (ddd, J = 8.9, 8.1, 2.4 Hz, 1H), 6.81 (s, 1H).
$^{13}$C NMR (126 MHz, Chloroform-d) δ 177.57, 165.83 (d, $J = 255.1$ Hz), 163.83, 157.34 (d, $J = 13.3$ Hz), 131.89, 131.51, 129.22, 128.33 (d, $J = 10.5$ Hz), 126.36, 120.92, 114.10 (d, $J = 22.8$ Hz), 107.74, 104.92 (d, $J = 25.3$ Hz).

$^{19}$F NMR (471 MHz, Chloroform-d) δ -102.71.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{10}$F$_1$O$_2$ 241.0665; Found 241.0670.

The characterization of the compound matched up with the data previously reported.$^2$

7-chloro-2-phenyl-4H-chromen-4-one 3c

![3c](image)

White solid (45.5 mg, 84%).

$^1$H NMR (400 MHz, Chloroform-d) δ 8.18 (d, $J = 8.6$ Hz, 1H), 7.92 (dd, $J = 7.9$, 1.8 Hz, 2H), 7.62 (d, $J = 1.9$ Hz, 1H), 7.59 – 7.50 (m, 3H), 7.40 (dd, $J = 8.5$, 1.9 Hz, 1H), 6.83 (s, 1H).

$^{13}$C NMR (126 MHz, Chloroform-d) δ 178.39, 162.33, 156.27, 138.00, 134.04, 130.34, 129.49, 127.65, 125.85, 125.50, 118.15, 107.79.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{10}$Cl$_1$O$_2$ 257.0369; Found 257.0371.

The characterization of the compound matched up with the data previously reported.$^2$

7-bromo-2-phenyl-4H-chromen-4-one 3d

![3d](image)

White solid (46.4 mg, 92%).

$^1$H NMR (400 MHz, Chloroform-d) δ 8.10 (d, $J = 8.5$ Hz, 1H), 7.91 (dd, $J = 7.9$, 1.8 Hz, 2H), 7.80 (d, $J = 1.8$ Hz, 1H), 7.59 – 7.50 (m, 3H), 7.40 (dd, $J = 8.5$, 1.9 Hz, 1H), 6.83 (s, 1H).

$^{13}$C NMR (126 MHz, Chloroform-d) δ 177.75, 163.58, 156.38, 131.97, 131.44, 129.23, 128.97, 128.06, 127.23, 126.39, 122.95, 118.34, 107.89.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{10}$Br$_1$O$_2$ 300.9864; Found 300.9863.

The characterization of the compound matched up with the data previously reported.$^3$

4-oxo-2-phenyl-4H-chromen-7-yl trifluoromethanesulfonate 3e

![3e](image)

White solid (48 mg, 72%).

$^1$H NMR (400 MHz, Chloroform-d) δ 8.35 (d, $J = 8.8$ Hz, 1H), 7.93 (dd, $J = 8.0$, 1.6 Hz, 2H), 7.63 – 7.51 (m, 4H), 7.35 (dd, $J = 8.8$, 2.3 Hz, 1H), 6.86 (s, 1H).

$^{13}$C NMR (126 MHz, Chloroform-d) δ 176.99, 164.34, 156.55, 152.35, 132.24, 131.10, 129.32, 128.54, 126.47, 123.81, 120.06, 118.71, 117.51, 111.68, 108.06.

$^{19}$F NMR (471 MHz, Chloroform-d) δ -72.42.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{10}$Br$_1$O$_2$S$_1$ 371.0201; Found 371.0196.

The characterization of the compound matched up with the data previously reported.$^4$

4-oxo-2-phenyl-4H-chromen-7-yl pivalate 3f
Yellow solid (34 mg, 55%).

\(^1\)H NMR (400 MHz, Chloroform-d) \(\delta 8.25\) (d, \(J = 8.6\) Hz, 1H), 7.90 (dd, \(J = 7.7, 1.9\) Hz, 2H), 7.57 – 7.49 (m, 3H), 7.39 (d, \(J = 2.1\) Hz, 1H), 7.14 (dd, \(J = 8.7, 2.1\) Hz, 1H), 6.83 (s, 1H), 1.40 (s, 9H).

\(^{13}\)C NMR (126 MHz, Chloroform-d) \(\delta 177.89, 176.44, 163.75, 156.84, 155.28, 131.82, 131.63, 129.18, 127.13, 126.36, 121.71, 119.54, 111.16, 107.71, 39.42, 27.15.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{20}\)H\(_{19}\)O\(_4\) 323.1283; Found 323.1279.

The characterization of the compound matched up with the data previously reported.\(^1\)

7-methyl-2-phenyl-4\(H\)-chromen-4-one 3g

Yellow solid (42 mg, 93%).

\(^1\)H NMR (400 MHz, Chloroform-d) \(\delta 8.12\) (d, \(J = 8.1\) Hz, 1H), 7.98 – 7.88 (m, 2H), 7.56 – 7.51 (m, 3H), 7.39 (s, 1H), 7.25 (dd, \(J = 8.4, 1.2\) Hz, 1H), 6.81 (s, 1H), 2.52 (s, 3H).

\(^{13}\)C NMR (126 MHz, Chloroform-d) \(\delta 178.53, 163.21, 156.49, 145.23, 131.99, 131.59, 129.12, 126.83, 126.33, 125.53, 125.19, 117.96, 107.61, 21.95.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{16}\)H\(_{13}\)O\(_2\) 237.0916; Found 237.0915.

The characterization of the compound matched up with the data previously reported.\(^2\)

6-nitro-2-phenyl-4\(H\)-chromen-4-one 3h

White solid (20 mg, 41%).

\(^1\)H NMR (400 MHz, Chloroform-d) \(\delta 9.12\) (d, \(J = 2.8\) Hz, 1H), 8.55 (dd, \(J = 9.1, 2.8\) Hz, 1H), 7.98 – 7.91 (m, 2H), 7.74 (d, \(J = 9.1\) Hz, 1H), 7.62 – 7.55 (m, 3H), 6.90 (s, 1H).

\(^{13}\)C NMR (126 MHz, Chloroform-d) \(\delta 176.79, 164.24, 159.17, 144.93, 132.48, 130.85, 129.39, 128.25, 126.54, 124.19, 122.62, 119.93, 107.97.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{10}\)N\(_2\)O\(_2\) 268.0610; Found 268.0615.

The characterization of the compound matched up with the data previously reported.\(^1\)

7-hydroxy-2-phenyl-4\(H\)-chromen-4-one 3i
Yellow solid (37.5 mg, 59%).

\(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 10.85 (s, 1H), 8.08 (dd, \(J = 7.7, 2.0\) Hz, 2H), 7.90 (d, \(J = 8.7\) Hz, 1H), 7.62 – 7.55 (m, 3H), 7.02 (d, \(J = 2.3\) Hz, 1H), 6.95 (dd, \(J = 8.7, 2.3\) Hz, 1H), 6.92 (s, 1H).

\(^1\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 176.95, 163.33, 162.47, 158.05, 132.09, 131.85, 129.63, 127.09, 126.72, 116.71, 115.62, 107.18, 103.10.

HRMS (ESI\(^+\)) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{11}\)O\(_3\) 239.0708; Found 239.0708.

The characterization of the compound matched up with the data previously reported.\(^5\)

7-methoxy-2-phenyl-4H-chromen-4-one \(3j\)

\[
\begin{array}{c}
\text{MeO} \\
\text{7-methoxy-2-phenyl-4H-chromen-4-one} \quad 3j
\end{array}
\]

White solid (42.1 mg, 83%).

\(^1\)H NMR (400 MHz, Chloroform-\(d\)) \(\delta\) 8.13 (d, \(J = 8.7\) Hz, 1H), 7.94 – 7.84 (m, 2H), 7.57 – 7.46 (m, 3H), 7.02 – 6.93 (m, 2H), 6.76 (s, 1H), 3.93 (s, 3H).

\(^1\)C NMR (126 MHz, Chloroform-\(d\)) \(\delta\) 177.97, 164.28, 163.09, 158.09, 131.93, 131.52, 129.10, 127.13, 126.24, 117.91, 114.53, 107.61, 100.49, 55.94.

HRMS (ESI\(^+\)) m/z: [M+H]\(^+\) Calcd for C\(_{16}\)H\(_{13}\)O\(_3\) 253.0865; Found 253.0856.

The characterization of the compound matched up with the data previously reported.\(^1\)

7-(benzyloxy)-2-phenyl-4H-chromen-4-one \(3k\)

\[
\begin{array}{c}
\text{BnO} \\
\text{7-(benzyloxy)-2-phenyl-4H-chromen-4-one} \quad 3k
\end{array}
\]

White solid (44.2 mg, 77%).

\(^1\)H NMR (400 MHz, Chloroform-\(d\)) \(\delta\) 8.16 (d, \(J = 8.6\) Hz, 1H), 7.95 – 7.86 (m, 2H), 7.57 – 7.50 (m, 3H), 7.49 – 7.37 (m, 5H), 7.12 – 7.03 (m, 2H), 6.77 (s, 1H), 5.20 (s, 2H).

\(^1\)C NMR (126 MHz, Chloroform-\(d\)) \(\delta\) 177.99, 163.36, 163.19, 158.03, 135.82, 131.93, 131.55, 129.12, 128.89, 128.53, 127.63, 127.25, 126.29, 118.12, 115.05, 107.66, 101.59, 70.64.

HRMS (ESI\(^+\)) m/z: [M+H]\(^+\) Calcd for C\(_{22}\)H\(_{17}\)O\(_3\) 329.1178; Found 329.1168.

The characterization of the compound matched up with the data previously reported.\(^6\)

6-methoxy-2-phenyl-4H-chromen-4-one \(3l\)

\[
\begin{array}{c}
\text{MeO} \\
\text{6-methoxy-2-phenyl-4H-chromen-4-one} \quad 3l
\end{array}
\]

White solid (34 mg, 79%).

\(^1\)H NMR (400 MHz, Chloroform-\(d\)) \(\delta\) 7.98 – 7.89 (m, 2H), 7.61 (d, \(J = 3.1\) Hz, 1H), 7.57 – 7.49 (m, 4H), 7.30 (dd, \(J = 9.1, 3.1\) Hz, 1H), 6.84 (s, 1H), 3.92 (s, 3H).

\(^1\)C NMR (126 MHz, Chloroform-\(d\)) \(\delta\) 178.45, 163.28, 157.11, 151.19, 131.97, 131.61, 129.13, 126.35, 124.66, 123.94, 119.63, 106.94, 104.90, 56.04.

HRMS (ESI\(^+\)) m/z: [M+H]\(^+\) Calcd for C\(_{16}\)H\(_{13}\)O\(_3\) 253.0865; Found 253.0851.

The characterization of the compound matched up with the data previously reported.\(^1\)
5,7-dimethoxy-2-phenyl-4H-chromen-4-one 3m

White solid (38 mg, 71%).

$^1$H NMR (400 MHz, Chloroform-d) $\delta$ 7.92 – 7.84 (m, 2H), 7.56 – 7.45 (m, 3H), 6.70 (s, 1H), 6.59 (d, $J$ = 2.2 Hz, 1H), 6.39 (d, $J$ = 2.2 Hz, 1H), 3.97 (s, 3H), 3.92 (s, 3H).

$^{13}$C NMR (126 MHz, Chloroform-d) $\delta$ 177.73, 164.15, 160.99, 160.71, 160.01, 131.62, 131.28, 129.03, 126.02, 109.39, 109.16, 96.27, 92.90, 56.53, 55.86.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{17}$H$_{15}$O$_4$ 283.0970; Found 283.0947.

The characterization of the compound matched up with the data previously reported.$^1$

2-(4-methoxyphenyl)-4H-chromen-4-one 3n

White solid (46.6 mg, 80%).

$^1$H NMR (400 MHz, Chloroform-d) $\delta$ 8.23 (dd, $J$ = 7.9, 1.7 Hz, 1H), 7.94 – 7.86 (m, 2H), 7.69 (ddd, $J$ = 8.7, 7.1, 1.7 Hz, 1H), 7.56 (ddd, $J$ = 8.5, 1.2 Hz, 1H), 7.42 (ddd, $J$ = 8.1, 7.1, 1.1 Hz, 1H), 7.08 – 7.00 (m, 2H), 6.76 (s, 1H), 3.90 (s, 3H).

$^{13}$C NMR (126 MHz, Chloroform-d) $\delta$ 178.49, 163.50, 162.50, 156.27, 133.67, 128.09, 125.74, 125.17, 124.09, 118.06, 114.55, 106.25, 55.60.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{16}$H$_{13}$O$_3$ 253.0865; Found 253.0853.

The characterization of the compound matched up with the data previously reported.$^1$

2-(4-hydroxyphenyl)-4H-chromen-4-one 3o

Yellow solid (23 mg, 47% isolated yield), 72% yield determined by $^1$H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard.

$^1$H NMR (400 MHz, DMSO-d$_6$) $\delta$ 10.35 (s, 1H), 8.04 (dd, $J$ = 7.8, 1.5 Hz, 1H), 7.98 (d, $J$ = 8.8 Hz, 2H), 7.82 (ddd, $J$ = 8.6, 7.1, 1.6 Hz, 1H), 7.76 (d, $J$ = 8.4 Hz, 1H), 7.53 – 7.45 (m, 1H), 6.96 (d, $J$ = 8.8 Hz, 2H), 6.89 (s, 1H).

$^{13}$C NMR (126 MHz, DMSO-d$_6$) $\delta$ 177.42, 163.60, 161.52, 156.12, 134.57, 128.91, 125.85, 125.72, 123.85, 122.11, 118.90, 116.48, 106.25, 105.34.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{11}$O$_3$ 239.0708; Found 239.0703.

The characterization of the compound matched up with the data previously reported.$^7$

2-(3-hydroxyphenyl)-4H-chromen-4-one 3p
Yellow solid (65.3 mg, 95%).

$^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 9.91 (s, 1H), 8.06 (dd, $J = 7.9, 1.6$ Hz, 1H), 7.84 (ddd, $J = 8.6, 7.0, 1.7$ Hz, 1H), 7.78 (d, $J = 8.4$ Hz, 1H), 7.57 – 7.47 (m, 2H), 7.46 (ddd, $J = 8.1, 2.5, 1.0$ Hz, 1H), 6.94 (s, 1H).

$^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 177.62, 163.25, 158.45, 156.20, 134.86, 132.97, 130.80, 126.06, 125.34, 123.88, 119.03, 117.74, 113.38, 107.45.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{11}$O$_3$ 239.0708; Found 239.0694.

The characterization of the compound matched up with the data previously reported.

2-(3,4-dimethoxyphenyl)-4$^H$-chomen-4-one 3q

Pale yellow solid (69 mg, 87%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 8.24 (dd, $J = 7.9, 1.7$ Hz, 1H), 7.70 (ddd, $J = 8.7, 7.1, 1.7$ Hz, 1H), 7.59 (d, $J = 2.1$ Hz, 1H), 7.57 (d, $J = 2.2$ Hz, 1H), 7.47 – 7.38 (m, 2H), 7.00 (d, $J = 8.5$ Hz, 1H), 6.77 (s, 1H), 4.00 (s, 3H), 3.98 (s, 3H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 178.47, 163.47, 156.28, 152.16, 149.36, 134.97, 125.76, 125.25, 124.32, 124.01, 120.11, 118.08, 111.23, 108.88, 106.57, 56.18, 56.17.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{17}$H$_{15}$O$_4$ 283.0970; Found 283.0953.

The characterization of the compound matched up with the data previously reported.

2-(3,5-dimethoxyphenyl)-4$^H$-chomen-4-one 3r

Brown solid (55.6 mg, 70%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 8.22 (d, $J = 7.9$ Hz, 1H), 7.70 (t, 1H), 7.57 (d, $J = 8.4$ Hz, 1H), 7.43 (t, $J = 7.4$ Hz, 1H), 7.04 (d, $J = 2.3$ Hz, 2H), 6.80 (s, 1H), 6.62 (s, 1H), 3.87 (s, 6H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 178.58, 163.27, 161.27, 156.31, 133.91, 133.76, 125.77, 125.36, 124.05, 120.03, 104.54, 103.58, 55.68.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{17}$H$_{15}$O$_4$ 283.0970; Found 283.0945.

The characterization of the compound matched up with the data previously reported.

2-(3,4,5-trimethoxyphenyl)-4$^H$-chomen-4-one 3s
Yellow solid (59.5 mg, 75%).

\[ \text{H NMR (400 MHz, Chloroform-}d\text{)} \delta 8.24 (dd, J = 7.9, 1.7 Hz, 1H), 7.72 (ddd, J = 8.7, 7.1, 1.7 Hz, 1H), 7.60 (dd, J = 8.4, 1.1 Hz, 1H), 7.44 (ddd, J = 8.3, 7.1, 1.1 Hz, 1H), 7.15 (s, 2H), 6.79 (s, 1H), 3.97 (s, 6H), 3.94 (s, 3H).
\]

\[ \text{C NMR (126 MHz, Chloroform-}d\text{)} \delta 178.47, 163.35, 156.29, 153.67, 141.26, 133.86, 127.09, 125.79, 125.39, 123.99, 118.16, 107.47, 103.79, 61.15, 56.43.
\]

\[ \text{HRMS (ESI\textsuperscript{+}) m/z: [M+H\textsuperscript{+}] Calcd for } C_{18}H_{17}O_{5} 313.1076; \text{ Found 313.1056.}
\]

The characterization of the compound matched up with the data previously reported.

5,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one 3t

Yellow oil (62 mg, 79%).

\[ \text{H NMR (400 MHz, Chloroform-}d\text{)} \delta 7.87 – 7.78 (m, 2H), 7.04 – 6.96 (m, 2H), 6.60 (d, J = 2.3 Hz, 1H), 6.38 (d, J = 2.3 Hz, 1H), 3.96 (s, 3H), 3.91 (s, 3H), 3.88 (s, 3H).
\]

\[ \text{C NMR (126 MHz, Chloroform-}d\text{)} \delta 177.79, 163.99, 162.12, 160.90, 160.76, 159.89, 127.66, 123.83, 114.40, 109.22, 107.66, 96.14, 92.87, 56.48, 55.83, 55.55.
\]

\[ \text{HRMS (ESI\textsuperscript{+}) m/z: [M+H\textsuperscript{+}] Calcd for } C_{18}H_{17}O_{5} 313.1076; \text{ Found 313.1054.}
\]

The characterization of the compound matched up with the data previously reported.

2-(naphthalen-2-yl)-4H-chromen-4-one 3u

Brown solid (35 mg, 72%).

\[ \text{H NMR (400 MHz, Chloroform-}d\text{)} \delta 8.51 (s, 1H), 8.27 (dd, J = 7.9, 1.7 Hz, 1H), 8.03 – 7.88 (m, 4H), 7.74 (ddd, J = 8.7, 7.1, 1.7 Hz, 1H), 7.66 (dd, J = 8.5, 1.1 Hz, 1H), 7.64 – 7.56 (m, 2H), 7.45 (ddd, J = 7.9, 7.0, 1.1 Hz, 1H), 6.98 (s, 1H).
\]

\[ \text{C NMR (126 MHz, Chloroform-}d\text{)} \delta 178.57, 163.43, 161.96, 160.44, 134.76, 133.92, 133.00, 129.16, 129.05, 128.14, 127.94, 127.19, 127.03, 125.84, 125.36, 124.12, 118.23, 107.99.
\]

\[ \text{HRMS (ESI\textsuperscript{+}) m/z: [M+H\textsuperscript{+}] Calcd for } C_{19}H_{13}O_{2} 273.0916; \text{ Found 273.0887.}
\]

The characterization of the compound matched up with the data previously reported.

2-(4-fluorophenyl)-4H-chromen-4-one 3v
White solid (25 mg, 78%).

\(^1\)H NMR (400 MHz, Chloroform-\(d\)) \(\delta\) 8.24 (dd, \(J = 7.9, 1.7\) Hz, 1H), 8.00 – 7.90 (m, 2H), 7.72 (ddd, \(J = 8.6, 7.1, 1.7\) Hz, 1H), 7.57 (d, \(J = 8.0\) Hz, 1H), 7.48 – 7.40 (m, 1H), 7.23 (t, \(J = 8.6\) Hz, 2H), 6.78 (s, 1H).

\(^13\)C NMR (126 MHz, Chloroform-\(d\)) \(\delta\) 178.41, 164.86 (d, \(J = 253.3\) Hz), 162.51, 156.27, 133.96, 128.60 (d, \(J = 8.9\) Hz), 128.07 (d, \(J = 3.2\) Hz), 125.84, 125.43, 123.95, 118.12, 116.41 (d, \(J = 22.2\) Hz), 107.46.

\(^19\)F NMR (471 MHz, Chloroform-\(d\)) \(\delta\) -107.33.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{10}\)F\(_2\)O\(_2\) 241.0665; Found 241.0650.

The characterization of the compound matched up with the data previously reported.\(^1\)

2-(4-chlorophenyl)-4\(H\)-chromen-4-one \(3w\)

White solid (36 mg, 75%).

\(^1\)H NMR (400 MHz, Chloroform-\(d\)) \(\delta\) 8.24 (dd, \(J = 7.9, 1.7\) Hz, 1H), 7.92 – 7.84 (m, 2H), 7.72 (ddd, \(J = 8.7, 7.1, 1.7\) Hz, 1H), 7.58 (dd, \(J = 8.5, 0.6\) Hz, 1H), 7.55 – 7.49 (m, 2H), 7.44 (ddd, \(J = 8.1, 7.1, 1.1\) Hz, 1H), 6.81 (s, 1H).

\(^13\)C NMR (126 MHz, Chloroform-\(d\)) \(\delta\) 178.39, 162.33, 156.27, 138.00, 134.04, 130.34, 129.49, 127.65, 125.85, 125.50, 124.00, 118.15, 107.79.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{10}\)Cl\(_1\)O\(_2\) 257.0369; Found 257.0353.

The characterization of the compound matched up with the data previously reported.\(^1\)

2-(4-bromophenyl)-4\(H\)-chromen-4-one \(3x\)

White solid (34 mg, 75%).

\(^1\)H NMR (400 MHz, Chloroform-\(d\)) \(\delta\) 8.24 (dd, \(J = 7.9, 1.7\) Hz, 1H), 7.81 (d, \(J = 8.7\) Hz, 2H), 7.72 (ddd, \(J = 8.7, 7.1, 1.7\) Hz, 1H), 7.68 (d, \(J = 8.7\) Hz, 2H), 7.58 (d, \(J = 8.1\) Hz, 1H), 7.49 – 7.40 (m, 1H), 6.81 (s, 1H).

\(^13\)C NMR (126 MHz, Chloroform-\(d\)) \(\delta\) 178.39, 162.40, 156.26, 134.05, 132.46, 130.80, 127.81, 125.86, 125.51, 124.01, 118.16, 107.80.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{10}\)Br\(_1\)O\(_2\) 300.9864; Found 300.9838.

The characterization of the compound matched up with the data previously reported.\(^1\)

2-(4-iodophenyl)-4\(H\)-chromen-4-one \(3y\)
White solid (36 mg, 65%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 8.24 (dd, $J = 7.9$, 1.8 Hz, 1H), 7.89 (d, $J = 8.6$ Hz, 2H), 7.72 (ddd, $J = 8.7$, 7.2, 1.7 Hz, 1H), 7.66 (d, $J = 8.6$ Hz, 2H), 7.57 (d, $J = 8.4$ Hz, 1H), 7.49 – 7.40 (m, 1H), 6.82 (s, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 178.39, 162.55, 156.26, 138.42, 134.05, 131.38, 127.78, 125.85, 125.51, 124.03, 118.18, 107.79, 98.62.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{10}$I$_1$O$_3$ 348.9726; Found 348.9700.

2-methyl-4H-chromen-4-one 3z

Yellow solid (15 mg, 30%). This compound was synthesized from 1-(2-hydroxyphenyl)butan-1-one$^{10}$.

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 8.18 (d, $J = 7.9$ Hz, 1H), 7.69 – 7.60 (m, 1H), 7.42 (d, $J = 8.5$ Hz, 1H), 7.38 (t, $J = 7.5$ Hz, 1H), 6.18 (s, 1H), 2.39 (s, 3H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 178.38, 166.30, 156.57, 133.55, 125.74, 125.02, 123.64, 117.88, 110.67, 20.72.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{10}$H$_9$O$_2$ 161.0603; Found 161.0595.

The characterization of the compound matched up with the data previously reported.$^{11}$

2-(1-methyl-1H-indol-3-yl)-4H-chromen-4-one 3aa

Yellow solid (27 mg, 32%). This compound was synthesized from 1-(2-hydroxyphenyl)-3-(1-methyl-1H-indol-3-yl)propan-1-one$^{11}$.

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 8.23 (dd, $J = 7.9$, 1.7 Hz, 1H), 8.15 – 8.08 (m, 1H), 7.76 (s, 1H), 7.65 (ddd, $J = 8.7$, 7.1, 1.7 Hz, 1H), 7.52 (dd, $J = 8.5$, 1.1 Hz, 1H), 7.41 – 7.29 (m, 4H), 6.74 (s, 1H), 3.89 (s, 3H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 178.12, 162.14, 156.16, 137.85, 133.25, 131.28, 125.69, 124.93, 124.84, 124.23, 123.29, 122.08, 120.94, 117.74, 110.40, 108.35, 105.36, 33.67.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{18}$H$_{14}$N$_1$O$_2$ 276.1025; Found 276.1018.

2-(thiophen-2-yl)-4H-chromen-4-one 3ab

Yellow solid (37 mg, 54%).
\( ^1\)H NMR (400 MHz, Chloroform-d) \( \delta \) 8.20 (dd, \( J = 7.9, 1.6 \) Hz, 1H), 7.71 (dd, \( J = 3.8, 1.2 \) Hz, 1H), 7.68 (ddd, \( J = 8.7, 7.1, 1.7 \) Hz, 1H), 7.57 (dd, \( J = 5.0, 1.2 \) Hz, 1H), 7.54 – 7.48 (m, 1H), 7.40 (ddd, \( J = 8.1, 7.1, 1.1 \) Hz, 1H), 7.17 (dd, \( J = 5.0, 3.8 \) Hz, 1H), 6.69 (s, 1H).

\( ^1\)C NMR (126 MHz, Chloroform-d) \( \delta \) 178.00, 159.11, 155.98, 135.21, 133.85, 130.39, 128.61, 128.56, 125.75, 125.36, 124.05, 118.04, 106.25.

HRMS (ESI+) m/z: [M+H]+ Calcd for C\(_{13}\)H\(_9\)O\(_2\)S\(_2\) 229.0323; Found 229.0336.

2-(furan-2-yl)-4H-chromen-4-one 3ac

![3ac](image)

Yellow solid (9.5 mg, 15%).

\( ^1\)H NMR (500 MHz, Chloroform-d) \( \delta \) 8.22 (dd, \( J = 7.9, 1.7 \) Hz, 1H), 7.68 (ddd, \( J = 8.6, 7.1, 1.7 \) Hz, 1H), 7.64 (dd, \( J = 1.8, 0.8 \) Hz, 1H), 7.50 (dd, \( J = 8.5, 1.0 \) Hz, 1H), 7.41 (ddd, \( J = 8.1, 7.1, 1.1 \) Hz, 1H), 7.15 (dd, \( J = 3.6, 0.8 \) Hz, 1H), 6.75 (s, 1H), 6.62 (dd, \( J = 3.5, 1.8 \) Hz, 1H).

\( ^1\)C NMR (126 MHz, Chloroform-d) \( \delta \) 177.96, 155.90, 155.27, 146.49, 145.91, 133.84, 125.87, 125.30, 124.31, 117.99, 113.16, 112.63, 105.60.

HRMS (ESI+) m/z: [M+H]+ Calcd for C\(_{13}\)H\(_9\)O\(_3\) 213.0552; Found 213.0571.

2-(3,4-dimethoxyphenyl)-7-methoxy-4H-chromen-4-one (Geraldone dimethyl ether) 5a

![5a](image)

White solid (30 mg, 88%). This compound was synthesized from 1aa.

\( ^1\)H NMR (400 MHz, Chloroform-d) \( \delta \) 8.14 (d, \( J = 8.6 \) Hz, 1H), 7.56 (dd, \( J = 8.4, 2.2 \) Hz, 1H), 7.38 (d, \( J = 2.2 \) Hz, 1H), 7.03 – 6.95 (m, 3H), 6.71 (s, 1H), 4.00 (s, 3H), 3.97 (s, 3H), 3.95 (s, 3H).

\( ^1\)C NMR (126 MHz, Chloroform-d) \( \delta \) 177.92, 164.17, 163.10, 157.99, 151.98, 149.32, 127.09, 124.41, 119.90, 117.86, 114.34, 111.19, 108.78, 106.50, 100.51, 56.17, 55.93.

HRMS (ESI+) m/z: [M+H]+ Calcd for C\(_{18}\)H\(_{17}\)O\(_5\) 313.1076; Found 313.1063.

The characterization of the compound matched up with the data previously reported.

2-(4-iodophenyl)-4H-chromen-4-one (Tithonine) 5c

![5c](image)

White solid (25 mg, 70%). This compound was synthesized from 1ab.

\( ^1\)H NMR (400 MHz, Chloroform-d) \( \delta \) 8.12 (d, \( J = 8.7 \) Hz, 1H), 7.51 (d, \( J = 2.3 \) Hz, 1H), 7.44 (dd, \( J = 8.5, 2.3 \) Hz, 1H), 7.01 – 6.91 (m, 3H), 6.68 (s, 1H), 6.25 (s, 1H), 3.97 (s, 3H), 3.93 (s, 3H).

\( ^1\)C NMR (126 MHz, Chloroform-d) \( \delta \) 178.09, 164.19, 163.05, 158.02, 149.44, 146.10, 127.19, 125.07, 119.02, 117.86, 114.40, 112.44, 110.79, 106.50, 100.44, 56.19, 55.93, 29.79.

HRMS (ESI+) m/z: [M+H]+ Calcd for C\(_{17}\)H\(_{15}\)O\(_5\) 299.0920; Found 299.0904.

The characterization of the compound matched up with the data previously reported.
2.2 Synthesis of flavanone derivatives (4a-4r and 5b)

2.2.1 General procedure for the synthesis of flavanones from 2'-hydroxydihydrochalcones 1

A mixture of 2'-hydroxydihydrochalcones 1 (50 mg, 0.221 mmol), Pd(TFA)$_2$ (7.3 mg, 0.022 mmol), Cu(OAc)$_2$ (40.1 mg, 0.221 mmol) in DMSO (0.1 M, 2.2 mL) was stirred in a 10-mL round-bottomed flask under an Ar atmosphere, the reaction mixture was heated at 100 °C in oil bath until complete conversion of dihydrochalcone to chalcone on TLC. Then, the reaction flask was fitted with a reflux condenser and a solution of aq. HCl (2 N, 20 mL) and EtOAc (10 mL) was added to the flask. The reaction mixture was stirred for 24 h. After cooling, water was added and the mixture was extracted with EtOAc. The combined organic layers were dried with MgSO$_4$, filtered, and concentrated in vacuo. The residue was purified by chromatography on silica gel column.

2-phenylchroman-4-one 4a

![4a](image)

White solid (46.2 mg, 79%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.94 (d, $J = 8.1$ Hz, 1H), 7.54 – 7.38 (m, 6H), 7.10 – 7.02 (m, 2H), 5.49 (dd, $J = 13.4$, 2.9 Hz, 1H), 3.10 (dd, $J = 16.9$, 13.4 Hz, 1H), 2.90 (dd, $J = 16.9$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 192.10, 161.67, 138.85, 136.33, 128.98, 128.91, 127.17, 126.28, 121.04, 118.26, 79.71, 44.78.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{13}$O$_2$ 225.0916; Found 225.0916.

The characterization of the compound matched up with the data previously reported.

7-chloro-2-phenylchroman-4-one 4b

![4b](image)

Brown oil (24 mg, 69%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.87 (d, $J = 8.5$ Hz, 1H), 7.49 – 7.39 (m, 5H), 7.09 (d, $J = 1.9$ Hz, 1H), 7.04 (dd, $J = 8.5$, 1.9 Hz, 1H), 5.50 (dd, $J = 13.1$, 2.9 Hz, 1H), 3.09 (dd, $J = 16.9$, 13.1 Hz, 1H), 2.91 (dd, $J = 16.8$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 191.00, 161.94, 142.16, 138.31, 129.07, 129.02, 128.40, 126.24, 122.56, 119.60, 118.42, 80.11, 44.45.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{12}$ClO$_2$ 259.0526; Found 259.0489.

The characterization of the compound matched up with the data previously reported.

4-oxo-2-phenylchroman-7-yl pivalate 4c
Yellow oil (21.2 mg, 32%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.96 (d, $J = 8.5$ Hz, 1H), 7.51 – 7.37 (m, 5H), 6.84 – 6.74 (m, 2H), 5.51 (dd, $J = 13.2$, 2.9 Hz, 1H), 3.08 (dd, $J = 16.9$, 13.3 Hz, 1H), 2.90 (dd, $J = 16.9$, 3.0 Hz, 1H), 1.35 (s, 9H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 191.06, 176.40, 162.57, 157.36, 138.57, 128.97, 128.94, 128.55, 126.20, 118.78, 115.80, 111.21, 80.05, 44.53, 39.34, 27.12.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{20}$H$_{21}$O$_4$ 325.1440; Found 325.1436.

The characterization of the compound matched up with the data previously reported. 

7-methyl-2-phenylchroman-4-one 4d

Yellow solid (30.5 mg, 68%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.83 (d, $J = 8.2$ Hz, 1H), 7.51 – 7.38 (m, 5H), 6.91 – 6.85 (m, 2H), 5.47 (dd, $J = 13.3$, 2.9 Hz, 1H), 3.07 (dd, $J = 16.9$, 13.3 Hz, 1H), 2.87 (dd, $J = 16.9$, 3.0 Hz, 1H), 2.38 (s, 3H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 191.82, 161.70, 147.90, 138.99, 128.94, 128.82, 127.04, 126.25, 123.11, 118.80, 118.23, 79.68, 44.71, 22.08.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{16}$H$_{15}$O$_2$ 239.1072; Found 239.1070.

The characterization of the compound matched up with the data previously reported. 

7-methoxy-2-phenylchroman-4-one 4e

Yellow solid (51.6 mg, 74%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.88 (d, $J = 8.8$ Hz, 1H), 7.51 – 7.38 (m, 5H), 6.63 (dd, $J = 8.8$, 2.4 Hz, 1H), 6.51 (d, $J = 2.4$ Hz, 1H), 5.48 (dd, $J = 13.4$, 3.0 Hz, 1H), 3.84 (s, 3H), 3.05 (dd, $J = 16.9$, 13.3 Hz, 1H), 2.84 (dd, $J = 16.9$, 3.0 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 190.74, 166.31, 163.64, 138.89, 128.96, 128.88, 126.27, 114.93, 110.40, 101.01, 80.12, 55.76, 44.43.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{16}$H$_{15}$O$_2$ 255.1021; Found 255.1016.

The characterization of the compound matched up with the data previously reported. 

7-(benzyloxy)-2-phenylchroman-4-one 4f
Yellow solid (26 mg, 74%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.88 (d, $J = 8.8$ Hz, 1H), 7.51 – 7.34 (m, 10H), 6.70 (d, $J = 2.3$ Hz, 1H), 5.47 (dd, $J = 13.3$, 2.9 Hz, 1H), 5.10 (s, 2H), 3.05 (dd, $J = 16.9$, 13.3 Hz, 1H), 2.83 (dd, $J = 16.9$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 190.71, 165.37, 163.58, 138.86, 135.95, 128.96, 128.92, 128.89, 128.82, 128.42, 127.58, 126.28, 115.10, 110.95, 102.00, 80.12, 70.39, 44.44.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{22}$H$_{19}$O$_3$ 331.1334; Found 331.1349.

The characterization of the compound matched up with the data previously reported.

6-methoxy-2-phenylchroman-4-one 4g

![6-methoxy-2-phenylchroman-4-one](image)

Yellow solid (37 mg, 81%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.53 – 7.33 (m, 6H), 7.13 (dd, $J = 9.0$, 3.2 Hz, 1H), 7.00 (d, $J = 9.0$ Hz, 1H), 5.45 (dd, $J = 13.4$, 2.9 Hz, 1H), 3.83 (s, 3H), 3.08 (dd, $J = 17.0$, 13.5 Hz, 1H), 2.88 (dd, $J = 16.9$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 192.19, 156.38, 154.33, 138.94, 128.94, 128.85, 126.25, 125.52, 120.85, 119.55, 107.42, 79.82, 55.91, 44.68.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{16}$H$_{15}$O$_3$ 255.1021; Found 255.1011.

The characterization of the compound matched up with the data previously reported.

2-(4-methoxyphenyl)chroman-4-one 4h

![2-(4-methoxyphenyl)chroman-4-one](image)

Yellow solid (37 mg, 75%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.93 (dd, $J = 7.7$, 2.0 Hz, 1H), 7.55 – 7.46 (m, 1H), 7.42 (d, $J = 8.8$ Hz, 2H), 7.09 – 7.00 (m, 2H), 6.96 (d, $J = 8.7$ Hz, 2H), 5.43 (dd, $J = 13.4$, 2.8 Hz, 1H), 3.83 (s, 3H), 3.11 (dd, $J = 16.8$, 13.4 Hz, 1H), 2.86 (dd, $J = 17.0$, 2.8 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 192.37, 161.74, 160.07, 136.28, 130.85, 127.85, 127.14, 121.64, 121.00, 118.25, 114.30, 79.45, 55.46, 44.56.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{16}$H$_{15}$O$_3$ 255.1021; Found 255.1010.

The characterization of the compound matched up with the data previously reported.

2-(4-hydroxyphenyl)chroman-4-one 4i

![2-(4-hydroxyphenyl)chroman-4-one](image)

Yellow solid (33 mg, 67%).

$^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 9.60 (s, 1H), 7.79 (dd, $J = 7.8$, 1.8 Hz, 1H), 7.58 (ddd, $J = 8.5$, 7.2, 1.8 Hz, 1H), 7.35 (d, $J = 8.5$ Hz, 2H), 7.12 – 7.03 (m, 2H), 6.80 (d, $J = 8.6$ Hz, 2H), 5.53 (dd, $J = 13.1$, 2.8 Hz, 1H), 3.28 (dd, $J = 16.9$, 13.2 Hz, 1H), 2.74 (dd, $J = 16.8$, 2.8 Hz, 1H).

$^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 192.54, 161.80, 158.24, 136.76, 129.63, 128.89, 126.84, 121.84, 121.14, 118.58, 115.69, 79.36, 43.90.
HRMS (ESI+) m/z: [M+H]+ Calcd for C_{15}H_{13}O_{3} 241.0865; Found 241.0868.
The characterization of the compound matched up with the data previously reported.^{15}

2-(3-hydroxyphenyl)chroman-4-one 4j

![4j](image)

Yellow solid (48.7 mg, 70%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.94 (dd, $J = 8.0$, 1.8 Hz, 1H), 7.57 – 7.48 (m, 1H), 7.31 (t, $J = 7.9$ Hz, 2H), 7.11 – 6.97 (m, 4H), 6.94 – 6.82 (m, 1H), 5.45 (dd, $J = 13.2$, 3.0 Hz, 1H), 5.08 (s, 1H), 3.07 (dd, $J = 16.9$, 13.2 Hz, 1H), 2.90 (dd, $J = 16.9$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 192.13, 161.59, 158.02, 140.88, 136.83, 130.14, 126.85, 121.96, 121.22, 118.58, 117.58, 115.89, 113.94, 79.23, 44.10.

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{15}H_{13}O_{3} 241.0865; Found 241.0863.
The characterization of the compound matched up with the data previously reported.^{15}

2-(3,4-dimethoxyphenyl)chroman-4-one 4k

![4k](image)

Yellow solid (55 mg, 69%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.94 (dd, $J = 8.1$, 1.7 Hz, 1H), 7.57 – 7.47 (m, 1H), 7.11 – 6.98 (m, 4H), 6.91 (d, $J = 8.3$ Hz, 1H), 5.44 (dd, $J = 13.3$, 2.8 Hz, 1H), 3.93 (s, 3H), 3.91 (s, 3H), 3.13 (dd, $J = 16.9$, 13.3 Hz, 1H), 2.89 (dd, $J = 16.9$, 2.8 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 192.27, 161.65, 149.52, 149.35, 136.30, 131.25, 127.14, 121.70, 121.01, 118.93, 118.24, 111.21, 109.48, 79.67, 56.08, 56.05, 44.68.

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{17}H_{17}O_{4} 285.1127; Found 285.1119.
The characterization of the compound matched up with the data previously reported.^{15}

2-(3,5-dimethoxyphenyl)chroman-4-one 4l

![4l](image)

Yellow oil (30.7 mg, 48%).

$^1$H NMR (400 MHz, Chloroform-$d$) $\delta$ 7.93 (dd, $J = 8.2$, 1.7 Hz, 1H), 7.57 – 7.48 (m, 1H), 7.11 – 7.03 (m, 2H), 6.63 (d, $J = 2.3$ Hz, 2H), 6.47 (t, $J = 2.2$ Hz, 1H), 5.42 (dd, $J = 13.3$, 2.9 Hz, 1H), 3.83 (s, 6H), 3.07 (dd, $J = 16.9$, 13.3 Hz, 1H), 2.89 (dd, $J = 16.9$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-$d$) $\delta$ 192.06, 161.56, 161.24, 141.15, 136.34, 127.15, 121.77, 121.02, 118.26, 104.24, 100.49, 79.66, 55.54, 44.86.

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{17}H_{17}O_{4} 285.1127; Found 285.1119.
The characterization of the compound matched up with the data previously reported.^{15}
2-[(3,4,5-trimethoxyphenyl)chroman-4-one 4m

Yellow solid (36 mg, 52%).

$^1$H NMR (400 MHz, Chloroform-\textit{d}) $\delta$ 7.94 (dd, $J = 8.1$, 1.8 Hz, 1H), 7.57 – 7.48 (m, 1H), 7.12 – 7.03 (m, 2H), 6.71 (s, 2H), 6.11 (d, $J = 8.2$ Hz, 1H), 5.42 (dd, $J = 13.5$, 3.9 Hz, 1H), 3.90 (s, 3H), 3.87 (s, 3H), 3.10 (dd, $J = 16.3$, 13.3 Hz, 1H), 2.89 (dd, $J = 16.9$, 2.8 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-\textit{d}) $\delta$ 192.04, 161.53, 153.66, 138.30, 136.36, 134.39, 127.17, 121.84, 120.99, 118.23, 103.33, 79.96, 60.96, 56.29, 44.94.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{18}$H$_{19}$O$_5$ 315.1233; Found 315.1225.

The characterization of the compound matched up with the data previously reported.$^{15}$

2-(naphthalen-2-yl)chroman-4-one 4n

Yellow solid (25.2 mg, 51%).

$^1$H NMR (400 MHz, Chloroform-\textit{d}) $\delta$ 7.99 – 7.91 (m, 3H), 7.91 – 7.85 (m, 2H), 7.61 (d, $J = 8.5$ Hz, 1H), 7.57 – 7.50 (m, 3H), 7.14 – 7.04 (m, 2H), 5.67 (dd, $J = 13.3$, 2.5 Hz, 1H), 3.20 (dd, $J = 16.9$, 13.2 Hz, 1H), 2.99 (dd, $J = 16.9$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-\textit{d}) $\delta$ 192.06, 161.67, 136.38, 136.16, 133.48, 133.27, 128.92, 128.28, 127.89, 126.68, 125.53, 123.78, 121.80, 121.09, 118.29, 79.81, 44.77.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{19}$H$_{15}$O$_2$ 275.1072; Found 275.1052.

The characterization of the compound matched up with the data previously reported.$^{17}$

2-(4-fluorophenyl)chroman-4-one 4o

Yellow solid (16.2 mg, 65%).

$^1$H NMR (400 MHz, Chloroform-\textit{d}) $\delta$ 7.94 (d, $J = 8.0$ Hz, 1H), 7.57 – 7.44 (m, 3H), 7.18 – 7.02 (m, 4H), 5.48 (dd, $J = 13.2$, 2.9 Hz, 1H), 3.07 (dd, $J = 16.9$, 13.3 Hz, 1H), 2.88 (dd, $J = 16.9$, 2.9 Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-\textit{d}) $\delta$ 191.85, 162.93 (d, $J = 247.7$ Hz), 161.49, 136.40, 134.69 (d, $J = 3.3$ Hz), 128.19, 121.87, 120.98, 118.19, 115.92 (d, $J = 21.7$ Hz), 79.03, 44.77.

$^{19}$F NMR (471 MHz, Chloroform-\textit{d}) $\delta$ -112.68.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{15}$H$_{12}$F$_2$O$_2$ 243.0821; Found 243.0817.

The characterization of the compound matched up with the data previously reported.$^{15}$

2-(4-chlorophenyl)chroman-4-one 4p
Yellow solid (9 mg, 22%).

1H NMR (400 MHz, Chloroform-d) δ 7.94 (dd, J = 7.8, 1.8 Hz, 1H), 7.53 (ddd, J = 8.1, 1.8, 1.8 Hz, 1H), 7.47 – 7.38 (m, 4H), 7.12 – 7.02 (m, 2H), 5.47 (dd, J = 13.2, 3.0 Hz, 1H), 3.05 (dd, J = 16.8, 13.2 Hz, 1H), 2.89 (dd, J = 16.8, 2.9 Hz, 1H).

13C NMR (126 MHz, Chloroform-d) δ 191.68, 161.41, 137.35, 136.43, 134.70, 129.16, 127.61, 127.20, 121.93, 120.98, 118.20, 78.92, 44.70.

HRMS (ESI+) m/z: [M]+ Calcd for C15H11ClO2 258.0448; Found 258.0393.

The characterization of the compound matched up with the data previously reported.15

2-methylchroman-4-one 4q

Colorless oil (10 mg, 18%). This compound was synthesized from 1-(2-hydroxyphenyl)butan-1-one.11

1H NMR (400 MHz, Chloroform-d) δ 7.89 (d, J = 7.8 Hz, 1H), 7.48 (t, J = 7.8 Hz, 1H), 7.06 – 6.94 (m, 2H), 4.67 – 4.54 (m, 1H), 2.69 (d, J = 8.4 Hz, 2H), 1.53 (d, J = 6.2 Hz, 3H).

13C NMR (126 MHz, Chloroform-d) δ 192.64, 161.78, 136.10, 127.06, 121.31, 120.90, 117.98, 74.38, 44.69, 21.09.

HRMS (ESI+) m/z: [M]+ Calcd for C10H11O2 163.0759; Found 163.0799.

The characterization of the compound matched up with the data previously reported.21

2-(thiophen-2-yl)chroman-4-one 4r

Yellow solid (20 mg, 29%).

1H NMR (400 MHz, Chloroform-d) δ 7.92 (dd, J = 8.3, 1.8 Hz, 1H), 7.51 (ddd, J = 8.2, 7.3, 1.8 Hz, 1H), 7.37 (dd, J = 5.1, 1.2 Hz, 1H), 7.14 (dt, J = 3.6, 1.1 Hz, 1H), 7.08 – 7.01 (m, 3H), 5.75 (ddd, J = 11.8, 3.5, 0.8 Hz, 1H), 3.20 (dd, J = 16.9, 11.8 Hz, 1H), 3.07 (dd, J = 16.8, 3.4 Hz, 1H).

13C NMR (126 MHz, Chloroform-d) δ 191.35, 161.01, 141.54, 136.40, 127.11, 127.00, 126.54, 126.05, 121.94, 121.06, 118.33, 75.19, 44.43.

HRMS (ESI+) m/z: [M]+ Calcd for C13H11O2S 231.0480; Found 231.0480.

2-(3,4-dimethoxyphenyl)-7-methoxychroman-4-one (Butin trimethyl ether) 5b

Yellow solid (20 mg, 48%). This compound was synthesized from 1aa.
$^1$H NMR (400 MHz, Chloroform-d) δ 7.87 (d, $J = 8.8$ Hz, 1H), 7.05 – 6.98 (m, 2H), 6.91 (d, $J = 8.8$ Hz, 1H), 6.62 (dd, $J = 8.8, 2.4$ Hz, 1H), 6.50 (d, $J = 2.4$ Hz, 1H), 5.42 (dd, $J = 13.3, 2.8$ Hz, 1H), 3.93 (s, 3H), 3.91 (s, 3H), 3.84 (s, 3H), 3.07 (dd, $J = 17.0, 13.3$ Hz, 1H), 2.82 (dd, $J = 16.9, 3.0$ Hz, 1H).

$^{13}$C NMR (126 MHz, Chloroform-d) δ 190.90, 166.28, 163.63, 149.51, 149.33, 131.30, 128.86, 118.95, 114.90, 111.19, 110.36, 109.45, 101.01, 80.10, 56.09, 56.05, 55.76, 44.36.

HRMS (ESI+) m/z: [M+H]$^+$ Calcd for C$_{18}$H$_{19}$O$_{5}$ 315.1233; Found 315.1218.

The characterization of the compound matched up with the data previously reported.
2.3. Preparation of 2′-hydroxydihydrochalcones 1

The starting materials 1n-1t, 1aa, and 1ab were prepared by using the method reported in literature.22

2.3.1 General procedure for the preparation of substrate 1b-1d, 1g, 1l, and 1u-1y 23

To an oven-dried round-bottom flask was added LiO\textsubscript{t}Bu (1 mmol, 80 mg), the ketones (0.5 mmol, 1 equiv), benzyl alcohol (0.75 mmol, 1.5 equiv). The flask was purged with argon and stirred at 80-110 °C for 12 h. After cooling, the reaction mixture was quenched by a saturated aq. NH\textsubscript{4}Cl solution and extracted with EtOAc. The organic phase was combined and dried with anhydrous MgSO\textsubscript{4}. The mixture was filtered and evaporated under reduced pressure. The residue was purified by silica gel flash column chromatography.

**1-(4-fluoro-2-hydroxyphenyl)-3-phenylpropan-1-one 1b**

\[
\begin{align*}
\text{O} & \hspace{1cm} \text{O} \\
F & \hspace{1cm} \text{H}
\end{align*}
\]

The compound was prepared using the **general procedure 2.3.1** described above.

White solid (130 mg, 27%).

\textsuperscript{1}H NMR (400 MHz, Chloroform-\textit{d}) \(\delta\) 12.63 (d, \(J = 1.5\) Hz, 1H), 7.73 (dd, \(J = 8.9, 6.4\) Hz, 1H), 7.35 – 7.27 (m, 2H), 7.25 – 7.18 (m, 3H), 6.66 (dd, \(J = 10.3, 2.5\) Hz, 1H), 6.58 (ddd, \(J = 8.8, 8.1, 2.5\) Hz, 1H), 3.28 (t, 2H), 3.06 (t, 2H).

\textsuperscript{13}C NMR (126 MHz, Chloroform-\textit{d}) \(\delta\) 204.31, 167.43 (d, \(J = 256.5\) Hz), 165.13 (d, \(J = 14.7\) Hz), 140.65, 132.26 (d, \(J = 12.1\) Hz), 128.75, 128.49, 126.50, 116.55, 107.31 (d, \(J = 23.1\) Hz), 105.18 (d, \(J = 23.9\) Hz), 40.18, 30.08.

\textsuperscript{19}F NMR (471 MHz, Chloroform-\textit{d}) \(\delta\) -99.19.

HRMS (ESI+) m/z: [M+H]\textsuperscript{+} Calcd for C\textsubscript{15}H\textsubscript{14}F\textsubscript{1}O\textsubscript{2} 245.0978; Found 245.0973.

The characterization of the compound matched up with the data previously reported.24

**1-(4-chloro-2-hydroxyphenyl)-3-phenylpropan-1-one 1c**

\[
\begin{align*}
\text{O} & \hspace{1cm} \text{Cl} \\
\text{O} & \hspace{1cm} \text{H}
\end{align*}
\]

The compound was prepared using the **general procedure 2.3.1** described above.
Yellow solid (90 mg, 17%).  

\(^1\)H NMR (400 MHz, Chloroform-d) \( \delta \) 12.43 (s, 1H), 7.66 (d, \( J = 8.7 \) Hz, 1H), 7.36 – 7.28 (m, 2H), 7.26 – 7.20 (m, 3H), 7.00 (d, \( J = 1.9 \) Hz, 1H), 6.86 (dd, \( J = 8.6, 1.9 \) Hz, 1H), 3.30 (t, 2H), 3.06 (t, \( J = 7.6 \) Hz, 2H).  

\(^1\)C NMR (126 MHz, Chloroform-d) \( \delta \) 204.76, 163.22, 142.17, 140.57, 130.90, 128.75, 128.48, 126.51, 119.71, 118.72, 117.94, 40.23, 30.00.  
HRMS (ESI\(^+\)) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{14}\)Cl\(_2\)O\(_2\) 261.0682; Found 261.0677.  

1-(4-bromo-2-hydroxyphenyl)-3-phenylpropan-1-one 1d

\[
\text{The compound was prepared using the general procedure 2.3.1 described above.}
\]

Yellow solid (122 mg, 20%).  

\(^1\)H NMR (400 MHz, Chloroform-d) \( \delta \) 12.38 (s, 1H), 7.57 (d, \( J = 8.6 \) Hz, 1H), 7.35 – 7.27 (m, 2H), 7.27 – 7.20 (m, 3H), 7.18 (d, \( J = 1.9 \) Hz, 1H), 7.01 (dd, \( J = 8.5, 1.9 \) Hz, 1H), 3.28 (t, \( J = 7.6 \) Hz, 2H), 3.06 (t, 2H).  

\(^1\)C NMR (126 MHz, Chloroform-d) \( \delta \) 204.97, 163.00, 140.56, 130.85, 130.77, 128.76, 128.48, 126.52, 122.57, 121.86, 118.25, 40.22, 29.98.  
HRMS (ESI\(^+\)) m/z: [M]\(^+\) Calcd for C\(_{15}\)H\(_{13}\)Br\(_1\)O\(_2\) 304.0099; Found 304.0070.  

3-hydroxy-4-(3-phenylpropanoyl)phenyl trifluoromethanesulfonate 1e

To a solution of 1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one 1i (50 mg, 0.206 mmol), pyridine (0.206 mmol) and dimethylaminopyridine (0.02 mmol) in dry CH\(_2\)Cl\(_2\) (1.5 ml) was added trifluoromethanesulfonic anhydride (0.227 mmol) at 0 °C for 20 min. Then, the reaction mixture was cooled and quenched with 2 N HCl aqueous solution, extracted with CH\(_2\)Cl\(_2\), dried over MgSO\(_4\), filtered and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column.  
White solid (57.3 mg, 74%).  

\(^1\)H NMR (400 MHz, Chloroform-d) \( \delta \) 12.53 (s, 1H), 7.83 (d, \( J = 8.9 \) Hz, 1H), 7.36 – 7.28 (m, 2H), 7.26 – 7.20 (m, 3H), 6.91 (d, \( J = 2.5 \) Hz, 1H), 6.80 (dd, \( J = 8.9, 2.5 \) Hz, 1H), 3.33 (t, \( J = 7.6 \) Hz, 2H), 3.08 (t, \( J = 7.6 \) Hz, 2H).  

\(^1\)C NMR (126 MHz, Chloroform-d) \( \delta \) 204.64, 164.11, 153.94, 140.33, 131.96, 128.80, 128.48, 126.52, 122.57, 121.86, 118.25, 40.46, 29.84.  
\(^{19}\)F NMR (471 MHz, Chloroform-d) \( \delta \) -72.67.  
HRMS (ESI\(^+\)) m/z: [M+NH\(_4\)]\(^+\) Calcd for C\(_{16}\)H\(_{17}\)F\(_3\)N\(_2\)O\(_5\)S\(_1\) 392.0780; Found 392.0811.  

3-hydroxy-4-(3-phenylpropanoyl)phenyl pivalate 1f

To a solution of 1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one 1i (50 mg, 0.206 mmol) and triethylamine (0.413 mmol) in acetone (1.5 ml) was added pivaloyl chloride (0.227 mmol) at room temperature for 30 min. Then the reaction mixture was
The compound was prepared using the general procedure 2.3.1 described above. Yellow solid (70 mg, 15%).

1H NMR (400 MHz, Chloroform-d) δ 12.33 (s, 1H), 7.62 (d, J = 8.2 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.26 – 7.22 (m, 3H), 7.09 (d, J = 9.2 Hz, 1H), 3.30 (t, J = 7.5 Hz, 2H), 3.11 (t, J = 7.5 Hz, 2H).

13C NMR (126 MHz, Chloroform-d) δ 205.05, 167.27, 157.09, 131.06, 128.85, 128.52, 127.56, 126.71, 126.20, 119.75, 118.25, 40.25, 29.73.

HRMS (ESI+) m/z: [M+H]+ Calcd for C16H17NO2 241.1229; Found 241.1235.

The characterization of the compound matched up with the data previously reported.25

1-(2-hydroxy-5-nitrophenyl)-3-phenylpropan-1-one 1h

To a solution of commercially available 1a (0.6 ml) in acetic acid (1.2 ml) at 0 °C was added dropwise nitric acid (0.9 ml) and the resulting mixture was refluxed for 3 h. Then the solution was poured to ice and the resulting precipitate was filtered, washed with water and dried to give 1h. White solid (201 mg, 30%).

1H NMR (400 MHz, Chloroform-d) δ 12.91 (s, 1H), 8.69 (d, J = 2.7 Hz, 1H), 8.34 (dd, J = 9.2, 2.7 Hz, 1H), 7.36 – 7.27 (m, 3H), 7.26 – 7.22 (m, 2H), 7.09 (d, J = 9.2 Hz, 1H), 3.43 (t, J = 7.5 Hz, 2H), 3.11 (t, J = 7.5 Hz, 2H).

13C NMR (126 MHz, Chloroform-d) δ 205.05, 167.27, 140.02, 139.63, 131.06, 128.85, 128.52, 127.56, 126.71, 126.20, 119.75, 118.25, 40.25, 29.73.

HRMS (ESI+) m/z: [M+NH]+ Calcd for C15H17N2O4 289.1188; Found 289.1190.

1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one 1i

This compound was synthesized by a previously reported procedure.27 Resorcinol (1.50 g, 13.62 mmol) and 3-phenylpropanoic acid (2.05 g, 13.62 mmol) in boron trifluoride etherate (7 ml) were stirred at 60 °C for 3 h. Then, the reaction mixture was cooled and diluted with sodium acetate aqueous solution, stirred for 3 h at room temperature. The mixture was extracted

quenched with water, extracted with EtOAc, dried over MgSO₄, filtered and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column.

White solid (44.2 mg, 66%).

1H NMR (400 MHz, Chloroform-d) δ 12.47 (s, 1H), 7.74 (d, J = 8.8 Hz, 1H), 7.35 – 7.20 (m, 5H), 6.70 (d, J = 2.3 Hz, 1H), 6.61 (dd, J = 8.8, 2.3 Hz, 1H), 3.29 (dd, J = 8.5, 6.9 Hz, 2H), 3.06 (dd, J = 8.4, 6.9 Hz, 2H).

13C NMR (126 MHz, Chloroform-d) δ 204.53, 176.30, 164.13, 157.25, 140.73, 131.11, 128.74, 128.49, 126.47, 117.22, 113.00, 111.27, 40.21, 39.34, 30.07, 27.12.

HRMS (ESI+) m/z: [M+H]+ Calcd for C20H23O4 327.1596; Found 327.1611.

1-(2-hydroxy-4-methylphenyl)-3-phenylpropan-1-one 1g

The compound was prepared using the general procedure 2.3.1 described above. Yellow solid (70 mg, 15%).

1H NMR (400 MHz, Chloroform-d) δ 12.33 (s, 1H), 7.62 (d, J = 8.2 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.26 – 7.20 (m, 3H), 6.79 (s, 1H), 6.69 (dd, J = 8.2, 1.1 Hz, 1H), 3.30 (t, 2H), 3.06 (t, 2H), 2.34 (s, 3H).

13C NMR (126 MHz, Chloroform-d) δ 204.88, 162.69, 148.07, 140.93, 129.82, 128.70, 128.49, 126.39, 120.33, 118.65, 117.18, 40.00, 30.23, 22.04.

HRMS (ESI+) m/z: [M+H]+ Calcd for C16H17O2 241.1229; Found 241.1235.

The characterization of the compound matched up with the data previously reported.25

1-(2-hydroxy-5-nitrophenyl)-3-phenylpropan-1-one 1h

Resorcinol (1.50 g, 13.62 mmol) and 3-phenylpropanoic acid (2.05 g, 13.62 mmol) in boron trifluoride etherate (7 ml) were stirred at 60 °C for 3 h. Then, the reaction mixture was cooled and diluted with sodium acetate aqueous solution, stirred for 3 h at room temperature. The mixture was extracted
with EtOAc, dried over MgSO₄, filtered and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column.

White solid (1162 mg, 35%).

1H NMR (400 MHz, Chloroform-d) δ 12.75 (s, 1H), 7.64 (d, J = 8.4 Hz, 1H), 7.35 – 7.27 (m, 2H), 7.26 – 7.19 (m, 3H), 6.40 – 6.32 (m, 2H), 5.52 (s, 1H), 3.24 (t, 2H), 3.05 (t, J = 7.7 Hz, 2H).

13C NMR (126 MHz, DMSO-d₆) δ 204.09, 165.31, 164.75, 141.59, 133.54, 128.93, 128.82, 126.46, 113.07, 108.71, 102.94, 39.44, 30.22.

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{15}H_{15}O₃ 243.1021; Found 243.1024.

The characterization of the compound matched up with the data previously reported.

1-(2-hydroxy-4-methoxyphenyl)-3-phenylpropan-1-one 1j

![Structure of 1j](image)

To a solution of 1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one 1i (50 mg, 0.206 mmol) and cesium carbonate (67 mg, 0.206 mmol) in DMF (1 ml) was added methyl iodide (0.206 mmol) at room temperature for 30 min. Then the reaction mixture was quenched with water, extracted with EtOAc, dried over MgSO₄, filtered and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column.

White solid (41.5 mg, 78%).

1H NMR (400 MHz, Chloroform-d) δ 12.80 (s, 1H), 7.64 (d, J = 9.5 Hz, 1H), 7.35 – 7.27 (m, 2H), 7.26 – 7.17 (m, 3H), 6.45 – 6.38 (m, 2H), 3.83 (s, 3H), 3.24 (t, 2H), 3.05 (t, J = 7.7 Hz, 2H).

13C NMR (126 MHz, Chloroform-d) δ 203.64, 166.11, 165.49, 140.98, 131.54, 128.68, 128.49, 126.37, 113.50, 107.78, 101.05, 55.67, 39.78, 30.40.

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{16}H_{17}O₃ 257.1178; Found 257.1195.

The characterization of the compound matched up with the data previously reported.

1-(4-(benzyloxy)-2-hydroxyphenyl)-3-phenylpropan-1-one 1k

![Structure of 1k](image)

To a solution of 1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one 1i (50 mg, 0.206 mmol) and potassium carbonate (29 mg, 0.206 mmol) in CH₃CN (1.5 ml) was added benzyl bromide (0.227 mmol) at room temperature. The reaction mixture was refluxed for 2 h. After cooling, the reaction mixture was quenched with water, extracted with EtOAc, dried over MgSO₄, filtered and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column.

White solid (64.1 mg, 94%).

1H NMR (400 MHz, Chloroform-d) δ 12.78 (s, 1H), 7.65 (d, J = 8.6 Hz, 1H), 7.45 – 7.21 (m, 11H), 6.53 – 6.46 (m, 2H), 5.09 (s, 2H), 3.24 (t, J = 7.7 Hz, 2H), 3.05 (t, J = 7.7 Hz, 2H).

13C NMR (126 MHz, Chloroform-d) δ 203.66, 165.41, 165.19, 140.98, 135.96, 131.62, 128.83, 128.70, 128.50, 128.44, 127.66, 126.39, 113.70, 108.28, 102.09, 70.31, 39.79, 30.39.

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{22}H_{21}O₃ 333.1491; Found 333.1519.

1-(2-hydroxy-5-methoxyphenyl)-3-phenylpropan-1-one 1l

1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one 1i
The compound was prepared using the general procedure 2.3.1 described above.

Yellow oil (75 mg, 15%).

1H NMR (400 MHz, Chloroform-d) δ 11.91 (s, 1H), 7.36 – 7.28 (m, 2H), 7.28 – 7.21 (m, 3H), 7.15 (d, J = 3.0 Hz, 1H), 7.10 (dd, J = 9.0, 3.1 Hz, 1H), 6.93 (d, J = 9.0 Hz, 1H), 3.76 (s, 3H), 3.31 (t, J = 7.7 Hz, 2H), 3.07 (t, J = 7.7 Hz, 2H).

13C NMR (126 MHz, Chloroform-d) δ 204.95, 156.96, 151.83, 140.85, 128.74, 128.54, 126.46, 124.35, 119.52, 118.83, 112.48, 56.09, 40.32, 30.07.

HRMS (ESI+) m/z: [M+H]+ Calcd for C16H17O3 257.1178; Found 257.1174.

1-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenylpropan-1-one

This compound was synthesized using a previously reported procedure. 3,5-Dimethoxyphenol (462 mg, 3 mmol) and 3-phenylpropanoic acid (451 mg, 3 mmol) in boron trifluoride etherate (2 ml) were stirred at 90 °C for 2 h. Then, the reaction mixture was cooled and diluted with sodium acetate aqueous solution, stirred for 3 h at room temperature. The mixture was extracted with EtOAc, dried over MgSO4, filtered and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column.

White solid (555 mg, 65%).

1H NMR (400 MHz, Chloroform-d) δ 14.03 (s, 1H), 7.33 – 7.18 (m, 6H), 6.08 (d, J = 2.5 Hz, 1H), 5.93 (d, J = 2.4 Hz, 1H), 3.83 (s, 3H), 3.32 (t, 2H), 3.00 (t, 2H).

13C NMR (126 MHz, Chloroform-d) δ 204.60, 167.79, 166.05, 141.81, 128.56, 128.53, 126.03, 105.81, 93.73, 90.93, 55.70, 55.66, 45.81, 30.78.

HRMS (ESI+) m/z: [M+H]+ Calcd for C17H19O4 287.1283; Found 287.1289.

3-(3,5-dimethoxyphenyl)-1-(2-hydroxyphenyl)propan-1-one

To a solution of 3-(3,5-dimethoxyphenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one which was prepared by a previously reported procedure (150 mg, 0.528 mmol) and catalytic amounts of palladium on carbon in EtOAc (2 ml) and ethanol (2 ml) was injected H2 gas at room temperature. The reaction mixture was stirred for 1 h. Then, the reaction mixture was diluted with EtOAc and filtered over a celite pad and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column.

White solid (79.3 mg, 53%).

1H NMR (400 MHz, Chloroform-d) δ 12.29 (s, 1H), 7.74 (dd, J = 8.1, 1.7 Hz, 1H), 7.46 (ddd, J = 8.6, 7.1, 1.6 Hz, 1H), 6.99 (ddd, J = 8.4, 1.2 Hz, 1H), 6.88 (ddd, J = 8.2, 7.2, 1.2 Hz, 1H), 6.40 (d, J = 2.3 Hz, 2H), 6.33 (t, J = 2.3 Hz, 1H), 3.78 (s, 6H), 3.32 (t, 2H), 3.01 (t, 2H).

13C NMR (126 MHz, Chloroform-d) δ 205.45, 162.53, 161.04, 143.23, 136.48, 129.93, 119.37, 119.05, 118.65, 106.57, 98.21, 55.38, 39.96, 30.36.

HRMS (ESI+) m/z: [M+H]+ Calcd for C17H19O4 287.1283; Found 287.1284.
1-(2-hydroxyphenyl)-3-(naphthalen-2-yl)propan-1-one 1u

![1u](image)

The compound was prepared using the general procedure 2.3.1 described above. Yellow solid (53 mg, 26%).

\[ \text{H NMR (400 MHz, Chloroform-d)} \delta 12.32 (s, 1H), 7.85 - 7.74 (m, 4H), 7.69 (s, 1H), 7.51 - 7.41 (m, 3H), 7.39 (dd, \ J = 8.4, 1.8 Hz, 1H), 6.99 (dd, \ J = 8.4, 1.2 Hz, 1H), 6.88 (ddd, \ J = 8.2, 7.2, 1.2 Hz, 1H), 3.43 (t, \ J = 7.7 Hz, 2H), 3.24 (t, \ J = 7.6 Hz, 2H). \]

\[ 13C \text{ NMR (126 MHz, Chloroform-d)} \delta 205.44, 162.60, 138.35, 136.52, 133.73, 132.27, 129.97, 128.38, 127.97, 127.60, 127.17, 126.68, 126.26, 125.59, 119.40, 119.09, 118.70, 40.05, 30.23. \]

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{19}H_{17}O_{2} 277.1229; Found 277.1223.

3-(4-fluorophenyl)-1-(2-hydroxyphenyl)propan-1-one 1v

![1v](image)

The compound was prepared using the general procedure 2.3.1 described above. White solid (87 mg, 18%).

\[ \text{H NMR (400 MHz, DMSO-d6)} \delta 12.27 (s, 1H), 7.74 (dd, \ J = 8.1, 1.7 Hz, 1H), 7.47 (ddd, \ J = 8.6, 7.2, 1.6 Hz, 1H), 7.21 (dd, \ J = 8.5, 5.6 Hz, 2H), 7.03 - 6.95 (m, 3H), 6.88 (ddd, \ J = 8.1, 7.1, 1.1 Hz, 1H), 3.31 (t, \ J = 7.6 Hz, 2H), 3.05 (t, \ J = 7.6 Hz, 2H). \]

\[ 13C \text{ NMR (126 MHz, DMSO-d6)} \delta 205.24, 162.56, 160.62, 136.53, 136.42 (d, \ J = 3.1 Hz), 129.95, 129.88 (d, \ J = 4.2 Hz), 119.33, 119.05, 118.71, 115.46 (d, \ J = 21.2 Hz), 40.13, 29.24. \]

\[ \text{19F NMR (471 MHz, Chloroform-d)} \delta -116.79. \]

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{15}H_{14}F_{1}O_{2} 245.0978; Found 245.0962.

The characterization of the compound matched up with the data previously reported.30

3-(4-chlorophenyl)-1-(2-hydroxyphenyl)propan-1-one 1w

![1w](image)

The compound was prepared using the general procedure 2.3.1 described above. White solid (70 mg, 13%).

\[ \text{H NMR (400 MHz, Chloroform-d)} \delta 12.24 (s, 1H), 7.73 (dd, \ J = 8.1, 1.7 Hz, 1H), 7.47 (ddd, \ J = 8.7, 7.2, 1.6 Hz, 1H), 7.27 (zd, \ J = 8.6 Hz, 2H), 7.18 (d, \ J = 8.4 Hz, 2H), 6.99 (dd, \ J = 8.4, 1.2 Hz, 1H), 6.88 (ddd, \ J = 8.2, 7.2, 1.2 Hz, 1H), 3.31 (t, \ J = 7.6 Hz, 2H), 3.04 (t, \ J = 7.5 Hz, 2H). \]

\[ 13C \text{ NMR (126 MHz, Chloroform-d)} \delta 205.04, 162.55, 139.26, 136.57, 136.42 (d, \ J = 3.1 Hz), 129.95, 129.88 (d, \ J = 4.2 Hz), 119.33, 119.05, 118.71, 39.84, 29.33. \]

HRMS (ESI+) m/z: [M+H]+ Calcd for C_{15}H_{14}ClO_{2} 261.0682; Found 261.0634.

The characterization of the compound matched up with the data previously reported.30

3-(4-bromophenyl)-1-(2-hydroxyphenyl)propan-1-one 1x

![1x](image)
The compound was prepared using the general procedure 2.3.1 described above.

White solid (90 mg, 15%)

\(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 12.24 (s, 1H), 7.73 (dd, \(J = 8.0, 1.7\) Hz, 1H), 7.50 – 7.44 (m, 1H), 7.42 (d, \(J = 8.3\) Hz, 2H), 7.13 (d, \(J = 8.3\) Hz, 2H), 6.99 (dd, \(J = 8.4, 1.2\) Hz, 1H), 6.93 – 6.84 (m, 1H), 3.31 (t, \(J = 7.6\) Hz, 2H), 3.03 (t, \(J = 7.5\) Hz, 2H).

\(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 205.00, 162.55, 139.81, 136.58, 131.75, 130.31, 129.83, 120.19, 119.30, 119.09, 118.72, 39.76, 29.37.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{14}\)BrO\(_2\) 305.0177; Found 305.0160.

The characterization of the compound matched up with the data previously reported.\(^{31}\)

1-(2-hydroxyphenyl)-3-(4-iodophenyl)propan-1-one 1y

The compound was prepared using the general procedure 2.3.1 described above.

White solid (84 mg, 12%)

\(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 12.23 (s, 1H), 7.73 (dd, \(J = 8.1, 1.6\) Hz, 1H), 7.62 (d, \(J = 8.3\) Hz, 2H), 7.51 – 7.43 (m, 1H), 7.05 – 6.95 (m, 3H), 6.88 (ddd, \(J = 8.1, 7.2, 1.2\) Hz, 1H), 3.31 (t, \(J = 7.6\) Hz, 2H), 3.02 (t, \(J = 7.5\) Hz, 2H).

\(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 205.38, 161.04, 141.45, 137.51, 136.53, 131.49, 131.25, 120.90, 119.73, 118.17, 92.05, 40.61, 29.31.

HRMS (ESI+) m/z: [M+H]\(^+\) Calcd for C\(_{15}\)H\(_{14}\)I\(_2\)O\(_2\) 353.0039; Found 353.0046.
3. Optimization of the Reaction Conditions

3.1. Optimization for Flavone

Table S1. Ligand investigation

<table>
<thead>
<tr>
<th>entry</th>
<th>ligand (20 mol %)</th>
<th>1b</th>
<th>1c</th>
<th>1d</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>none</td>
<td>14</td>
<td>12</td>
<td>31</td>
</tr>
<tr>
<td>2</td>
<td>KOAc</td>
<td>0</td>
<td>45</td>
<td>17</td>
</tr>
<tr>
<td>3</td>
<td>K₂CO₃</td>
<td>8</td>
<td>28</td>
<td>20</td>
</tr>
<tr>
<td>4</td>
<td>4-DMAP</td>
<td>6</td>
<td>29</td>
<td>36</td>
</tr>
<tr>
<td>5</td>
<td>Pyridine</td>
<td>5</td>
<td>41</td>
<td>37</td>
</tr>
<tr>
<td>6</td>
<td>Pyrimidine</td>
<td>7</td>
<td>48</td>
<td>32</td>
</tr>
<tr>
<td>7</td>
<td>1,10-Phenanthroline</td>
<td>9</td>
<td>31</td>
<td>25</td>
</tr>
<tr>
<td>8</td>
<td>2,2'-Bipyridine</td>
<td>5</td>
<td>55</td>
<td>10</td>
</tr>
<tr>
<td>9</td>
<td>5-Nitro-1,10-phenanthroline</td>
<td>3</td>
<td>81</td>
<td>2</td>
</tr>
</tbody>
</table>

Table S2. Catalyst investigation

<table>
<thead>
<tr>
<th>entry</th>
<th>Pd(II) catalyst (10 mol %)</th>
<th>1b</th>
<th>1c</th>
<th>1d</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Pd(OPiv)₂</td>
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<td>64</td>
<td>4</td>
</tr>
<tr>
<td>2</td>
<td>Pd(OAc)₂</td>
<td>2</td>
<td>59</td>
<td>6</td>
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<tr>
<td>3</td>
<td>Pd(acac)₂</td>
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<td>38</td>
<td>10</td>
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Table S3. Temperature investigation

<table>
<thead>
<tr>
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<th>Temperature (°C)</th>
<th>1b</th>
<th>1c</th>
<th>1d</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>60</td>
<td>5</td>
<td>12</td>
<td>3</td>
</tr>
</tbody>
</table>
### 3.2. Optimization for Flavanone

**Table S4. Ligand investigation**

![Chemical structure image]

<table>
<thead>
<tr>
<th>entry</th>
<th>ligand (20 mol %)</th>
<th>isolated yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>None</td>
<td>33</td>
</tr>
<tr>
<td>2</td>
<td>1,10-Phenanthroline</td>
<td>23</td>
</tr>
<tr>
<td>3</td>
<td>Pyridine</td>
<td>14</td>
</tr>
<tr>
<td>4</td>
<td>4-DMAP</td>
<td>25</td>
</tr>
<tr>
<td>5</td>
<td>K₂CO₃</td>
<td>7</td>
</tr>
<tr>
<td>6</td>
<td>AcOH</td>
<td>20</td>
</tr>
<tr>
<td>7</td>
<td>HCO₂H</td>
<td>9</td>
</tr>
<tr>
<td>8</td>
<td>p-TsOH</td>
<td>24</td>
</tr>
<tr>
<td>9</td>
<td>H₃PO₄</td>
<td>15</td>
</tr>
<tr>
<td>10</td>
<td>PivOH</td>
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</tr>
<tr>
<td>11</td>
<td>N-Acetyl glycine</td>
<td>29</td>
</tr>
</tbody>
</table>
4. Supplementary Figure

Figure S1. Kinetic experiment of the flavanone synthesis from 4-methoxy-2'-hydroxydihydrochalcone 1n. Initial time part of the reaction.
5. Kinetic Study

Relative amounts of the compounds were determined by HPLC with a ZORBAX Eclipse Plus C18 4.6x250mm (A) or Poroshell 120 EC-C18 4.6x150mm (B) (0.5 % formic acid in H₂O:ACN = 35:65, 0.9 ml/min, RID detector). The conversion yield was converted to the area ratio obtained by the RID detector. For A column; starting material \( t_r = 13.787 \) min, chalcone \( t_r = 15.969 \) min, flavanone \( t_r = 8.906 \) min, flavone \( t_r = 7.239 \) min. For B column; starting material \( t_r = 6.143 \) min, chalcone \( t_r = 6.943 \) min, flavanone \( t_r = 4.237 \) min, flavone \( t_r = 3.554 \) min.

![Signal 1: RID1 A, Refractive Index Signal](image_url)
6. References


7. Spectral Data

2-phenyl-4H-chromen-4-one 3a

$\text{3a}$

$^1$H-NMR

$(400 \text{ MHz, CDCl}_3)$

$\text{13C-NMR}$

$(125 \text{ MHz, CDCl}_3)$
7-fluoro-2-phenyl-4H-chromen-4-one 3b
$^{19}$F NMR
(470 MHz, CDCl$_3$)
7-chloro-2-phenyl-4H-chromen-4-one 3c
7-bromo-2-phenyl-4H-chromen-4-one 3d

$\text{Br} \quad \text{O} \quad \text{O} \quad 3d \quad \text{H-NMR} \\
(400 \text{ MHz, CDCl}_3)$

$\text{Br} \quad \text{O} \quad \text{O} \quad 3d \quad \text{C-NMR} \\
(125 \text{ MHz, CDCl}_3)$
4-oxo-2-phenyl-4H-chromen-7-yl trifluoromethanesulfonate 3e

\[ \text{H-NMR} \]
\[
\text{(400 MHz, CDCl}_3) \]

\[ \text{C-NMR} \]
\[
\text{(125 MHz, CDCl}_3) \]
4-oxo-2-phenyl-4H-chromen-7-yl pivalate 3f

1H-NMR (400 MHz, CDCl3)

13C-NMR (125 MHz, CDCl3)
7-methyl-2-phenyl-4H-chromen-4-one 3g

$\text{Me}$

$\text{O}$

$\text{O}$

$\text{3g}$

$\text{H}$-

$\text{N}$-

$\text{M}$-

$\text{R}$

$\text{Me}$

$\text{O}$

$\text{O}$

$\text{3g}$

$\text{3C-NMR}$

$\text{(125 MHz, CDCl}_3\text{)}$

$\text{1H-NMR}$

$\text{(400 MHz, CDCl}_3\text{)}$
6-nitro-2-phenyl-4\(H\)-chromen-4-one 3h
7-hydroxy-2-phenyl-4H-chromen-4-one 3i
7-methoxy-2-phenyl-4H-chromen-4-one 3j

\[ \text{\(\text{MeO} \quad \text{O} \quad \text{O} \quad \text{O} \quad \text{H} \quad \text{N} \quad \text{MeO} \)} \]

\[ \text{\(^{1}H\text{-NMR} \)}
\[ (400 \text{ MHz, CDCl}\_3) \]

\[ \text{\(^{13}C\text{-NMR} \)}
\[ (125 \text{ MHz, CDCl}\_3) \]
7-(benzyloxy)-2-phenyl-4H-chromen-4-one 3k

$\text{\(3k\)}$

$^1H$-NMR
(400 MHz, CDCl$_3$)

$^{13}C$-NMR
(125 MHz, CDCl$_3$)
6-methoxy-2-phenyl-4H-chromen-4-one 3I
5,7-dimethoxy-2-phenyl-4H-chromen-4-one 3m
2-(4-methoxyphenyl)-4H-chromen-4-one 3n

\[ \text{\textsuperscript{1}H-NMR} \]
(400 MHz, CDCl\textsubscript{3})

\[ \text{\textsuperscript{13}C-NMR} \]
(125 MHz, CDCl\textsubscript{3})
2-(4-hydroxyphenyl)-4H-chromen-4-one 3o

\[
\text{\textsuperscript{1}H-NMR} \\
(400 MHz, DMSO-d_6)
\]

\[
\text{\textsuperscript{13}C-NMR} \\
(125 MHz, DMSO-d_6)
\]
2-(3-hydroxyphenyl)-4H-chromen-4-one 3p

(400 MHz, DMSO-d$_6$)

(125 MHz, DMSO-d$_6$)
2-(3,4-dimethoxyphenyl)-4H-chromen-4-one 3q
2-(3,5-dimethoxyphenyl)-4H-chromen-4-one 3r

$\text{H-NMR}$

$(400 \text{ MHz, CDCl}_3)$

$\text{C-NMR}$

$(125 \text{ MHz, CDCl}_3)$
2-(3,4,5-trimethoxyphenyl)-4H-chromen-4-one 3s

\[ \text{3s} \]

\[ ^1\text{H-NMR} \]
(400 MHz, CDCl\textsubscript{3})

\[ \text{3s} \]

\[ ^1\text{C-NMR} \]
(125 MHz, CDCl\textsubscript{3})
5,7-dimethoxy-2-(4-methoxyphenyl)-4H-chromen-4-one $3t$

$\text{H-NMR}$

(400 MHz, CDCl$_3$)

$\text{C-NMR}$

(125 MHz, CDCl$_3$)
2-(naphthalen-2-yl)-4H-chromen-4-one 3u
2-(4-fluorophenyl)-4H-chromen-4-one 3v

\[
\begin{align*}
\text{1H-NMR} \\
(400 \text{ MHz, CDCl}_3)
\end{align*}
\]

\[
\begin{align*}
\text{13C-NMR} \\
(125 \text{ MHz, CDCl}_3)
\end{align*}
\]
2-(4-chlorophenyl)-4H-chromen-4-one 3w
2-(4-bromophenyl)-4H-chromen-4-one 3x

$\text{H-NMR}$
$(400 \text{ MHz, CDCl}_3)$

$\text{C-NMR}$
$(125 \text{ MHz, CDCl}_3)$
2-(4-iodophenyl)-4H-chromen-4-one 3y

$\text{3y}$

$^1\text{H-NMR}$

(400 MHz, CDCl$_3$)

$\text{13C-NMR}$

(125 MHz, CDCl$_3$)
2-methyl-4H-chromen-4-one 3z

\[
\begin{align*}
\text{\(3z\)} & \quad \text{\(\text{\(1^H\)-NMR}\)} \\
& \quad \text{(400 MHz, CDCl$_3$)}
\end{align*}
\]

\[
\begin{align*}
\text{\(3z\)} & \quad \text{\(\text{\(1^C\)-NMR}\)} \\
& \quad \text{(125 MHz, CDCl$_3$)}
\end{align*}
\]
2-(1-methyl-1H-indol-3-yl)-4H-chromen-4-one 3aa

$\text{H-NMR (400 MHz, CDCl}_3$)

$\text{C-NMR (125 MHz, CDCl}_3$)
2-(thiophen-2-yl)-4H-chromen-4-one 3ab
2-(furan-2-yl)-4H-chromen-4-one 3ac

$\text{H-NMR (400 MHz, CDCl}_3\text{)}$

$\text{C-NMR (125 MHz, CDCl}_3\text{)}$
2-(3,4-dimethoxyphenyl)-7-methoxy-4H-chromen-4-one 5a

*$^1$H-NMR
(400 MHz, CDCl$_3$)

*$^{13}$C-NMR
(125 MHz, CDCl$_3$)
2-(3-hydroxy-4-methoxyphenyl)-7-methoxy-4H-chromen-4-one 5c

\[ \text{5c} \]

$^1$H-NMR
(400 MHz, CDCl$_3$)

$^{13}$C-NMR
(125 MHz, CDCl$_3$)
2-phenylchroman-4-one 4a

$^{1}H$-NMR
(400 MHz, CDCl$_3$)

$^{13}C$-NMR
(125 MHz, CDCl$_3$)
7-chloro-2-phenylchroman-4-one 4b

\[ \text{\(4b\)} \]

\[ ^1\text{H-NMR (400 MHz, CDCl}_3) \]

\[ ^{13}\text{C-NMR (125 MHz, CDCl}_3) \]
4-oxo-2-phenylchroman-7-yl pivalate 4c

$\text{\[4c\]}$

$\text{\[1H-NMR \ (400 MHz, CDCl\textsubscript{3})\]}$

$\text{\[13C-NMR \ (125 MHz, CDCl\textsubscript{3})\]}$
7-methoxy-2-phenylchroman-4-one 4e

$^1$H-NMR
(400 MHz, CDCl$_3$)

$^{13}$C-NMR
(125 MHz, CDCl$_3$)
7-(benzyloxy)-2-phenylchroman-4-one 4f

$\text{\textsuperscript{1}H-NMR}$
(400 MHz, CDCl$_3$)

$\text{\textsuperscript{13}C-NMR}$
(125 MHz, CDCl$_3$)
6-methoxy-2-phenylchroman-4-one 4g

$\text{MeO}$

$\text{O}$

$\text{H-NMR}$

(400 MHz, CDCl$_3$)

$\text{MeO}$

$\text{O}$

$\text{13C-NMR}$

(125 MHz, CDCl$_3$)
2-(4-methoxyphenyl)chroman-4-one 4h

$\text{\H\O\O\4h}$

$^1\text{H-NMR}$

(400 MHz, CDCl$_3$)

$\text{\O\M\e\O\O\4h}$

$^1\text{C-NMR}$

(125 MHz, CDCl$_3$)
2-(4-hydroxyphenyl)chroman-4-one 4i

\[
\begin{align*}
\text{4i} \\
\text{\textsuperscript{1}H-NMR} \\
(400 MHz, CDCl\textsubscript{3}) \\
\end{align*}
\]

\[
\begin{align*}
\text{\textsuperscript{13}C-NMR} \\
(125 MHz, DMSO-d\textsubscript{6}) \\
\end{align*}
\]
2-(3-hydroxyphenyl)chroman-4-one 4j

1H-NMR (400 MHz, CDCl3)

13C-NMR (125 MHz, DMSO-d6)
2-(3,4-dimethoxyphenyl)chroman-4-one 4k

$\text{H-NMR}$

(400 MHz, CDCl$_3$)

$\text{C-NMR}$

(125 MHz, CDCl$_3$)
2-(3,5-dimethoxyphenyl)chroman-4-one 4I

$\text{\textsuperscript{1}H-NMR}$

(400 MHz, CDCl$_3$)

$\text{\textsuperscript{13}C-NMR}$

(125 MHz, CDCl$_3$)
2-(3,4,5-trimethoxyphenyl)chroman-4-one 4m

$\text{^1H-NMR}$

(400 MHz, CDCl$_3$)

$\text{^13C-NMR}$

(125 MHz, CDCl$_3$)
2-(naphthalen-2-yl)chroman-4-one 4n
2-(4-fluorophenyl)chroman-4-one 4o
$^1$H-NMR
(400 MHz, CDCl$_3$)
2-(4-chlorophenyl)chroman-4-one 4p

\[ \text{H-NMR} \]
(400 MHz, CDCl$_3$)

\[ \text{C-NMR} \]
(125 MHz, CDCl$_3$)
2-methylchroman-4-one 4q

$\text{Me}$

$^1$H-NMR
(400 MHz, CDCl$_3$)

$^{13}$C-NMR
(125 MHz, CDCl$_3$)
2-(thiophen-2-yl)chroman-4-one 4r

$^{1}H$-NMR (400 MHz, CDCl$_3$)

$^{13}C$-NMR (125 MHz, CDCl$_3$)
2-(3,4-dimethoxyphenyl)-7-methoxychroman-4-one 5b

\[ \text{MeO} \quad \text{O} \quad \text{OMe} \]

\[ \text{MeO} \quad \text{O} \quad \text{OMe} \]

\[ 5b \quad \text{H-NMR} \]

(400 MHz, CDCl₃)

\[ \text{MeO} \quad \text{O} \quad \text{OMe} \]

\[ \text{MeO} \quad \text{O} \quad \text{OMe} \]

\[ 5b \quad \text{C-NMR} \]

(125 MHz, CDCl₃)
1-(4-fluoro-2-hydroxyphenyl)-3-phenylpropan-1-one 1b

$\text{H-NMR}$

$\text{(400 MHz, CDCl}_3\text{)}$

$\text{C-NMR}$

$\text{(125 MHz, CDCl}_3\text{)}$
1-(4-chloro-2-hydroxyphenyl)-3-phenylpropan-1-one 1c

\[
\begin{align*}
\text{1c} & \\
\text{\textsuperscript{1}H-NMR} & \\
(400 MHz, CDCl\textsubscript{3})
\end{align*}
\]

\[
\begin{align*}
\text{1c} & \\
\text{\textsuperscript{13}C-NMR} & \\
(125 MHz, CDCl\textsubscript{3})
\end{align*}
\]
1-(4-bromo-2-hydroxyphenyl)-3-phenylpropan-1-one **1d**
3-hydroxy-4-(3-phenylpropanoyl)phenyl trifluoromethanesulfonate 1e

$^{1}H$-NMR  
$(400 \text{ MHz, CDCl}_3)$

$^{13}C$-NMR  
$(125 \text{ MHz, CDCl}_3)$
$^{1}$H-NMR
(400 MHz, CDCl$_3$)
3-hydroxy-4-(3-phenylpropanoyl)phenyl pivalate 1f

$\text{H-NMR}$
$(400 \text{ MHz, CDCl}_3)$

$\text{C-NMR}$
$(125 \text{ MHz, CDCl}_3)$
1-(2-hydroxy-4-methylphenyl)-3-phenylpropan-1-one 1g

$\text{Me}$

1H-NMR
(400 MHz, CDCl$_3$)

$\text{O}$

$\text{H}$

$\text{Me}$

$\text{1g}$

$^{13}$C-NMR
(125 MHz, CDCl$_3$)

$\text{O}$

$\text{H}$

$\text{Me}$
1-(2-hydroxy-5-nitrophenyl)-3-phenylpropan-1-one 1h

$\text{H-NMR}$
(400 MHz, CDCl$_3$)

$\text{C-NMR}$
(125 MHz, CDCl$_3$)
1-(2,4-dihydroxyphenyl)-3-phenylpropan-1-one \textbf{1i}

$^{1}$H-NMR
(400 MHz, CDCl$_3$)

$^{13}$C-NMR
(125 MHz, DMSO-d$_6$)
1-(2-hydroxy-4-methoxyphenyl)-3-phenylpropan-1-one 1j

`\text{MeO}\ O\ \text{MeO}\`

$^1\text{H-}{\text{NMR}}$

$(400 \text{ MHz, CDCl}_3)$

$\text{MeO}\ O\ \text{MeO}\$

$^{13}\text{C-}{\text{NMR}}$

$(125 \text{ MHz, CDCl}_3)$
1-(4-(benzyloxy)-2-hydroxyphenyl)-3-phenylpropan-1-one 1k

$\text{1H-NMR}$

(400 MHz, CDCl$_3$)

$\text{13C-NMR}$

(125 MHz, CDCl$_3$)
1-(2-hydroxy-5-methoxyphenyl)-3-phenylpropan-1-one 1l
1-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenylpropan-1-one **1m**

![1H-NMR](image1)

**1H-NMR**

(400 MHz, CDCl₃)

![13C-NMR](image2)

**13C-NMR**

(125 MHz, CDCl₃)
3-(3,5-dimethoxyphenyl)-1-(2-hydroxyphenyl)propan-1-one 1r

$^1$H-NMR (400 MHz, CDCl$_3$)

$^{13}$C-NMR (125 MHz, CDCl$_3$)
1-(2-hydroxyphenyl)-3-(naphthalen-2-yl)propan-1-one **1u**

**1H-NMR**
(400 MHz, CDCl₃)

**13C-NMR**
(125 MHz, CDCl₃)
3-(4-fluorophenyl)-1-(2-hydroxyphenyl)propan-1-one 1v

\[
\begin{align*}
\text{1H-NMR} \\
(400 \text{ MHz, DMSO-}d_6)
\end{align*}
\]

\[
\begin{align*}
\text{13C-NMR} \\
(125 \text{ MHz, CDCl}_3)
\end{align*}
\]
$^1$H-NMR

(470 MHz, CDCl$_3$)
3-(4-chlorophenyl)-1-(2-hydroxyphenyl)propan-1-one $1w$

$1w$

$^1$H-NMR
(400 MHz, CDCl$_3$)

$12$C-NMR
(125 MHz, CDCl$_3$)
3-(4-bromophenyl)-1-(2-hydroxyphenyl)propan-1-one \textbf{1x}

\begin{align*}
\text{\textsuperscript{1}H-NMR} \\
(400 \text{ MHz, DMSO-d}_6)
\end{align*}

\begin{align*}
\text{\textsuperscript{13}C-NMR} \\
(125 \text{ MHz, DMSO-d}_6)
\end{align*}
1-(2-hydroxyphenyl)-3-(4-iodophenyl)propan-1-one 1y

$\text{1y}$

$^1\text{H-NMR}$
(400 MHz, DMSO-$d_6$)

$\text{1y}$

$^{13}\text{C-NMR}$
(125 MHz, DMSO-$d_6$)