Supporting Information:

A Mild Method for Generation of o-Quinone Methides Under the Basic Conditions. The Facile Synthesis of trans-2,3-Dihydrobenzofurans

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1. General
All reactions were carried out under an atmosphere of nitrogen using standard Schlenk techniques, unless otherwise noted. 1H NMR, 13C NMR and 19F NMR spectra were recorded at room temperature in CDCl3 on 400 MHz instrument with tetramethylsilane (TMS) as internal standard. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC analysis.

2. General Procedure for Synthesis of 2-(1-Tosylalkyl)phenols

1) Under N2, solution of Grignard reagent 5 (25.0 mmol) was added to phthalimide 6 (10.0 mmol) in THF (10 mL). After being stirred at room temperature for 3 h, the reaction mixture was quenched by a saturated NH4Cl (20 mL) and extracted with CH2Cl2. The combined organic phases were washed with brine, then dried over Na2SO4, filtered and concentrated. A short silica gel column filtration of the crude mixture (hexane/ethyl acetate) afforded 2-hydroxyalkylphenols.

2) TolSO2Na (2.047 g, 11.5 mmol) and TsOH (3.360 g, 17.5 mmol) were placed in a dried Schlenk tube, and dry CH2Cl2 (40 mL) was added, and the mixture was stirred at room temperature for 5 min. Then, the solution (30 mL) of 2-hydroxyalkylphenols 7 (10.0 mmol) in...
CH₂Cl₂ was added and stirred for 1.5 h, the reaction mixture was quenched and adjusted to pH = 8 by a saturated NaHCO₃. After extracted with CH₂Cl₂, the combined organic phases were washed with 1N HCl and brine, then dried over Na₂SO₄, filtered and concentrated. A short silica gel column filtration of the crude mixture (hexane/ethyl acetate) afforded 2-(1-tosylalkyl)phenols 1.

2-(Phenyl(tosyl)methyl)phenol (1a) Pale solid, mp = 151-152 °C (decompose), yield: 79%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:2); ¹H NMR (400 MHz, CDCl₃) δ 7.72-7.52 (m, 5H), 7.27-7.11 (m, 6H), 6.91-6.73 (m, 3H), 5.94 (s, 1H), 2.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.4, 144.8, 135.1, 132.6, 130.6, 130.4, 130.1, 129.4, 129.0, 128.7, 121.1, 112.0, 117.3, 110.1, 69.5, 21.7; HRMS Calculated For C₂₀H₁₇O₃S [M-H]- 337.0898, found: 337.0896.

2-(p-Tolyl(tosyl)methyl)phenol (1b) Pale solid, mp = 170-171 °C (decompose), yield: 86%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:2); ¹H NMR (400 MHz, CDCl₃) δ 7.58-7.41 (m, 5H), 7.21-7.09 (m, 5H), 6.93-6.82 (m, 2H), 6.67 (s, 1H), 5.84 (s, 1H), 2.37 (s, 3H), 2.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.5, 144.8, 138.8, 131.1, 130.3, 130.2, 129.53, 129.49, 129.3, 129.1, 121.5, 120.5, 118.1, 110.2, 70.4, 21.8, 21.3; HRMS Calculated For C₂₁H₁₉O₃S [M-H]- 351.1055, found: 351.1059.

2-(m-Tolyl(tosyl)methyl)phenol (1c) Pale solid, mp = 147-148 °C (decompose), yield: 66%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:2); ¹H NMR (400 MHz, CDCl₃) δ 7.66-7.55 (m, 3H), 7.37-7.32 (m, 2H), 7.19-7.10 (m, 5H), 6.92-6.64 (m, 2H), 6.64 (s, 1H), 5.89 (s, 1H), 2.36 (s, 3H), 2.29 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.5, 144.8, 138.5, 135.3, 132.4, 131.2, 131.0, 130.2, 129.6, 129.5, 129.1, 128.7, 127.5, 121.4, 120.3, 117.7, 70.1, 21.8, 21.6; HRMS Calculated For C₂₁H₁₉O₃S [M-H]- 351.1055, found: 351.1048.

2-(o-Tolyl(tosyl)methyl)phenol (1d) Pale solid, mp = 156-157 °C (decompose), yield: 81%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:2); ¹H NMR (400 MHz, CDCl₃) δ 8.07 (dd, J = 7.8, 1.0 Hz, 1H), 7.68-7.52 (m, 3H), 7.23-7.10 (m, 5H), 7.01-6.74 (m, 3H), 6.29 (s, 1H), 6.18 (s, 1H), 2.34 (s, 3H), 2.04 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.5, 144.8, 137.7, 135.7, 131.5, 130.9, 130.8, 130.0, 129.6, 129.5, 129.0, 128.6, 126.3, 121.6, 120.3, 117.4, 64.5, 21.8, 19.6; HRMS Calculated For C₂₁H₁₉O₃S [M-H]- 351.1055, found: 351.1050.

2-((4-Methoxyphenyl)(tosyl)methyl)phenol (1e) Pale solid, mp = 163-164 °C (decompose), yield: 49%, Rf: 0.40 (ethyl acetate/petroleum ether = 1:2); ¹H NMR (400 MHz, CDCl₃) δ 7.56-7.43 (m, 5H), 7.17-7.13 (m, 3H), 6.83-6.76 (m, 5H), 5.88 (s, 1H), 3.76 (s, 3H), 2.35 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 159.9, 154.5, 144.8, 135.3, 131.8, 130.6, 130.1, 129.5, 129.1, 124.5, 121.2, 120.4, 117.5, 114.2, 69.2, 55.4, 21.8; HRMS Calculated For C₂₁H₁₉O₄S [M-H]- 367.1011, found: 367.1004.
2-((4-(Trifluoromethyl)phenyl)(tosyl)methyl)phenol (1f) Pale solid, mp = 179-180 °C (decompose), yield: 59%, Rf: 0.70 (ethyl acetate/petroleum ether = 1:2); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.70-7.62 (m, 3H), 7.58-7.26 (m, 7H), 7.19-6.80 (m, 2H), 6.11 (s, 1H), 5.94 (s, 1H), 2.37 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 154.2, 145.2, 136.8, 135.0, 130.8, 130.6, 130.5, 129.7, 129.1, 125.7, 125.66, 122.7, 121.6, 119.6, 117.4, 69.1, 21.8; $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -62.77; HRMS Calculated For C$_{21}$H$_{16}$O$_3$SF$_3$ [M-H]$^-$ 405.0772, found: 405.0765.

2-((4-Fluorophenyl)(tosyl)methyl)phenol (1g) Pale solid, mp = 181-182 °C (decompose), yield: 56%, Rf: 0.45 (ethyl acetate/petroleum ether = 1:3); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.65 (dd, $J$ = 7.8, 1.2 Hz, 1H), 7.58 – 7.46 (m, 4H), 7.22 – 7.10 (m, 3H), 6.95 (dt, $J$ = 15.2, 8.0 Hz, 3H), 6.76 (d, $J$ = 8.1 Hz, 1H), 6.51 (s, 1H), 2.36 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.0 ($J$ = 247.0 Hz), 154.3, 145.1, 132.3, 132.3, 130.6, 130.4, 129.6, 129.1, 128.5, 121.5, 120.0, 117.6, 115.7, 69.0, 21.8; $^{19}$F NMR (376 MHz, CDCl$_3$) $\delta$ -112.77; HRMS Calculated For C$_{20}$H$_{17}$O$_3$SFNa [M+Na]$^+$ 379.0780, found: 379.0781.

5-Bromo-2-(phenyl(tosyl)methyl)phenol (1h) Pale solid, mp = 166-167 °C (decompose), yield: 83%, Rf: 0.40 (ethyl acetate/petroleum ether = 1:2); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.02 (s, 1H), 7.53-7.12 (m, 11H), 6.49 (d, $J$ = 8.5 Hz, 1H), 6.00 (s, 1H), 2.32 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 153.8, 145.3, 134.7, 132.9, 132.5, 132.3, 130.4, 129.7, 129.1, 129.0, 121.9, 118.2, 112.7, 110.2, 67.9, 21.9; HRMS Calculated For C$_{20}$H$_{16}$O$_3$SBr [M-H]$^-$ 415.0004, found: 415.0013.

5-Methoxy-2-(phenyl(tosyl)methyl)phenol (1i) Pale solid, mp = 129-130 °C (decompose), yield: 35%, Rf: 0.40 (ethyl acetate/petroleum ether = 1:2); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.55-7.51 (m, 5H), 7.26-7.13 (m, 6H), 6.45-6.32 (m, 2H), 5.87 (s, 1H), 3.65 (s, 3H), 2.32 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 161.2, 155.9, 144.8, 135.2, 133.0, 131.5, 130.4, 129.5, 129.1, 128.8, 128.7, 112.0, 107.5, 102.9, 69.6, 55.4, 21.8; HRMS Calculated For C$_{21}$H$_{19}$O$_4$S [M-H]$^-$ 367.1004, found: 367.1012.

5-Methoxy-2-(phenyl(tosyl)methyl)phenol (1i) Pale solid, mp = 129-130 °C (decompose), yield: 35%, Rf: 0.40 (ethyl acetate/petroleum ether = 1:2); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.55-7.51 (m, 5H), 7.26-7.13 (m, 6H), 6.45-6.32 (m, 2H), 5.87 (s, 1H), 3.65 (s, 3H), 2.32 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 161.2, 155.9, 144.8, 135.2, 133.0, 131.5, 130.4, 129.5, 129.1, 128.8, 128.7, 112.0, 107.5, 102.9, 69.6, 55.4, 21.8; HRMS Calculated For C$_{21}$H$_{19}$O$_4$S [M-H]$^-$ 367.1004, found: 367.1012.
2-(1-Tosylpentyl)phenol (1l) Colorless oil, yield: 53%, Rf 0.30 (ethyl acetate/petroleum ether = 1:2); 1H NMR (400 MHz, CDCl3) δ 7.48 (d, J = 8.0 Hz, 2H), 7.21-7.15 (m, 3H), 6.85 (brs, 3H), 4.56 (s, 1H), 2.39 (s, 3H), 2.32-2.28 (m, 1H), 1.37-1.10 (m, 4H), 0.81 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 155.7, 144.8, 134.1, 130.2, 129.5, 129.2, 121.1, 119.33, 119.28, 110.2, 61.0, 29.9, 22.4, 21.8, 14.4, 13.9; HRMS Calculated For C18H21O3S [M-H]- 317.1211, found: 317.1216.

3. General Procedure for Synthesis of 2,3-Dihydrobenzofurans

Under the nitrogen, 2-(1-tosylalkyl)phenol 1 (0.20 mmol), sulfonium salt 2 (0.24 mmol) and Cs2CO3 (0.50 mmol) were placed in the Schlenk tube, and dry CH2Cl2 (3 mL) was added. The mixture was stirred at room temperature for 12 h. Then 5 mL water was added, the organic phase was separated and the aqueous layer was extracted with CH2Cl2. The combined organic phases were dried over Na2SO4, concentrated under the reduced pressure, and purified by flash chromatography on silica gel to afford the corresponding product trans-2,3-dihydrobenzofuran 3.

trans-Ethyl 3-phenyl-2,3-dihydrobenzofuran-2-carboxylate (3a). Pale solid, mp = 59-60 °C, yield: 99%, Rf 0.50 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.35-7.20 (m, 6H), 7.02-6.91 (m, 3H), 5.03 (d, J = 6.6 Hz, 1H), 4.81 (d, J = 6.7 Hz, 1H), 4.31-4.26 (m, 2H), 1.31 (t, J = 7.1 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 170.8, 159.4, 142.2, 129.2, 129.1, 128.1, 127.7, 125.5, 121.9, 110.3, 87.4, 61.9, 52.9, 14.4; HRMS Calculated For C17H16O3Na [M+Na]+ 291.0997, found: 291.0994.

trans-Ethyl 3-p-tolyl-2,3-dihydrobenzofuran-2-carboxylate (3b). Colorless oil, yield: 98% Rf 0.60 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.23 -7.12 (m, 5H), 7.02-6.91 (m, 3H), 5.02 (d, J = 6.6 Hz, 1H), 4.81 (d, J = 6.7 Hz, 1H), 4.31-4.26 (m, 2H), 2.36 (s, 3H), 1.34 (t, J = 7.1 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 170.8, 159.4, 139.2, 137.4, 129.8, 129.1, 128.0, 125.4, 121.8, 110.21, 110.16, 87.6, 61.9, 52.6, 21.3, 14.4. HRMS Calculated
trans-Ethyl 3-m-tolyl-2,3-dihydrobenzofuran-2-carboxylate (3c). Colorless oil, yield: 91% Rf: 0.60 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.24-7.19 (m, 2H), 7.09-6.89 (m, 6H), 5.02 (d, J = 6.5 Hz, 1H), 4.75 (d, J = 6.5 Hz, 1H), 4.34-4.24 (m, 2H), 2.32 (s, 3H), 1.31 (t, J = 7.1 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 170.8, 159.4, 142.1, 138.8, 129.1, 129.0, 128.9, 128.7, 128.4, 125.4, 125.2, 121.8, 110.2, 61.9, 52.9, 21.6, 14.4; HRMS Calculated For C18H18O3Na [M+Na]+ 305.1154, found: 305.1152.

trans-Ethyl 3-o-tolyl-2,3-dihydrobenzofuran-2-carboxylate (3d). Colorless oil, yield: 98% Rf: 0.50 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.27-7.12 (m, 4H), 7.03-6.90 (m, 4H), 5.09 (d, J = 5.6 Hz, 1H), 5.03 (d, J = 5.7 Hz, 1H), 4.32-4.27 (m, 2H), 2.48 (s, 3H), 1.33 (t, J = 7.1 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 170.9, 159.6, 140.7, 136.0, 130.8, 129.3, 129.1, 128.3, 127.4, 126.9, 125.3, 121.9, 110.2, 87.1, 61.9, 49.0, 20.0, 14.4; HRMS Calculated For C18H18O3Na [M+Na]+ 305.1154, found: 305.1158.

trans-Ethyl 3-(4-methoxyphenyl)-2,3-dihydrobenzofuran-2-carboxylate (3e). Colorless oil, yield: 98% Rf: 0.40 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.27-7.13 (m, 3H), 7.02-6.87 (m, 5H), 4.99 (d, J = 6.8 Hz, 1H), 4.77 (d, J = 6.7 Hz, 1H), 4.39-4.21 (m, 2H), 3.81 (s, 3H), 1.33 (t, J = 7.1 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 170.8, 159.4, 159.1, 134.2, 129.2, 129.1, 125.4, 121.8, 114.4, 110.2, 87.6, 61.9, 55.5, 52.2, 14.4; HRMS Calculated For C18H18O4Na [M+Na]+ 321.1103, found: 321.1109.

trans-Ethyl 3-(4-(trifluoromethyl)phenyl)-2,3-dihydrobenzofuran-2-carboxylate (3f). Colorless oil, yield 91%, Rf: 0.35 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.61 (d, J = 7.9 Hz, 2H), 7.37-7.24 (m, 3H), 7.04-6.92 (m, 3H), 5.01 (d, J = 6.5 Hz, 1H), 4.89 (d, J = 6.5 Hz, 1H), 4.40-4.23 (m, 2H), 1.34 (t, J = 7.1 Hz, 3H); 19F NMR (376 MHz, CDCl3) δ -62.55; HRMS Calculated For C18H15F3O3Na [M+Na]+ 359.0871, found: 359.0862.

trans-Ethyl 3-(4-fluorophenyl)-2,3-dihydrobenzofuran-2-carboxylate (3g). Colorless oil, yield 93%, Rf: 0.45 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.27 – 7.16 (m, 3H), 7.02 (m, 4H), 6.93 (t, J = 7.4 Hz, 1H), 4.98 (d, J = 6.7 Hz, 1H), 4.80 (d, J = 6.7 Hz, 1H), 4.30 (m, 2H), 1.33 (t, J = 7.1 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 170.6, 163.5 (J = 245.0 Hz), 159.3, 137.90 (d, J = 3.2 Hz), 129.71 (d, J = 8.1 Hz), 129.4, 128.5, 125.4, 122.1, 110.5, 87.0, 62.1, 52.6, 14.4; 19F NMR (376 MHz, CDCl3) δ -114.98; HRMS Calculated For C17H16FO3Na [M+Na]+ 287.1083, found: 287.1072.
trans-Ethyl 6-bromo-3-phenyl-2,3-dihydrobenzofuran-2-carboxylate (3h). Colorless oil, yield: 99%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:10); \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.38-7.12 (m, 7H), 6.89 (d, \(J = 8.5\) Hz, 1H), 5.06 (d, \(J = 6.5\) Hz, 1H), 4.78 (d, \(J = 6.5\) Hz, 1H), 4.33-4.25 (m, 2H), 1.52 (t, \(J = 7.1\) Hz, 3H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 170.3, 158.6, 141.4, 132.1, 131.3, 129.3, 128.4, 128.0, 127.7, 111.7, 87.9, 62.1, 52.7, 14.4; HRMS Calculated For C\(_{17}\)H\(_{15}\)BrO\(_3\)Na [M+Na]\(^+\) 369.0102, found: 369.0110.

trans-Ethyl 6-methoxy-3-phenyl-2,3-dihydrobenzofuran-2-carboxylate (3i). Colorless oil, yield: 90%, Rf: 0.40 (ethyl acetate/petroleum ether = 1:10); \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.36-7.21 (m, 5H), 6.91-6.47 (m, 3H), 5.03 (d, \(J = 6.2\) Hz, 1H), 4.72 (d, \(J = 6.2\) Hz, 1H), 4.28-4.29 (m, 2H), 3.80 (s, 3H), 1.33 (t, \(J = 7.1\) Hz, 3H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 170.8, 161.2, 160.8, 142.6, 129.1, 128.0, 127.6, 125.5, 120.7, 107.9, 96.5, 88.2, 86.6, 81.9, 55.7, 52.4, 14.4; HRMS Calculated For C\(_{18}\)H\(_{18}\)O\(_4\)Na [M+Na]\(^+\) 321.1103, found: 321.1106.

trans-Ethyl 3-methyl-2,3-dihydrobenzofuran-2-carboxylate (3j). Colorless oil, yield: 80%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:10); \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.15-7.12 (m, 2H), 6.93-6.89 (m, 2H), 4.70 (d, \(J = 6.3\) Hz, 1H), 4.28 (q, \(J = 6.6\) Hz, 2H), 3.64-3.61 (m, 1H), 1.49 (d, \(J = 5.5\) Hz, 3H), 1.32 (t, \(J = 6.3\) Hz, 3H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 171.1, 158.8, 130.5, 128.6, 123.8, 121.5, 110.1, 86.6, 61.7, 41.7, 20.2, 14.4.

trans-Ethyl 3-ethyl-2,3-dihydrobenzofuran-2-carboxylate (3k). Colorless oil, yield: 77%, Rf: 0.60 (ethyl acetate/petroleum ether = 1:10); \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.18-7.14 (m, 2H), 6.91-6.88 (m, 2H), 4.82 (d, \(J = 5.4\) Hz, 1H), 4.33-4.18 (m, 2H), 3.52-3.48 (m, 1H), 1.85-1.75 (m, 2H), 1.29 (t, \(J = 7.1\) Hz, 3H), 1.03 (t, \(J = 7.4\) Hz, 3H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 171.6, 159.1, 129.0, 128.7, 124.5, 121.3, 110.0, 84.2, 61.7, 48.5, 28.5, 14.3, 11.0; HRMS Calculated For C\(_{13}\)H\(_{16}\)O\(_3\)Na [M+Na]\(^+\) 243.0997, found: 243.0995.

trans-Ethyl 3-butyl-2,3-dihydrobenzofuran-2-carboxylate (3l). Colorless oil, yield: 82%, Rf: 0.60 (ethyl acetate/petroleum ether = 1:10); \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.26-7.13 (m, 2H), 6.91-6.87 (m, 2H), 4.82 (d, \(J = 5.3\) Hz, 1H), 4.27-4.21 (m, 2H), 3.55-3.48 (m, 1H), 1.80-1.70 (m, 2H), 1.49-1.35 (m, 4H), 1.31-1.26 (m, 3H), 0.92 (t, \(J = 7.1\) Hz, 3H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 171.6, 159.1, 129.3, 128.7, 124.5, 121.3, 110.0, 84.6, 61.7, 47.0, 35.6, 28.8, 22.7, 14.3, 14.1; HRMS Calculated For C\(_{15}\)H\(_{20}\)O\(_3\)Na [M+Na]\(^+\) 271.1310, found: 271.1317.

trans-Methyl 3-phenyl-2,3-dihydrobenzofuran-2-carboxylate (3m). Colorless oil, yield: 94%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:10); \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.35-7.19 (m, 6H), 7.02-6.89 (m, 3H), 5.05 (d, \(J = 6.4\) Hz, 1H), 4.81 (d, \(J = 6.3\) Hz, 1H), 3.82 (s, 3H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 171.3, 159.3, 142.1, 129.2, 129.1, 128.7, 128.0, 127.7, 125.5, 121.9, 110.3, 87.3, 52.9, 52.8;

trans-Benzyl 3-phenyl-2,3-dihydrobenzofuran-2-carboxylate (3n). Colorless oil, yield: 67%, Rf: 0.70 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.38-7.30 (m, 8H), 7.26-7.21 (m, 1H), 7.19-7.17 (m, 2H), 7.02-6.93 (m, 3H), 5.34 (d, J = 12.3 Hz, 1H), 5.24 (d, J = 12.3 Hz, 1H), 5.10 (d, J = 6.6 Hz, 1H), 4.79 (d, J = 6.5 Hz, 1H); 13C NMR (100 MHz, CDCl3) δ 170.6, 159.4, 142.0, 135.5, 129.2, 129.1, 128.8, 128.7, 128.5, 128.1, 127.7, 125.4, 121.9, 110.3, 110.2, 87.4, 67.4, 53.0; HRMS Calculated For C22H18O3Na [M+Na]+ 353.1154, found:353.1152.

trans-Phenyl (-3-phenyl-2,3-dihydrobenzofuran-2-yl)methanone (3o). yield: 95%, Rf: 0.50 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.97 (d, J = 8.3 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.8 Hz, 2H), 7.40-7.17 (m, 6H), 7.01 (t, J = 7.8 Hz, 2H), 6.91 (t, J = 7.4 Hz, 1H), 5.84 (d, J = 6.4 Hz, 1H), 5.01 (d, J = 6.4 Hz, 1H); 13C NMR (100 MHz, CDCl3) δ 194.9, 159.3, 142.4, 134.0, 133.9, 129.51, 129.45, 129.2, 129.1, 128.9, 128.3, 127.7, 125.5, 121.8, 110.2, 90.8, 51.0.

trans-N,N-diethyl-3-phenyl-2,3-dihydrobenzofuran-2-carboxamide (3p). Colorless oil, yield: 90%, Rf: 0.30 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.37-7.26 (m, 5H), 7.24-7.26 (m, 4H), 5.24 (d, J = 7.7 Hz, 1H), 5.18 (d, J = 7.7 Hz, 1H), 3.46-3.36 (m, 4H), 1.19-1.12 (m, 6H); 13C NMR (100 MHz, CDCl3) δ 167.8, 159.1, 142.2, 130.1, 129.1, 128.7, 128.6, 127.5, 125.4, 121.6, 109.8, 87.3, 51.5, 42.0, 40.9, 14.7, 13.0; HRMS Calculated For C19H21NO2Na [M+Na]+ 318.1470, found: 318.1466.

3-phenyl-2,3-dihydrobenzofuran (3q). Colorless oil, yield: 95%, Rf: 0.70 (ethyl acetate/petroleum ether = 1:10); 1H NMR (400 MHz, CDCl3) δ 7.35 (t, J = 7.2 Hz, 2H), 7.31 – 7.15 (m, 4H), 7.04 (d, J = 7.4 Hz, 1H), 6.90 (d, J = 15.7, 7.9 Hz, 2H), 4.93 (t, J = 9.2 Hz, 1H), 4.75 – 4.65 (m, 1H), 4.45 (dd, J = 8.6, 7.7 Hz, 1H); 13C NMR (101 MHz, CDCl3) δ 160.4, 143.0, 130.8, 129.0, 128.7, 128.0, 127.3, 125.5, 121.1, 109.9, 79.4, 48.7.
4. The synthesis of chiral 2,3-dihydrobenzofuran

![Chemical structure](image)

Under the nitrogen, 2-(1-tosylbenzyl)phenol 1 (0.20 mmol), chiral sulfonium salt (0.24 mmol) and Cs₂CO₃ (0.50 mmol) were placed in the Schlenk tube, and dry THF (3 mL) was added. The mixture was stirred at room temperature for 12 h. Then 5 mL water was added, the organic phase was separated and the aqueous layer was extracted with EtOAc. The combined organic phases were dried over Na₂SO₄, concentrated under the reduced pressure, and purified by flash chromatography on silica gel to afford the product trans-Ethyl 3-phenyl-2,3-dihydrobenzofuran-2-carboxylate (3a), 99% yield, 37% ee. The absolute configuration of 3a is not assigned. HPLC (AD-H, elute: Hexanes/i-PrOH = 95/5, detector: 254 nm, flow rate: 1.0 mL/min), t₁ = 5.8 min, t₂ = 6.6 min (maj).

5. References


6. Crystallographic Data of 3a

CCDC 876688 contains the structure and supplementary crystallographic data for the structure of trans-Ethyl 3-phenyl-2,3-dihydrobenzofuran-2-carboxylate 3a. These data can be obtained free of charge via [www.ccdc.com.ac.uk/data_request/cif](http://www.ccdc.com.ac.uk/data_request/cif) from the Cambridge Crystallographic Data Centre.
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
10 formula(s) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  S: 1-1  Re: 0-1

MC-4-22
12030311-2 23 (0.438) AM (Cen.2: 8.00; H:0.000;O,000.0,001.00; S:5(Mn, 2x1.00); Cen (11.28)

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</table>

S10
1H NMR MC-6-23G in CDCl₃/Yzo/gi/CQA-2011-03/4354/fid

1b. 1H NMR (CDCl₃, 400 MHz)

13C NMR MC-6-23G in CDCl₃/Yzo/gi/CQA-2011-03/4354/fid
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used
C: 0-150  H: 0-150  O: 3-3  S: 1-1  Re: 0-1

Minimum:  5.0  5.0  -200.0  200.0
Maximum: 5.0  5.0  200.0

Mass  Calc. Mass  mDa  PPM  DBE  i-PIT  Formula
351.1059  351.1055  0.4  1.1  12.5  1.4  C21 H19 O3 S

1b - HRMS
1H NMR MC-6-23H in CDCl3/Yzc/g/CQA-2011-03/4355/fid

1c - 1H NMR (CDCl3, 400 MHz)
13C NMR (CDCl3, 100 MHz)

13C NMR MC-6-23H in CDCl3/Yzc/g/CQA-2011-03/1409/fid
Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

21^{1} formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:
C: 0-150  H: 0-150  O: 3-3  S: 1-1  Re: 0-1

MC=6.23H
12030320 37 (0.677) AM (Cen.2, 50.50, H:0,000,0.0,01,00; Sm (Mn, 2x1.00); Crn (22.41)

Minimum:  
Maximum:  

Mass  Calc. Mass  mDa  PPM  DBE  t-FIT  Formula
351.1048  351.1055  -0.7  -2.0  12.5  5.0  C21 H19 O3 S
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron ions
21 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  S: 1-1  Re: 0-1

MC-6-23B
1203031429 (0.540) AM (C35.2, 80.00, H:5000.0,0.00,1.00); Sm (Mn, 2.1.00); Cn (1:137)
6
1: TOF MS ES-

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1d - HRMS

1d - HRMS

Electronic Supplementary Material (ESI) for Chemical Communications
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S16
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM  /  DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
21 formula(s) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 4-4  S: 1-1  Re: 0-1

MC-623A
12003013 37 (0.684) AM (Ca 2, 80.00, H 5, 5000 0.00 0.10 0.00; Sm, 2x1.00; Cm (30.47)

Minimum: 5.0  5.0
Maximum: -200.0  200.0

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OMe

SO2Tol

OH

1e - HRMS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  F: 3-3  S: 1-1  Re: 0-1

MC-6-23C
12030315 20 (0.372) AM (Cl:2. 89.02, H:5.000 0.00, 0.00, 1.00); Sm (Mn, 2x1.02); Cm (15:50)

Minimum:
5.0  5.0  -200.0
Maximum:
Calc. Mass mDa  ppm  DBE  I-FIT  Formula
405.0765  405.0772  -0.7  -1.7  12.5  9.1  C21 H16 O3 F3 S

1f HRMS

$^{19}$F NMR (CDCl$_3$, 377 MHz)

$^{19}$F NMR MC-6-23C in CDCl$_3$/Yzc/gl/CQA-2011-03/2527/fid
**S21**

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

**13C NMR (CDCl$_3$, 100 MHz)**

**Electronic Supplementary Material (ESI) for Chemical Communications**

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Elemental Composition Report
Single Mass Analysis (displaying only valid results)
Tolerance = 50.0 PPM   /   DBE: min = -200.0, max = 200.0
Selected filters: None
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100    H: 0-150    O: 3-3    Na: 1-1    S: 1-1    F: 1-1
Minimum:                  -200.0   Maximum:    5.0       50.0      200.0
Mass        Calc. Mass      mDa       PPM       DBE       i-FIT
Formula
379.0781    379.0780        0.1       0.3       11.5      0.9         C20
H17 03 Na S F
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 0-3  S: 1-1  Br: 1-1  Re: 0-1

MC-6-233
12000316 28 (0.521) AM (C63, 80.00, H6,5000, 0.005, 1.00), 9m (Mn, 2x1.00), Cm (2128)

Minimum: 5.0
Maximum: 200.0

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Br

SO₂Tol

1h +HRMS
Electronic Supplementary Material (ESI) for Chemical Communications
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1H NMR: 1H NMR (CDCl₃, 400 MHz)

13C NMR: 13C NMR (CDCl₃, 100 MHz)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
21 formula(s) evaluated with 1 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-150  H: 0-150  O: 4-4  S: 1-1  Re: 0-1

MC-6.23E
1200317 1 (0.019) AM (Cen,2, 80.00, H2,0000,0.00,1.00), Sm (Mn, 2x1 00), Cm (1:13)

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MeO

SO2Tol

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

$^{13}$C NMR (CDCl$_3$, 100 MHz)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 O: 3-3 S: 1-1 Cl: 1-1
MC-0-466
12030691 38 (0.710) AM (Cen,2, 80.00, H5,5000,0.0,1.00); Sm (Mn, 2x1.00); Cm (R:38)
144.9634

Minimum: 100
Maximum: 100
Mass Calc. Mass mDa PPM DBE 1-VIT Formula
311.0512 311.0509 0.3 1.0 7.5 0.1 CI5 HI6 O3 S CI

1j-HRMS
1H NMR for 4-methylbenzenesulfonic acid in CDCl₃ (400 MHz)

13C NMR for 4-methylbenzenesulfonic acid in CDCl₃ (100 MHz)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-150 H: 0-150 O: 3-3 S: 1-1 Re: 0-1

MC-6.35
12030321 15 (0.278) AM (Cn2. 80.00, H8.5000; 0.00; 1.00); Sm (Mm, 2x1.00); Cn (8.31)

1: TOF MS ES-
1.54e4

Min: 289.0001 289.0008 0.3 1.0 8.5 18.9 C16 H17 O3 5

SO2Tol

1k-I-HRMS
1H NMR DY-5-53B in CDCl3

1H NMR (CDCl3, 400 MHz)

13C NMR (CDCl3, 100 MHz)

13C NMR DY-5-53 in CDCl3
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  S: 1-1  Re: 0-1

MC-A-23F
12030318 25 (0.463) AM (Cen.2, 80.00, H,8000,0.0,00,1.00); Sm (Min, 2x1.00); Cm (18:29)

Minimum: 5.0 5.0 -200.0
Maximum: 200.0

Mass  Calc. Mass  m/z  PPM  DBE  I-FIT  Formula
317.1216 317.1211 0.5 1.6 8.6 1.3 C18 H21 O3 S

11-HRMS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-150 H: 0-150 O: 3-3 Na: 1-1 Re: 0-1

MC-6-28
12030121 11 (0.205) AM (Cen.2, 80.00, Hl,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Clm (7:12)

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3a - HMRS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Re: 0-1

MG-5-31A
12030213 70 (1.303) AM (Cen.2, 80.00, HI,5000.0,0.00,1.00); Sm (Ms, 2r1.00); Crn (45.83)

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3b - HRMS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Re: 0-1

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
 305.1156  305.1154  0.2  0.7  9.5  6.3  C18 H18 O3 Na

3c - HRMS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Re: 0-1

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3d - HRMS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 O: 4-4 Na: 1-1 Re: 0-1

MG-ESI-TOF MS ESI+
7.97e3

Minimum: 5.0 5.0 200.0
Mass Calc. Mass mDa PPM DBE 1-FIT Formula
321.1109 321.1103 0.6 1.9 9.5 6.4 C18 H18 O4 Na

3e - HRMS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass

Elements Used:
C: 0-150  H: 0-150  O: 3-3  F: 3-3  Na: 1-1  Re: 0-1

Minimum: 359.0862  Mass Calc. 359.0871  nDa -0.9  PPM -2.5  DBE 9.5  i-FIT 2.0  Formula C18 H15 O3 F3 Na

1H NMR (CDCl₃, 377 MHz)

19F NMR CDCl₃ 377 MHz in CDCl₃, CQUI-2011-03 treated with [19F]HCl in CDCl₃
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Br: 1-1  Re: 0-1

MC-6.31C
12000220 16 (0.288) AM (Cem,2, 80.00, H,5000.0, 0.00,1.00); Sm (Mn, 2x1.00); Cm (10.21)

Minimum: 100
Maximum: 260.0000

Mass Calc. Mass mDa PPM DBE i-FIT Formula
369.0110 369.0102 0.8 2.2 9.5 0.3 C17 H15 O3 Na Br

3h - HRMS
**Elemental Composition Report**

**Single Mass Analysis (displaying only valid results)**

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0  
Selected filters: None

Monoisotopic Mass, Even Electron Ions  
16 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass  
Elements Used:  
C: 0-150  
H: 0-150  
O: 4-4  
Na: 1-1  
Re: 0-1

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![3i-HRMS](image)

**MC-6-33A**

1203221 7 (0.130) AM (Cen, 2, 80.00, H1,9009, 0.00, 1.00); Sn (Min, 2x1.00, Cn (7:14)

1. TOF MS ES+ 10.0e4
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Re: 0-1

MC-6-39
12030218 22 (0.409) AM (Cen, 60.90, Hi, S, 0.00, 0.00, 1.00), Sm (Mn, 2x1.00); Cm (13.22)

Mass  Calc. Mass  mOA  PPM  DBE  1-FIT  Formula
243.0995  243.0997  -0.2  -0.8  5.5  2775043.8  C13 H16 O3 Na

\[ \text{3k - HRMS} \]

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Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Re: 0-1

MC-6-338
12030219 34 (0.633) AM (Cen,2, 80.00, H;0.00:0.00:0.00:1.00); Sm (Mn, 2x1.00); Cm (21:37)

1: TOF MS ES+ 8.49e3

Minimum:  5.0  Maximum:  200.0
Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
271.1317  271.1310  0.7  2.6  5.5  34.2  C15 H2O O3 Na

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

$^{13}C$ NMR (CDCl$_3$, 100 MHz)

$^\text{CO}_2\text{Me}$
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Re: 0-1

MC-6-33C
12030000 29 (0.538) AM (Cen:2, 50.00, H:5000.0, 0.0, 1.00); Sm (Mn, 2x1.0); Cm (15.31)
277.0846

Minimum: 
Maximum:
-200.0

Mass Calc. Mass mDa PPM DBE i-FIT Formula
277.0846 277.0841 0.5 1.8 9.5 27.7 C16 H14 O3 Na

3m - HRMS
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM  /  DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150  H: 0-150  O: 3-3  Na: 1-1  Re: 0-1

MC-6-34A
12030301 90 (0.922) AM (Cen.2, 80.00, Hc,5000.0.0.00:1.00); Sm (Mr, 2x1.00); Cn (28.57)
303.1152

100
%

187.0005  269.0200  321.1141  354.1207

0  200  250  275  300  325  350  375  400  425  450  475  500  525  550  575  600  625  650  675

Minimum:
5.0
Mass Calc. Mass mDa PPM DBE i-FIT Formula
353.1152  353.1154  +0.2  13.5  C22 H18 O3 Na

3n-HRMS
$^{30}$-$^1$H NMR (CDCl$_3$, 400 MHz)

$^{13}$C NMR (CDCl$_3$, 100 MHz)
1H NMR (CDCl₃, 400 MHz)

3p - 1H NMR (CDCl₃, 400 MHz)

13C NMR (CDCl₃, 100 MHz)
**Elemental Composition Report**

Single Mass Analysis (displaying only valid results)
Tolerance = 50.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron ions
12 formula(s) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100  H: 0-150  N: 1-1  O: 2-2  Na: 1-1

<table>
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<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>PPM</th>
<th>DBE</th>
<th>1-PPP</th>
<th>Formula</th>
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</thead>
<tbody>
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<td>318.1466</td>
<td>318.1470</td>
<td>-0.4</td>
<td>-1.3</td>
<td>9.4</td>
<td>C19 H21 N 02 Na</td>
</tr>
</tbody>
</table>

3p - HRMS

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