

Electronic Supporting Information

Stereoselective Construction of Fluorinated Indanone Derivatives via a Triple Cascade Lewis Acid-Catalyzed Reaction

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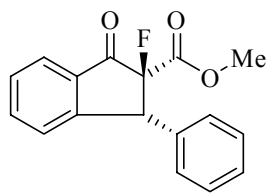
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General information: ^1H , ^{13}C , ^{19}F NMR were recorded on Varian Mercury Plus 500 and 400 instruments at 500 MHz and 400 MHz (^1H NMR), 125 MHz (^{13}C NMR), as well as 376 MHz (^{19}F NMR), or a Bruker AV 300 Spectrometer at 300 MHz (^1H NMR), 75 MHz (^{13}C NMR). Chemical shifts were reported in ppm down field from internal Me_4Si and external CCl_3F , respectively. MS were recorded on a VG-7070E or HP 5988A spectrometer using the ESI method. Elemental analyses were determined on an MT-3 elemental analyzer. HPLC analyses were carried out on a Hewlett Packard Model HP 1200 instrument. All of the reactions were carried out under an argon atmosphere with the exclusion of moisture.

Materials: THF and toluene were distilled from sodium and benzophenone under nitrogen. DCM, DCE, and MeNO_2 were distilled from calcium hydride before use. Analytical thin layer chromatography was performed on 0.20 mm Qingdao Haiyang silica gel plates. Silica gel (200-300 mesh) (from Qingdao Haiyang Chem. Company, Ltd.) was used for flash chromatography.



2a, yield 68%, M. p. 140-142 °C

¹⁹F-NMR (376MHz, CDCl₃) δ [ppm] -162.3 (d, *J* = 24.1 Hz);

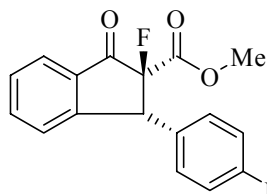
¹H-NMR (500MHz, CDCl₃) δ [ppm] 7.93 (d, *J* = 8.0 Hz, 1H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.36-7.35 (m, 3H), 7.24-7.22 (m, 2H), 4.94 (d, *J* = 24.5 Hz, 1H), 3.28 (s, 3H);

¹³C-NMR(125MHz, CDCl₃) δ [ppm] 195.3 (d, *J* = 18.3 Hz), 165.9 (d, *J* = 29.1 Hz), 151.8 (d, *J* = 6.8 Hz), 136.7, 135.6, 135.0 (d, *J* = 1.4 Hz), 129.6, 129.4, 128.8, 128.6, 127.1 (d, *J* = 1.5 Hz), 125.3 (d, *J* = 1.0 Hz), 99.9 (d, *J* = 204.8 Hz), 55.7 (d, *J* = 23.9 Hz), 52.3 (d, *J* = 1.1 Hz);

IR (KBr) ν (cm⁻¹) 1763, 1721, 1603, 1456, 1292, 1208, 1145, 924, 758, 706;

MS (EI) *m/z* (%) 307.42 [M+Na]⁺ (100%);

Anal Calcd for C₁₇H₁₃FO₃: C 71.82%, H 4.61%; Found: C 71.40%, H 4.22%.



2b, yield 62%, M. p. 118-119.8 °C

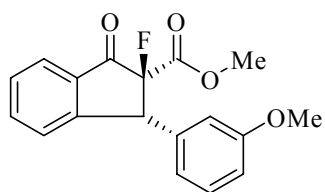
¹⁹F-NMR (376MHz, CDCl₃) δ [ppm] -162.7 (d, *J* = 24.1 Hz);

¹H-NMR (400MHz, CDCl₃) δ [ppm] 7.92 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 4.89 (d, *J* = 24.0 Hz, 1H), 3.29 (s, 3H), 2.35 (s, 3H);

¹³C-NMR (125MHz, CDCl₃) δ [ppm] 195.4 (d, *J* = 18.4 Hz), 166.0 (d, *J* = 29.1 Hz), 152.1 (d, *J* = 6.9 Hz), 138.4, 136.7 (d, *J* = 2.5 Hz), 135.0 (d, *J* = 1.4 Hz), 132.4, 129.5, 129.4, 129.3, 129.2, 127.1, 125.2, 100.0 (d, *J* = 204.3 Hz), 55.5 (d, *J* = 9.6 Hz), 52.3 (d, *J* = 7.4 Hz), 21.4 (d, *J* = 4.9 Hz);

IR (KBr) ν (cm⁻¹) 1769, 1730, 1603, 1450, 1293, 1240, 1209, 1071, 960, 806, 760, 689;

MS (EI) *m/z* (%) 321.47 [M+Na]⁺



2c, yield 60%, M. p. 93-94 °C

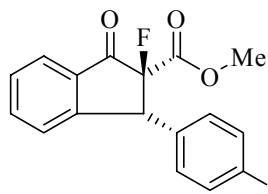
¹⁹F-NMR (376MHz, CDCl₃) δ [ppm] -162.4 (d, *J* = 24.4 Hz);

¹H-NMR (300MHz, CDCl₃) δ [ppm] 7.93 (d, *J* = 7.5 Hz, 1H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.30-7.25 (m, 1H), 6.90-6.75 (m, 3H), 4.90 (d, *J* = 24.0 Hz, 1H), 3.78 (s, 3H), 3.32 (s, 3H);

¹³C-NMR (125MHz, CDCl₃) δ [ppm] 195.3 (d, *J* = 18.1 Hz), 165.9 (d, *J* = 29.1 Hz), 160.0, 151.7 (d, *J* = 6.8 Hz), 136.7, 134.9 (d, *J* = 1.3 Hz), 129.8, 129.4, 127.2 (d, *J* = 1.5 Hz), 125.2 (d, *J* = 0.9 Hz), 121.9, 115.4, 113.9, 99.9 (d, *J* = 204.5 Hz), 55.6 (d, *J* = 23.9 Hz), 55.5, 52.4;

IR (KBr) ν (cm⁻¹) 1769, 1729, 1597, 1492, 1438, 1042, 962, 903, 812, 738, 697, 639;

MS (EI) *m/z* (%) 337.28 [M+Na]⁺ (40%), 315.25 [M+H]⁺ (100%).



2d, yield 70%, M. p. 166-166.5 °C

¹⁹F NMR (376 MHz, CDCl₃) δ [ppm] -162.5 (d, *J* = 24.1 Hz).

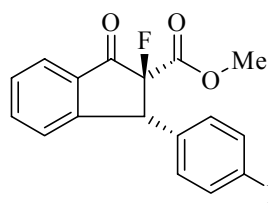
¹H NMR (400 MHz, CDCl₃) δ [ppm] 7.92 (d, *J* = 7.6 Hz, 1H), 7.73-7.77 (m, 1H), 7.55-7.59 (m, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 8.8 Hz, 2H), 7.16 (d, *J* = 8.8 Hz, 2H), 4.89 (d, *J* = 24.0 Hz, 1H), 3.32 (s, 3H);

¹³C NMR (75 MHz, CDCl₃), δ [ppm] 194.8 (d, *J* = 18.5 Hz), 165.8 (d, *J* = 29.2 Hz), 151.2, 151.1, 136.9, 134.9, 134.7, 134.0, 130.9, 129.6, 129.0, 126.9, 125.4, 98.7 (d, *J* = 205.6 Hz), 55.1 (d, *J* = 24.1 Hz), 52.5.

IR (KBr) ν (cm⁻¹) 1727, 1686, 1609, 1489, 1442, 1208, 1150, 854, 783.

MS (ESI) *m/z*: 319.07 [M+H]⁺.

Anal. Calcd. for C₁₇H₁₂ClFO₃: C 64.06%, H 3.79%; Found C 64.52%, H 4.01%.



2e, yield 71%, M. p. 130-133 °C (*trans*)

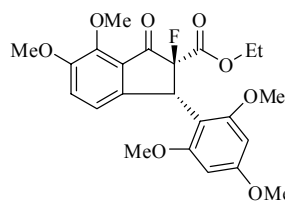
¹⁹F NMR (376 MHz, CDCl₃) δ -162.2 (d, *J* = 23.3 Hz).

¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, *J* = 8.8 Hz, 2H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.79 (t, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.44 (d, *J* = 8.8 Hz, 2H), 7.39 (d, *J* = 7.6 Hz, 1H), 5.03 (d, *J* = 23.2 Hz, 1H), 3.33 (s, 3H);

¹³C NMR (125 MHz, CDCl₃), 194.1 (d, *J* = 18.1 Hz), 165.5 (d, *J* = 28.8 Hz), 150.2, 150.0, 148.1, 142.9, 137.1, 134.8 (d, *J* = 1.4 Hz), 130.6, 130.0, 126.7 (d, *J* = 1.5 Hz), 125.7 (d, *J* = 1.0 Hz), 123.9, 99.4 (d, *J* = 207.6 Hz), 55.1 (d, *J* = 24.4 Hz), 52.7 (d, *J* = 1.1 Hz).

IR (KBr) ν (cm⁻¹) 1768, 1728, 1604, 1523, 1355, 1235, 1108, 766.

MS (ESI) *m/z*: 330.73 [M+H]⁺.



2f, yield 15%, M. p. 149-150.5 °C

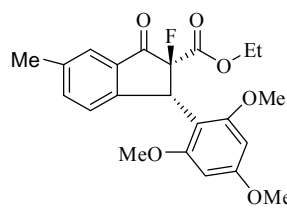
¹⁹F NMR (376 MHz, CDCl₃) δ -151.6 (d, *J* = 27.4 Hz).

¹H NMR (400 MHz, CDCl₃) δ 7.10 (d, *J* = 8.4 Hz, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 6.15 (d, *J* = 1.2 Hz, 1H), 5.93 (d, *J* = 1.5 Hz, 1H), 5.29 (d, *J* = 27.6 Hz, 1H), 4.07 (s, 3H), 4.05-3.81 (m, 8H), 3.77 (s, 3H), 3.30 (s, 3H), 0.95 (t, *J* = 6.8 Hz, 3H);

¹³C NMR (125 MHz, CDCl₃), δ 192.6 (d, *J* = 19.1 Hz), 165.9 (d, *J* = 27.1 Hz), 161.1, 159.7, 159.5, 151.0, 147.8, 146.9 (d, *J* = 4.3 Hz), 126.2, 120.7, 105.6 (d, *J* = 3.9 Hz), 99.1 (d, *J* = 197.0 Hz), 91.2, 90.8, 62.1, 61.6, 57.1, 56.4, 55.5, 55.0, 44.6 (d, *J* = 27.1 Hz), 13.9.

IR (KBr) ν (cm⁻¹) 1763, 1720, 1606, 1589, 1499, 1275, 1125, 1070, 814.

MS (ESI) *m/z*: 471.24 [M+Na]⁺, 449.36 [M+H]⁺.



2g, yield 12%, M. p. 126-132 °C (*trans/cis*: 3/1)

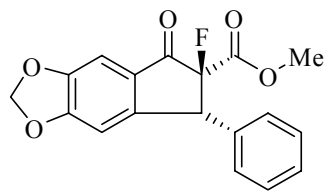
¹⁹F NMR (376 MHz, CDCl₃) δ -149.0 (*trans*) (d, *J* = 28.5 Hz), -152.1 (*cis*) (d, *J* = 27.4 Hz).

¹H NMR (500 MHz, CDCl₃) δ 7.64-7.71 (m, 1H), 7.29-7.38 (m, 2H), 6.18 (*cis*) and 6.15 (*trans*) (d, *J* = 2.5 Hz, 1H), 5.94 (*cis*) and 5.88 (*trans*) (d, *J* = 2.0 Hz, 1H), 5.36 (*cis*) and 5.33 (*trans*) (d, *J* = 28.5 Hz, 1H), 3.98-4.02 (m, 1H), 3.91 (*trans*) and 3.89 (*cis*) (s, 3H), 3.83-3.88 (m, 1H), 3.79 (*cis*) and 3.77 (*trans*) (s, 3H), 3.26 (*cis*) and 3.23 (*trans*) (s, 3H), 2.42 (*cis*) and 2.00 (*trans*) (s, 3H), 0.93-0.97 (m, 3H);

¹³C NMR (125 MHz, CDCl₃) (*trans / cis*), δ 195.4 (d, *J* = 18.6 Hz), 166.3 (d, *J* = 27.0 Hz), 166.2 (d, *J* = 26.4 Hz), 161.4, 160.1, 159.1, 153.4 (d, *J* = 1.5 Hz), 137.6, 137.0, 136.7, 136.0, 134.5, 134.0, 127.9, 125.5, 124.5, 122.2, 104.8 (d, *J* = 5.9 Hz), 98.9 (d, *J* = 195 Hz), 97.3 (d, *J* = 192.6 Hz), 91.1, 90.9, 90.8, 90.7, 61.6, 61.5, 56.5, 56.4, 55.5, 55.4, 55.1, 55.0, 45.7 (d, *J* = 27.8 Hz), 45.4 (d, *J* = 27.8 Hz), 21.3, 17.7, 13.9.

IR (KBr) ν (cm⁻¹) 1760, 1719, 1605, 1588, 1467, 1230, 1159, 1124, 812.

MS (ESI) *m/z*: 425.35 [M+Na]⁺, 403.14 [M+H]⁺.



2h, yield 72%, M. p. 241-241.5 °C

¹⁹F NMR (376 MHz, CDCl₃) δ -160.4 (d, *J* = 23.7 Hz).

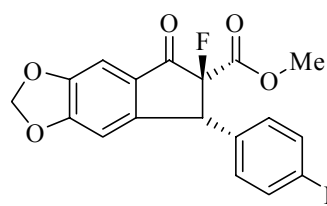
¹H NMR (400 MHz, CDCl₃) δ 7.19-7.34 (m, 6H), 6.75 (s, 1H), 6.15 (s, 1H), 6.13 (s, 1H), 4.79 (d, *J* = 23.6 Hz, 1H), 3.26 (s, 3H);

¹³C NMR (125 MHz, CDCl₃), δ 193.0 (d, *J* = 18.5 Hz), 166.1 (d, *J* = 29.3 Hz), 155.9, 150.0, 149.9, 149.8, 135.5, 129.8 (d, *J* = 1.4 Hz), 129.5, 128.8, 128.6, 106.3 (d, *J* = 1.5 Hz), 103.3 (d, *J* = 0.9 Hz), 103.0, 100.0 (d, *J* = 203.8 Hz), 55.4 (d, *J* = 24.4 Hz), 52.3 (d, *J* = 1.0 Hz).

IR (KBr) ν (cm⁻¹) 1767, 1709, 1608, 1497, 1415, 1314, 1262, 1033, 926, 704.

MS (ESI) m/z : 351.40 $[M+Na]^+$.

Anal. Calcd. For $C_{18}H_{13}FO_5$: C 65.85%, H 3.99%; Found C 65.62%, H 3.75%.



2i, yield 45%, M. p. 96-98 °C

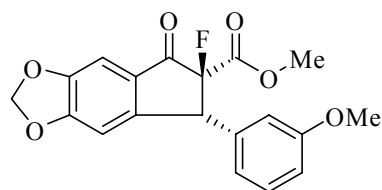
^{19}F NMR (376 MHz, $CDCl_3$) δ -160.7 (d, $J = 24.1$ Hz).

1H NMR (300 MHz, $CDCl_3$) δ 7.07-7.27 (m, 5H), 6.74 (s, 1H), 6.15 (s, 1H), 6.13 (s, 1H), 4.78 (d, $J = 23.7$ Hz, 1H), 3.29 (s, 3H), 2.34 (s, 3H);

^{13}C NMR (75 MHz, $CDCl_3$), δ 193.1 (d, $J = 18.5$ Hz), 166.1 (d, $J = 28.8$ Hz), 155.9, 150.3 (d, $J = 7.1$ Hz), 149.7, 138.4, 132.3, 130.0, 129.7, 129.4, 127.9, 106.3, 103.3, 103.0, 100.1 (d, $J = 203.1$ Hz), 55.1 (d, $J = 24.2$ Hz), 52.3, 21.3.

IR (KBr) ν (cm^{-1}) 1767, 1717, 1609, 1475, 1308, 1258, 1038, 1258, 1034, 937.

MS (ESI) m/z : 365.00 $[M+Na]^+$.



2j, yield 65%, M. p. 130-131 °C

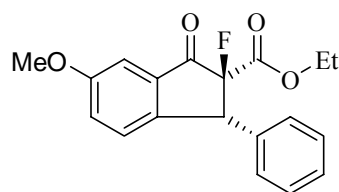
^{19}F NMR (376 MHz, $CDCl_3$) δ -160.3 (d, $J = 23.7$ Hz).

1H NMR (300 MHz, $CDCl_3$) δ 7.23-7.29 (m, 2H), 6.85-6.88 (m, 1H), 6.72-6.80 (m, 3H), 6.14-6.16 (m, 2H), 4.78 (d, $J = 23.7$ Hz, 1H), 3.79 (s, 3H), 3.32 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$), 193.0 (d, $J = 18.5$ Hz), 166.0 (d, $J = 28.1$ Hz), 159.9, 149.9 (d, $J = 7.0$ Hz), 149.7, 137.0, 129.8 (d, $J = 6.4$ Hz), 128.3, 127.0, 121.9, 115.4, 113.8, 106.4 (d, $J = 1.3$ Hz), 103.2, 99.9 (d, $J = 203.6$ Hz), 55.4 (d, $J = 24.8$ Hz), 52.3, 46.3.

IR (KBr) ν (cm^{-1}) 1770, 1714, 1609, 1478, 1313, 1271, 1032, 936.

MS (ESI) m/z : 381.21 $[M+Na]^+$, 358.55 $[M]^+$.



2k, yield 50%, M. p. 90-91.5 °C

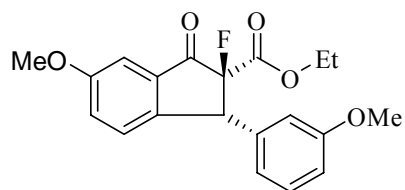
¹⁹F-NMR (376MHz, CDCl₃) δ [ppm] -161.1 (d, *J* = 24.4 Hz);

¹H-NMR (500MHz, CDCl₃) δ [ppm] 7.34-7.32 (m, 6H), 7.24-7.22 (m, 2H), 4.86 (d, *J* = 24.5 Hz, 1H), 3.91 (s, 3H), 3.85-3.77 (m, 1H), 3.69-3.63 (m, 1H), 0.84 (t, *J* = 7.0 Hz, 3H);

¹³C-NMR (125MHz, CDCl₃) δ [ppm] 195.6 (d, *J* = 18.4 Hz), 165.7 (d, *J* = 28.4 Hz), 160.7, 144.8 (d, *J* = 6.6 Hz), 136.3 (d, *J* = 1.3 Hz), 135.9, 129.6, 128.7, 128.5, 128.0 (d, *J* = 1.4 Hz), 126.1, 106.1, 100.0 (d, *J* = 205.5 Hz), 62.1, 56.0, 55.0 (d, *J* = 24 Hz), 13.8;

IR (KBr) ν (cm⁻¹) 1768, 1724, 1613, 1492, 1458, 1371, 1335, 1285, 1252, 1203, 1177, 1134, 1097, 1025, 966, 851, 824, 796, 706;

MS (EI) *m/z* (%) 327.21 [M-H]⁺.



2l, yield 59%

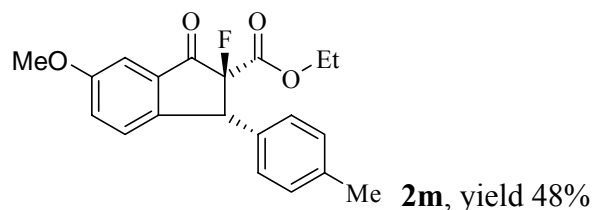
¹⁹F-NMR (376MHz, CDCl₃) δ [ppm] -160.9 (d, *J* = 24.1 Hz);

¹H-NMR (500MHz, CDCl₃) δ [ppm] 7.35-7.30 (m, 3H), 7.26-7.23 (d, *J* = 8.0 Hz, 1H), 6.87-6.85 (m, 1H), 6.82 (d, *J* = 7.5 Hz, 1H), 6.75 (t, *J* = 2.0 Hz, 1H), 4.83 (d, *J* = 24.0 Hz, 1H), 3.91 (s, 3H), 3.87-3.82 (m, 1H), 3.77 (s, 3H), 3.76-3.68 (m, 1H), 0.87 (t, *J* = 7.5 Hz, 3H);

¹³C-NMR (125MHz, CDCl₃) δ [ppm] 195.5 (d, *J* = 18.4 Hz), 165.7 (d, *J* = 28.4 Hz), 160.7, 159.9, 144.7 (d, *J* = 6.6 Hz), 136.2 (d, *J* = 1.3 Hz), 129.7, 128.1 (d, *J* = 1.5 Hz), 126.1, 122.0, 115.5, 113.8, 106.0, 99.9 (d, *J* = 205.3 Hz), 62.1, 56.0, 55.5, 55.0 (d, *J* = 24.0 Hz), 13.8;

IR (KBr) ν (cm⁻¹) 1763, 1727, 1610, 1495, 1435, 1370, 1336, 1283, 1172, 1042, 968, 860, 796, 738;

MS (EI) m/z (%) 339.77 $[M-F]^+$ (100%).



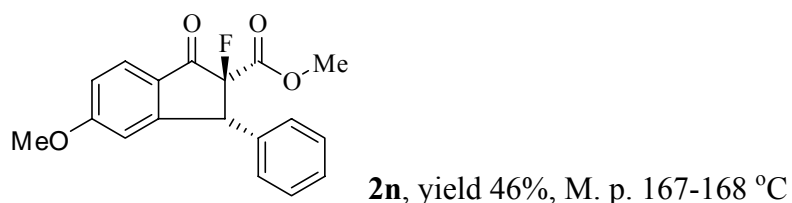
$^{19}\text{F-NMR}$ (376MHz, CDCl_3) δ [ppm] -161.2 (d, $J = 24.4$ Hz), -161.4 (d, $J = 24.1$ Hz);

$^1\text{H-NMR}$ (500MHz, CDCl_3) δ [ppm] 7.32-7.31 (m, 3H), 7.12 (m, 4H), 4.82 (d, $J = 24.0$ Hz, 1H), 3.90 (s, 3H), 3.86-3.80 (m, 1H), 3.71-3.65 (m, 1H), 2.34 (s, 3H), 0.87 (t, $J = 7.0$ Hz, 3H);

$^{13}\text{C-NMR}$ (125MHz, CDCl_3) δ [ppm] 195.7 (d, $J = 18.5$ Hz), 165.8 (d, $J = 28.5$ Hz), 160.7, 145.0 (d, $J = 6.8$ Hz), 138.3, 136.3 (d, $J = 1.4$ Hz), 132.8, 129.5, 129.4, 128.0 (d, $J = 1.4$ Hz), 126.0, 106.0, 100.1 (d, $J = 204.8$ Hz), 62.0, 56.0, 54.7 (d, $J = 24.0$ Hz), 21.3, 13.8;

IR (KBr) ν (cm^{-1}) 1763, 1727, 1610, 1495, 1435, 1370, 1336, 1283, 1172, 1042, 968, 860, 796, 738, 699, 641, 557, 527, 456, 416;

MS (EI) m/z (%) 341.27 $[M-H]^+$.



$^{19}\text{F-NMR}$ (376MHz, CDCl_3) δ [ppm] -161.1 (d, $J = 24.1$ Hz);

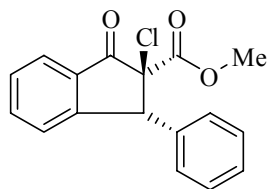
$^1\text{H-NMR}$ (300MHz, CDCl_3) δ [ppm] 7.88 (d, $J = 8.7$ Hz, 1H), 7.38-7.35 (m, 3H), 7.27-7.23 (m, 2H), 7.09 (dd, $J = 8.4$ Hz, $J = 1.5$ Hz, 1H), 6.83 (d, $J = 1.2$ Hz, 1H), 4.88 (d, $J = 24.0$ Hz, 1H), 3.88 (s, 3H), 3.28 (s, 3H);

$^{13}\text{C-NMR}$ (125MHz, CDCl_3) δ [ppm] 193.1 (d, $J = 18.3$ Hz), 167.0, 166.2 (d, $J = 29.4$ Hz), 155.0 (d, $J = 6.9$ Hz), 135.5, 129.6, 128.8, 128.6, 128.2 (d, $J = 1.4$ Hz), 127.2, 127.1, 117.4 (d, $J = 2.0$ Hz), 110.4 (d, $J = 5.9$ Hz), 101.2 (d, $J = 203.5$ Hz), 56.2 (d, $J = 7.1$ Hz), 55.7 (dd, $J = 24.4$ Hz, $J = 9.4$ Hz), 52.3 (d, $J = 7.4$ Hz);

IR (KBr) ν (cm^{-1}) 1768, 1714, 1597, 1493, 1447, 1307, 1284, 1250, 1093, 1019, 943,

839, 816;

MS (EI) m/z (%) 337 [M+Na]⁺ (100%).



3, yield 44%, M. p. 132-134 °C

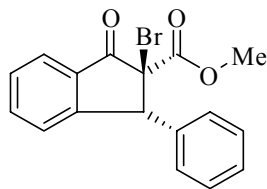
¹H-NMR (300MHz, CDCl₃) δ [ppm] 8.01 (d, *J* = 7.8 Hz, 1H), 7.81-7.76 (m, 1H), 7.64-7.59 (m, 1H), 7.46-7.37 (m, 4H), 7.25-7.22 (m, 2H), 5.13 (s, 1H), 3.25 (s, 3H);

¹³C-NMR (100MHz, CDCl₃) δ [ppm] 195.3, 166.2, 152.1, 136.5, 136.3, 134.7, 129.5, 129.4, 128.7, 126.9, 125.6, 61.3, 53.1;

IR (KBr) ν (cm⁻¹) 1754, 1726, 1599, 1496, 1455, 1323, 1272, 1206, 1101, 1074, 1024, 989, 879, 856, 822;

MS (EI) m/z (%) 339.59 [M+K]⁺ (100%).

Anal Calcd For C₁₇H₁₃ClO₃: C 67.89%, H 4.36%; Found C 67.44%, H 3.99%.



4, yield 60%, M. p. 131-133.5 °C

¹H-NMR (400MHz, CDCl₃) δ [ppm] 7.96 (d, *J* = 7.6 Hz, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.40-7.18 (m, 6H), 5.07 (s, 1H), 3.20 (s, 3H);

¹³C-NMR (75MHz, CDCl₃) δ [ppm] 195.3, 166.3, 152.1, 136.6, 136.3, 134.7, 129.5, 129.4, 128.8, 126.9, 125.6, 61.2 (d, *J* = 9.5 Hz), 53.1 (d, *J* = 9.3 Hz);

IR (KBr) ν (cm⁻¹) 1757, 1726, 1599, 1493, 1456, 1318, 1272, 1206, 1081, 1023, 989, 892, 797, 754, 704;

MS (EI) m/z (%) 265.45 [M-Br]⁺ (100%).

