Supporting Information for

Synthesis of Theaflavins
via Biomimetic Oxidative Coupling Reaction

Experimental Procedures

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General

Nuclear magnetic resonance [¹H NMR (500 MHz), ¹³C NMR (125 MHz)] spectra were determined on a JEOL ECA-500 and a JEOL α-500 instruments. Chemical shifts for ¹H NMR were reported in parts per million downfields from tetramethylsilane (δ) as the internal standard and coupling constants are in hertz (Hz). The following abbreviations are used for spin multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Chemical shifts for ¹³C NMR were referenced to solvent peaks: δC 77.0 for CDCl₃, δC 206.3 for acetone-d₆, δC 118.3 for CD₃CN and δC 49.0 for CD₃OD.

High-resolution mass spectra (HRMS) were obtained on JEOL MStation JMS-700, JMS-GCmate II and BRUKER DALTONICS microTOF (ESI). Fast atom bombardment (FAB) mass spectra were obtained with a mixture of 3-nitrobenzylalcohol and magic bullet as a matrix.

Analytical thin layer chromatography (TLC) was performed on Merck precoated analytical plates, 0.25 mm thick, silica gel 60 F254. Preparative TLC separations were made on 7 x 20 cm plates prepared with a 0.25 mm layer of Merck silica gel 60 F254. Compounds were eluted from the adsorbent with 10% methanol in chloroform.

Column chromatography was carried out with KANTO CHEMICAL Silica Gel 60 N (spherical, neutral) 63 - 210 μm. Reagents and solvents were commercial grades and were used as supplied with following exceptions:

- benzene, dichloromethane : dried over molecular sieves 4A.
- acetonitrile : dried over molecular sieves 3A.

All reactions sensitive to oxygen or moisture were conducted under an argon atmosphere.
Synthesis of 5,7-di-O-(2-nitrobenzenesulfonyl)catechin (12)

To a solution of boric acid (100 g, 1.6 mol) and NaOH (20.0 g) in H₂O (1.30 L) was added 9 (10.0 g, 34.5 mmol) and the resulting solution was adjusted to pH 9.0 by the addition of 1M NaOH. Then 2-nitrobenzenesulfonyl chloride (15.3 g, 69.0 mmol) in toluene (220 mL) was added dropwise over 30 min and the mixture was stirred at room temperature for 7 h. The reaction was quenched with 1M HCl and extracted with ethyl acetate. The organic phase was dried over anhydrous sodium sulfate and evaporated under reduced pressure. The residue was purified by silica gel flash column chromatography (1 ~ 3% MeOH in CH₂Cl₂) to afford 12 (15.9 g, 70 %) as a pale yellow amorphous solid.

**H NMR** (500 MHz, acetone-\(d_6\)) \(\delta\) 8.09-8.00 (m, 3H), 7.98-7.75 (m, 5H), 6.79 (d, \(J = 8.0\) Hz, 1H), 6.74 (dd, \(J = 6.5, 2.0\) Hz, 1H), 6.60 (dd, \(J = 8.0, 2.0\) Hz, 1H), 6.56 (d, \(J = 2.0\) Hz, 1H), 4.85 (d, \(J = 6.0\) Hz, 1H), 4.10-4.05 (m, 1H), 2.66 (dd, \(J = 17.0, 7.5\) Hz, 1H), 2.53 (dd, \(J = 17.0, 5.0\) Hz, 1H)

**C NMR** (125 MHz, acetone-\(d_6\)) \(\delta\) 157.0, 149.4, 149.2, 148.9, 148.4, 145.8, 145.7, 137.7, 137.6, 133.7, 133.5, 133.0, 132.4, 130.8, 128.1, 128.1, 126.1, 126.1, 119.3, 116.5, 116.0, 114.4, 110.2, 109.2, 82.6, 66.1, 27.5

**IR** (neat) 3398, 1701, 1618, 1591, 1545, 1439, 1389, 1366, 1196, 1110, 1032, 997, 780 cm\(^{-1}\)

**HRMS** (ESI) calculated for C₂₇H₂₀N₂O₁₄S₂Na [M+Na]⁺ 683.0248, found 683.0281

\([\alpha]_{D}^{20}\) = +13.3 (c 1.0, acetone)
Synthesis of 5,7-di-O-(2-nitrobenzenesulfonyl)epicatechin (13)

In a similar manner to that used to prepare 12, treatment of 10 (5.0 g) gave 13 (7.1 g, 63%) as a pale yellow amorphous solid.

$^1$H NMR (500 MHz, acetone-$d_6$) $\delta$ 8.17-8.08 (m, 4H), 8.06-8.01 (m, 2H), 8.00-7.91 (m, 4H), 7.01 (s, 1H), 6.80, (d, $J$ = 1.5 Hz, 2H), 6.77 (d, $J$ = 2.0 Hz, 1H), 6.47 (d, $J$ = 2.0 Hz, 1H), 5.02 (s, 1H), 4.30-4.26 (m, 1H), 3.00-2.85 (m, 2H)

$^{13}$C NMR (125 MHz, acetone-$d_6$) $\delta$ 157.7, 149.4, 149.2, 148.1, 145.5, 145.4, 137.6, 133.7, 133.5, 132.8, 132.5, 130.6, 128.2, 127.5, 126.1, 126.0, 119.2, 116.0, 115.5, 115.0, 110.2, 108.8, 80.1, 65.0, 29.8

IR (neat) 3421, 1691, 1617, 1385, 1195, 1110, 997, 781 cm$^{-1}$

HRMS (ESI) calculated for C$_{27}$H$_{20}$N$_2$O$_{14}$S$_2$Na [M+Na]$^+$ 683.0248, found 683.0255

$[\alpha]_{D}^{20} = +6.5$ (c 1.00, acetone)
Synthesis of 5,7-di-O-(2-nitrobenzenesulfonyl)epigallocatechin (14)

In a similar manner to that used to prepare 12, treatment of 11 (4.0 g) gave 14 (4.6 g, 52%) as a brown amorphous solid.

$^1$H NMR (500 MHz, acetone-$d_6$) δ 8.13-8.09 (m, 5H), 8.03-8.01 (m, 2H), 7.98-7.90 (m, 3H), 7.83 (brs, 2H), 7.44 (brs, 1H), 6.77 (d, $J = 2.0$ Hz, 1H), 6.52 (s, 2H), 6.48 (d, $J = 2.0$ Hz, 1H), 4.96 (brs, 1H), 4.25 (d, $J = 4.0$ Hz, 1H), 4.12 (d, $J = 4.0$ Hz, 1H), 2.93 (dd, $J = 16.5$, 4.0 Hz, 1H), 2.90 (dd, $J = 16.5$, 4.0 Hz, 1H)

$^{13}$C NMR (125 MHz, acetone-$d_6$) δ 157.2, 148.9, 148.7, 145.7, 137.2, 133.4, 133.1, 132.8, 132.5, 132.1, 129.4, 127.8, 127.0, 125.7, 125.7, 115.6, 109.9, 108.4, 106.2, 79.7, 64.6, 29.5

IR (neat) 3342, 1701, 1620, 1591, 1547, 1441, 1385, 1368, 1194, 1111, 997, 781 cm$^{-1}$

HRMS (ESI) calculated for C$_{27}$H$_{20}$N$_2$O$_{15}$S$_2$Na $[M+Na]^+$ 699.0197, found 699.0191

$[\alpha]_{D}^{20} = +4.1$ (c 1.00, acetone)
Synthesis of \((2R,3R)-5,7,5,7\text{-tetra-O–(2-nitrobenzenesulfonyl)}\) neotheaflavin (16)

To a solution of 12 (1.0 g, 1.5 mmol) in MeCN (15 mL) was added Pb(OAc)₄ (806 mg, 4.5 mmol) at 0 °C. The resulting suspension was stirred for 10 min at 0 °C. The reaction mixture was added to benzene, and then the mixture was filtered through a pad of celite. Then the filtrate was evaporated under reduced pressure, and the resulting crude product was used in the next reaction without further purification.

The crude product 15 was dissolved in MeCN / CH₂Cl₂ (1 : 4, 25 mL). To this solution were added MS3A (1.0 g) and Ns-epigallocatechin 14 (342 mg, 505 μmol) in MeCN / CH₂Cl₂ (1 : 4, 10 mL) at 0 °C. The resulting suspension was stirred for 20 min at 0 °C. After the addition of H₂O the mixture was stirred for 5 min at rt. The reaction mixture was filtered, and then the filtrate was extracted with AcOEt, the organic phase was washed with H₂O, and evaporated under reduced pressure. The residue was purified by silica gel flash column chromatography (CH₂Cl₂ : MeOH = 98 : 2) to afford 16 (327 mg, 50%) as an orange amorphous solid, and the mixture of product was used in the next reaction without further purification.

\(^1\)H NMR (500 MHz, acetone-\(d_6\)) \(\delta\) 8.18-7.86 (m, 21H), 7.53 (s, 1H), 6.94 (d, \(J = 2.3\) Hz, 1H), 6.93 (d, \(J = 2.3\) Hz, 1H), 6.51 (d, \(J = 2.3\) Hz, 1H), 6.50 (d, \(J = 2.3\) Hz, 1H), 6.02 (brs, 1H), 5.25 (s, 1H), 4.56 (brs, 1H), 4.48 (brs, 1H), 3.1-2.9 (m, 4H, H₂O peak was overlapped)

\(^13\)C NMR (125 MHz, acetone-\(d_6\)) \(\delta\) 184.8, 157.4, 157.1, 154.6, 149.4, 149.3, 149.2, 149.1, 149.1, 148.2, 148.1, 137.6, 137.5, 133.8, 133.5, 132.8, 132.5, 130.4, 129.7, 128.2, 128.2, 128.1, 127.5, 126.7, 126.1, 126.1, 126.0, 123.4, 121.5, 119.1, 118.4, 116.1, 115.7, 110.6, 110.5, 109.2, 109.0, 82.0, 81.9, 77.3, 77.3, 64.6, 63.2, 55.2, 29.6 (acetone peak was overlapped), 29.5 (acetone peak was overlapped)

IR (neat) 3352, 1701, 1618, 1591, 1547, 1477, 1437, 1384, 1361, 1232, 1190, 1106, 1058, 1030, 995 850, 775, 736 cm⁻¹

HRMS (ESI) calculated for C₅₃H₃₆N₄O₂₈S₄Na \([M+Na]^+\) 1327.0291, found 1327.0272

\([\alpha]^{20}_D = −7.4\ (c\ 0.50, \text{acetone})\)
Synthesis of neotheaflavin (2)

To a suspension of Cs$_2$CO$_3$ (501 mg, 0.17 mmol) and thiophenol (0.17 mL, 1.7 mmol) in MeCN / DMF (1 : 2, 2.7 mL) was added solution of crude 16 (223 mg, 0.17 mmol) in MeCN (3.0 mL) at 0 °C and the reaction mixture was stirred at the same temperature for 2 h. The reaction was quenched with 1M HCl aq. and extracted with AcOEt. The organic phase was evaporated under reduced pressure. The residue was purified by preparative TLC (CH$_2$Cl$_2$ : MeOH = 9 : 1) to afford 2 (53 mg, 55%) as an orange amorphous solid.

$^1$H NMR (500 MHz, acetone-$d_6$) δ 8.83 (brs, 1H), 8.27 (s, 1H), 7.77 (s, 1H), 7.67 (s, 1H), 6.08 (s, 1H), 6.04 (s, 1H), 5.96 (s, 1H), 5.95 (s, 1H), 5.62 (d, $J = 5.0$ Hz, 1H), 5.02 (s, 1H), 4.38 (brs, 1H), 4.16-4.10 (m, 1H), 3.00-2.75 (m, 3H), 2.66 (dd, $J = 16.0$, 9.0 Hz, 1H)

$^{13}$C NMR (125 MHz, acetone-$d_6$) δ 184.6, 157.4, 157.2, 157.2, 156.8, 156.5, 156.3, 154.1, 150.3, 146.0, 134.6, 132.1, 130.3, 128.4, 122.1, 121.4, 119.0, 100.5, 99.0, 96.1, 95.3, 95.1, 81.3, 79.0, 69.2, 66.4, 30.3, 29.1

IR (neat) 3362, 1699, 1622, 1607, 1506, 1472, 1429, 1361, 1236, 1193, 1143, 1099, 1076, 1046, 1012, 823 cm$^{-1}$

HRMS (ESI) calculated for C$_{29}$H$_{24}$O$_{12}$Na [M+Na]$^+$ 587.1159, found 587.1130

$[\alpha]_{D}^{20} = -122.1$ (c 0.20, acetone)

Analytical data for neotheaflavin (2) in Ref. 5b
Synthesis of (2R,3R)-5,7,7,7-tetra-O-(2-nitrobenzensulfonyl)theaflavin (26)

To a solution of 13 (500 mg, 757 mmol) in MeCN (7 mL) was added Pb(OAc)$_4$ (268 mg, 605 mmol) at 0 °C. The resulting suspension was stirred for 10 min at the same temperature. The reaction mixture was added benzene (20 mL), and then the mixture was filtered with celite pad. Then the filtrate was evaporated under reduced pressure, and the resulting crude product was used in the next reaction without further purification.

The crude product 21 was dissolved in MeCN / CH$_2$Cl$_2$ (1 : 4, 12 mL). The solution was added MS3A (300 mg), Ns-epigallocatechin 14 (171 mg, 252 mmol) in MeCN / CH$_2$Cl$_2$ (1 : 4, 4 mL) at 0 °C. The resulting suspension was stirred for 20 min at 0 °C. After the addition of H$_2$O, the mixture was stirred for 5 min at r.t. The reaction mixture was filtered, and then the filtrate was extracted with AcOEt, the organic phase was washed with H$_2$O, and evaporated under reduced pressure. The residue was purified by chromatography on silica gel column (CH$_2$Cl$_2$ : MeOH = 9 : 1) to afford mixture of 26 and 13 as an orange amorphous solid, and the mixture of product was used in the next reaction without further purification.
Synthesis of theaflavin (1)

![Synthesis diagram]

To a solution of crude 26 (249 mg) in MeCN / DMF (1 : 2, 3.0 mL) were added Cs$_2$CO$_3$ (257 mg, 789 mmol) and thiophenol (0.090 mL, 879 mmol) at 0 °C and the reaction mixture was stirred for 3 h at the same temperature. The reaction was quenched with 1 M HCl aq. and extracted with AcOEt. The organic layer was evaporated under reduced pressure and the residue was purified by HPLC to afford Theaflavin (1) (16 mg, 11% for two steps) as an orange amorphous solid.

$^1$H NMR (500 MHz, acetone-d$_6$) $\delta$ 8.30 (brs, 1H), 8.16 (brs, 1H), 8.05 (s, 1H), 8.01 (s, 1H), 7.59 (s, 1H), 6.08 (d, $J$ = 2.0 Hz, 1H), 6.06 (d, $J$ = 2.0 Hz, 1H), 6.03 (d, $J$ = 2.0 Hz, 1H), 5.99 (d, $J$ = 2.0 Hz, 1H), 5.76 (s, 1H), 4.49 (s, 1H), 4.42 (brs, 1H), 4.16 (brs, 1H), 3.84 (brs, 1H), 2.96 (dd, $J$ = 17.0, 4.0 Hz, 1H, H$_2$O peak was overlaped), 2.93 (dd, $J$ = 17.0, 4.0 Hz, 1H, H$_2$O peak was overlaped), 2.82 (brd, $J$ = 16.0 Hz, 1H, H$_2$O peak was overlaped), 2.80 (brd, $J$ = 16.0 Hz, 1H, H$_2$O peak was overlaped)

$^{13}$C NMR (125 MHz, acetone-d$_6$) $\delta$ 184.8, 157.7, 157.6, 157.5, 157.0, 156.5, 154.6, 150.5, 145.6, 135.1, 131.6, 128.7, 127.0, 123.8, 121.6, 119.1, 99.9, 99.3, 96.4, 95.7, 95.5, 81.2, 76.6, 66.3, 65.1, 30.5, 30.1

IR (neat) 3275, 1691, 1624, 1600, 1507, 1460, 1419, 1352, 1230, 1197, 1138, 1089, 1060, 1041, 1010, 891, 805, 706 cm$^{-1}$

HRMS (ESI) calculated for C$_{29}$H$_{24}$O$_{12}$Na [M+Na]$^+$ 587.1159, found 587.1164

$[\alpha]_{b}^{20}$ = -274.8 (c 0.20, acetone)

$^1$H NMR (500 MHz, CD$_3$OD) $\delta$ 7.94 (s, 1H), 7.81 (s, 1H), 7.33 (s, 1H), 6.00 (d, $J$ = 2.0 Hz, 1H), 5.97 (d, $J$ = 2.0 Hz, 1H), 5.95 (d, $J$ = 2.0 Hz, 1H), 5.94 (d, $J$ = 2.0 Hz, 1H), 5.62 (s, 1H), 4.86 (s, 1H), 4.47-4.41 (m, 1H), 4.32-4.25 (m, 1H), 2.96 (dd, $J$ = 17.0, 4.0 Hz, 1H), 2.93 (dd, $J$ = 17.0, 4.0 Hz, 1H), 2.82 (brd, $J$ = 16.0 Hz, 1H), 2.80 (brd, $J$ = 16.0 Hz, 1H)

$^{13}$C NMR (125 MHz, CD$_3$OD) $\delta$ 184.7, 157.0, 156.9, 156.6, 156.4, 156.1, 156.1, 155.4, 149.8, 145.2, 133.4, 130.2, 127.7, 125.0, 122.7, 120.9, 117.1, 99.0, 98.4, 95.8, 94.8, 94.3, 80.0, 75.9, 65.3, 64.4, 28.6, 28.1

Analytical data for theaflavin (1) in Ref. 5b.

To a solution of 12 (600 mg, 909 μmol) in MeCN (6 mL) was added Pb(OAc)_4 (483 mg, 1.09 mmol) at 0 °C. The resulting suspension was stirred for 10 min at 0 °C. To the reaction mixture was added benzene (40 mL), and then the mixture was filtered through a pad of celite. Then the filtrate was evaporated under reduced pressure, and the resulting crude product was used in the next reaction without further purification.

The crude product 15 was dissolved in MeCN / CH_2Cl_2 (1 : 4, 10 mL). To this solution were added MS3A (200 mg) and pyrogallol (22) (39 mg, 310 μmol) in MeCN / CH_2Cl_2 (1 : 4, 1.5 mL) at 0 °C. The resulting suspension was stirred for 20 min at 0 °C. After the addition of H_2O, the mixture was stirred for 5 min at rt. The reaction mixture was filtered, and then the filtrate was extracted with AcOEt, the organic phase was washed with H_2O and evaporated under reduced pressure. The residue was purified by preparative TLC (CH_2Cl_2 : MeOH = 98 : 2) to afford crude 27 (40 mg) as a orange amorphous solid, and the mixture of product was used in the next reaction without further purification.

To a suspension of Cs₂CO₃ (155 mg, 0.48 mmol) and thiophenol (55 μL, 0.53 mmol) in MeCN / DMF (1 : 2, 0.9 mL) was added solution of crude 27 in MeCN (1.0 mL) at 0 °C and the reaction mixture was stirred at the same temperature for 2 h. The reaction was quenched with 1M HCl aq. and extracted with AcOEt. The organic phase was evaporated under reduced pressure. The residue was purified by preparative TLC (CH₂Cl₂ : MeOH = 9 : 1) to afford 23 (16 mg, 13% for two steps) as a orange amorphous solid.

**¹H NMR** (500 MHz, methanol-d₄) δ 7.87 (d, J = 12.0 Hz, 1H), 7.62 (s, 1H), 7.17 (d, J = 9.0 Hz, 1H), 6.82 (dd, J = 12.0, 9.0 Hz, 1H), 5.98 (d, J = 2.3 Hz, 1H), 5.90 (d, J = 2.3 Hz, 1H), 5.45 (d, J = 7.5 Hz, 1H), 4.20-4.13 (m, 1H), 2.86 (dd, J = 16.4, 8.0 Hz, 1H), 2.62 (dd, J = 16.4, 8.6 Hz, 1H)

**¹³C NMR** (125 MHz, methanol-d₄) δ 186.3, 158.0, 157.7, 156.7, 156.6, 151.8, 147.0, 131.5, 130.0, 124.1, 122.9, 122.6, 118.6, 100.6, 96.7, 95.5, 80.2, 68.9, 28.9

**IR (neat)** 3319, 1602, 1411, 1327, 1253, 1070, 825 cm⁻¹

**HRMS** (ESI) calculated for C₂₀H₁₆O₈Na [M+Na]⁺ 407.0737, found 407.0748

[α]ᵈ₂⁰ = -24.8 (c 0.20, acetone)

To a solution of 12 (200 mg, 0.30 mmol) in MeCN (3 mL) was added Pb(OAc)$_4$ (161 mg, 0.36 mmol) at 0 °C. The resulting suspension was stirred for 10 min at 0 °C. The reaction mixture was added to benzene, and then the mixture was filtered through a pad of celite. Then the filtrate was evaporated under reduced pressure, and the resulting crude product was used in the next reaction without further purification.

The crude product 15 was dissolved in MeCN / CH$_2$Cl$_2$ (1 : 4, 5.0 mL). To the solution were added MS3A (200 mg) and methyl gallate 24 (18.6 mg, 101 μmol) in MeCN / CH$_2$Cl$_2$ (1 : 4, 2.0 mL) at 0 °C. The resulting suspension was stirred for 20 min at 0 °C. After the addition of H$_2$O, the mixture was stirred for 5 min at rt. The reaction mixture was filtered, and then the filtrate was extracted with AcOEt, the organic phase was washed with H$_2$O and evaporated under reduced pressure. The residue was purified by preparative TLC (CH$_2$Cl$_2$ : MeOH = 98 : 2) to afford 28 (41 mg, 50%) as an orange amorphous solid.

$^1$H NMR (500 MHz, acetone-d$_6$) δ 8.86 (s, 1H), 8.20-7.93 (m, 10H), 7.76 (s, 1H), 7.57 (s, 1H), 6.85 (d, $J = 2.3$ Hz, 1H), 6.63 (d, $J = 2.3$ Hz, 1H), 5.63 (d, $J = 7.5$ Hz, 1H), 4.33-4.26 (m, 1H), 3.86 (s, 3H), 2.90 (m, 1H, H$_2$O peak was overlaped), 2.74 (dd, $J = 17.2, 8.6$ Hz, 1H, H$_2$O peak was overlaped)

$^{13}$C NMR (125 MHz, acetone-d$_6$) δ 185.7, 167.4, 156.5, 154.3, 152.0, 149.2, 149.0, 148.9, 148.6, 148.3, 137.6, 133.6, 133.4, 133.2, 132.8, 132.5, 132.3, 128.0, 127.8, 127.2, 126.0, 126.0, 123.9, 122.4, 122.0, 116.4, 115.6, 110.3, 109.7, 81.0, 66.4, 53.2, 28.9

IR (neat) 3369, 1701, 1385, 1248, 1195, 1111, 999, 781 cm$^{-1}$

HRMS (ESI) calculated for C$_{34}$H$_{24}$N$_2$NaO$_{18}$S$_2$ [M+Na]$^+$ 835.0358, found 835.0343

$[\alpha]_D^{20} = +9.6$ (c 0.20, acetone)
To a suspension of Cs$_2$CO$_3$ (209 mg, 0.64 mmol) and thiophenol (66 μL, 0.64 mmol) in MeCN / DMF (1 : 2, 0.9 mL) was added solution of 28 (52 mg, 64 μmol) in MeCN (1.0 mL) at 0 °C and the reaction mixture was stirred at the same temperature for 30 min. The reaction was quenched with 1M HCl aq. and extracted with AcOEt. The organic phase was evaporated under reduced pressure. The residue was purified by preparative TLC (CH$_2$Cl$_2$ : MeOH = 9 : 1) to afford 25 (14 mg, 47%) as a orange amorphous solid.

$^1$H NMR (500 MHz, methanol-$d_4$) δ 8.96 (d, $J = 7.9$ Hz, 1H), 7.72 (m, 1H), 7.65 (d, $J = 3.4$ Hz, 1H), 5.99 (m, 1H), 5.92 (m, 1H), 5.34 (d, $J = 8.5$ Hz, 1H), 4.35-4.13 (m, 1H), 3.83 (s, 3H), 2.98 (ddd, $J = 15.9$, 9.1, 5.1 Hz, 1H), 2.61 (ddd, $J = 15.9$, 9.1 Hz, 1H)

$^{13}$C NMR (125 MHz, methanol-$d_4$) δ 186.8, 168.9, 158.1, 157.7, 156.6, 155.0, 152.4, 149.7, 134.6, 134.4, 128.8, 124.0, 123.5, 122.8, 115.9, 100.8, 96.7, 95.5, 81.3, 69.1, 53.5, 29.7

IR (neat) 3346, 1701, 1608, 1225 cm$^{-1}$

HRMS (ESI) calculated for C$_{22}$H$_{18}$O$_{10}$Na $[M+Na]^+$ 465.0792, found 465.0795

$[\alpha]_D^{20} = -44.6$ (c 0.20, acetone)
Supporting Information for

Synthesis of Theaflavins via Biomimetic Oxidative Coupling Reaction

Spectral Data

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X: parts per Million; 1H

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![Chemical Structure](image_url)
X: parts per million : 13C
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neotheaflavin (2)
Theaflavin (1)
Theaflavin (1)
23

X : parts per Million : 1H