Supporting Information
for DOI: 10.1055/s-0035-1560069
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Supporting Information

Copper(II)-Catalyzed Oxidative Esterification of Substituted
p-Cresols under Ligand- and Additive-Free Conditions

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1. General Information

Unless otherwise indicated, all reagents were obtained from commercial sources and used as received without further purification. All reactions were carried out in oven-dried glassware and monitored by thin layer chromatography (TLC, pre-coated silica gel plates containing HF254). All solvents were only dried over 4 Å molecular sieves. Most reaction products were purified by silica gel chromatography with elution of petroleum ether/ethyl acetate. Melting points were determined using an open capillaries and uncorrected. NMR spectra were determined on Bruker AV400 in CDCl₃ with TMS as internal standard for ¹H NMR (400 MHz) and ¹³C NMR (100 MHz), respectively. HRMS were carried out on a QSTAR Pulsar I LC/TOF MS mass spectrometer.

2. General Procedure for The Cu(OAc)₂-Catalyzed Esterification

A mixture of substrate (1.0 mmol), carboxylic acid (1.0 mmol) and Cu(OAc)₂ (10 mol%) in CH₃CN (4.0 mL) was stirred under ambient air at 75 °C for specified time. The reaction mixture was concentrated in vacuo to give a residue, to which were added hydrochloric acid (10 mL, 2%) and ethyl acetate (15 mL). The organic phase was separated, and the aqueous phase was further extracted with ethyl acetate (5 mL, twice). The combined organic layers were washed with saturated aqueous NaHCO₃ (20 mL) and brine (20 mL). The ethyl acetate was dried over anhydrous Na₂SO₄ and concentrated in vacuo to give a residue, which was purified by column chromatography on silica gel (eluents: petroleum ether / ethyl acetate, 30:1) to provide the corresponding product.

3. Experimental Data of Products (Table 2 and Table 3)

Table 2:

<table>
<thead>
<tr>
<th>Compound</th>
<th>Description</th>
<th>Mp</th>
<th>Yields (%)</th>
<th>¹H NMR (400 MHz, ppm)</th>
<th>¹³C NMR (100 MHz, ppm)</th>
<th>HRMS (EI): m/z [M⁺] calcd. for CₓHᵧOₘ</th>
<th>HRMS (EI): m/z [M⁺] found</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-hydroxy-3,5-dimethylbenzyl benzoate (3a)</td>
<td>Yellow solid, mp 60–63 °C</td>
<td>0.20 g (79%)</td>
<td>δ 2.26 (s, 6H), 4.67 (br s, 1H), 5.23 (s, 2H), 7.08 (s, 2H), 7.39–7.46 (m, 2H), 7.53–7.57 (m, 1H), 8.03–8.09 (m, 2H)</td>
<td>δ 16.0 (2C), 66.9, 123.2 (2C), 128.4 (2C), 128.5, 129.3 (2C), 129.7 (2C), 130.2, 133.0, 152.4, 166.7</td>
<td>m/z [M⁺] calcd. for C₁₆H₁₆O₃: 256.1099; found: 256.1100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4-hydroxy-3,5-dimethylbenzyl 4-methylbenzoate (3b)</td>
<td>Pale yellow solid, mp 98–100 °C</td>
<td>0.22 g (81%)</td>
<td>δ 2.26 (s, 6H), 2.40 (s, 3H), 4.66 (br s, 1H), 5.21 (s, 2H), 7.07 (s, 2H), 7.22 (d, J = 8.0 Hz, 2H), 7.94 (d, J = 8.0 Hz, 2H)</td>
<td>δ 16.0 (2C), 66.9, 123.2 (2C), 128.4 (2C), 128.5, 129.3 (2C), 129.7 (2C), 130.2, 133.0, 152.4, 166.7</td>
<td>m/z [M⁺] calcd. for C₁₆H₁₆O₃: 256.1099; found: 256.1100</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm), δ 16.0 (2C), 21.7, 66.7, 123.2 (2C), 127.6, 127.7, 129.1 (2C), 129.2 (2C), 129.8 (2C), 143.6, 152.4, 166.8; HRMS (EI): m/z [M$^+$] calcd. for C$_{17}$H$_{16}$O$_3$: 270.1256; found: 270.1257.

4-hydroxy-3,5-dimethylbenzyl 4-methoxybenzoate (3c): Pale yellow solid, mp 68–70 °C, 0.25 g (86%); $^1$H NMR (400 MHz, CDCl$_3$, ppm), δ 2.26 (s, 6H), 3.85 (s, 3H), 4.51 (br s, 1H), 5.20 (s, 2H), 6.90 (d, J = 8.8 Hz, 2H), 7.07 (s, 2H), 8.01 (d, J = 8.8 Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm), δ 16.0 (2C), 55.4, 66.6, 113.6 (2C), 122.7, 123.2 (2C), 127.8, 129.2 (2C), 131.8 (2C), 152.3, 163.4, 166.4; HRMS (ESI): m/z [M+Na$^+$] calcd. for C$_{17}$H$_{18}$O$_4$Na: 309.1103; found: 309.1107.

4-hydroxy-3,5-dimethylbenzyl 4-chlorobenzoate (3d): White solid, mp 90–92 °C, 0.21 g (73%); $^1$H NMR (400 MHz, CDCl$_3$, ppm), δ 2.26 (s, 6H), 4.69 (br s, 1H), 5.22 (s, 2H), 7.07 (s, 2H), 7.39 (d, J = 8.8 Hz, 2H), 7.99 (d, J = 8.8 Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm), δ 16.0 (2C), 67.1, 123.2 (2C), 127.3, 128.7 (2C), 128.8, 129.4 (2C), 131.1 (2C), 139.4, 152.5, 165.8; HRMS (EI): m/z [M$^+$] calcd. for C$_{16}$H$_{15}$O$_3$Cl: 290.0710; found: 290.0709.

4-hydroxy-3,5-dimethylbenzyl 4-fluorobenzoate (3e): Yellow solid, mp 83–86 °C, 0.19 g (69%); $^1$H NMR (400 MHz, CDCl$_3$, ppm), δ 2.26 (s, 6H), 4.66 (br s, 1H), 5.21 (s, 2H), 7.07–7.12 (m, 4H), 8.05–8.09 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm), δ 16.0 (2C), 67.0, 115.5 (d, J = 19.1 Hz, 2C), 123.2, 126.5, 127.4, 129.3 (2C), 132.2 (d, J = 9.2 Hz, 2C), 152.5, 165.7, 167.0; HRMS (EI): m/z [M$^+$] calcd. for C$_{16}$H$_{15}$O$_3$F: 274.1005; found: 274.1004.

4-hydroxy-3,5-dimethylbenzyl 4-nitrobenzoate (3f): Yellow
solid, mp 113–116 °C, 0.13 g (42%); ¹H NMR (400 MHz, CDCl₃, ppm), δ 2.27 (s, 6H), 4.73 (br s, 1H), 5.27 (s, 2H), 7.09 (s, 2H), 8.20–8.28 (m, 4H); ¹³C NMR (100 MHz, CDCl₃, ppm), δ 16.0 (2C), 67.8, 123.4 (2C), 123.5 (2C), 126.8, 129.5 (2C), 130.8 (2C), 135.7, 150.5, 152.7, 164.7; HRMS (EI): m/z [M⁺] calcd. for C₁₆H₁₃NO₅: 301.0950; found: 301.0951.

3g

**4-hydroxy-3,5-dimethylbenzyl 2-methylbenzoate (3g):** Pale yellow solid, mp 69–70 °C, 0.19 g (70%); ¹H NMR (400 MHz, CDCl₃, ppm), δ 2.26 (s, 6H), 2.60 (s, 3H), 4.64 (br s, 1H), 5.21 (s, 2H), 7.08 (s, 2H), 7.20–7.24 (m, 2H), 7.35–7.41 (m, 1H), 7.89–7.95 (m, 1H); ¹³C NMR (100 MHz, CDCl₃, ppm), δ 15.9 (2C), 21.8, 66.6, 123.2 (2C), 125.7, 127.7, 129.2 (2C), 129.7, 130.7, 131.7, 132.0, 140.3, 152.3, 167.7; HRMS (ESI): m/z [M+Na⁺] calcd. for C₁₇H₁₈O₃Na: 293.1154; found: 293.1160.

3h

**4-hydroxy-3,5-dimethylbenzyl 2-phenylacetate (3h):** Pale yellow solid, mp 52–53 °C, 0.18 g (66%); ¹H NMR (400 MHz, CDCl₃, ppm), δ 2.23 (s, 6H), 3.65 (s, 2H), 4.67 (br s, 1H), 5.00 (s, 2H), 6.94 (s, 2H), 7.27–7.35 (m, 5H); ¹³C NMR (100 MHz, CDCl₃, ppm), δ 15.9 (2C), 41.4, 66.7, 123.3 (2C), 127.1, 127.3, 128.6 (2C), 129.1 (2C), 129.4 (2C), 134.0, 152.4, 171.7; HRMS (ESI): m/z [M+Na⁺] calcd. for C₁₇H₁₈O₃Na: 293.1154; found: 293.1156.

3i

**4-hydroxy-3,5-dimethylbenzyl acrylate (3i):** Pale yellow solid, mp 46–48 °C, 0.15 g (72%); ¹H NMR (400 MHz, CDCl₃, ppm), δ 2.25 (s, 6H), 4.68 (br s, 1H), 5.01 (s, 2H), 5.82 (dd, J₁ = 1.6 Hz, J₂ = 10.4 Hz, 1H), 6.14 (dd, J₁ = 10.4 Hz, J₂ = 17.6 Hz, 1H), 6.43 (dd, J₁ = 1.6 Hz, J₂ = 17.6 Hz, 1H), 7.02 (s, 2H); ¹³C NMR (100 MHz, CDCl₃, ppm), δ 15.9 (2C), 66.5, 123.2 (2C), 127.3, 128.5, 129.3 (2C), 131.0, 152.5, 166.3; HRMS (EI): m/z [M⁺] calcd. for C₁₂H₁₄O₃: 206.0943; found: 206.0944.
4-hydroxy-3,5-dimethylbenzyl acetate (3j): Pale yellow solid, mp 73–75 °C, 0.15 g (76%); \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm), \(\delta\) 2.08 (s, 3H), 2.25 (s, 6H), 4.70 (br s, 1H), 4.97 (s, 2H), 7.00 (s, 2H); \(^1\)C NMR (100 MHz, CDCl\(_3\), ppm), \(\delta\) 15.9 (2C), 21.1, 66.5, 123.3 (2C), 127.4, 129.3 (2C), 152.4, 171.2; HRMS (EI): \(m/z\) [M\(^+\)] calcd. for C\(_{11}\)H\(_{14}\)O\(_3\): 194.0943; found: 194.0944.

4-hydroxy-3,5-dimethylbenzyl propionate (3k): Colorless oil, 0.14 g (69%); \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm), \(\delta\) 1.147 (t, \(J = 7.6\) Hz, 3H), 2.25 (s, 6H), 2.35 (q, \(J = 7.6\) Hz, 2H), 4.67 (br s, 1H), 4.98 (s, 2H), 6.99 (s, 2H); \(^1\)C NMR (100 MHz, CDCl\(_3\), ppm), \(\delta\) 9.1, 15.9 (2C), 27.7, 66.3, 123.3 (2C), 127.5, 129.2 (2C), 152.4, 174.4; HRMS (EI): \(m/z\) [M\(^+\)] calcd. for C\(_{12}\)H\(_{16}\)O\(_3\): 208.1099; found: 208.1098.

4-hydroxy-3,5-dimethylbenzyl isobutyrate (3l): Pale yellow solid, mp 50–52 °C, 0.13 g (58%); \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm), \(\delta\) 1.17 (d, \(J = 7.2\) Hz, 6H), 2.24 (s, 6H), 2.53–2.60 (m, 1H), 4.69 (br s, 1H), 4.97 (s, 2H), 6.98 (s, 2H); \(^1\)C NMR (100 MHz, CDCl\(_3\), ppm), \(\delta\) 15.9 (2C), 19.0 (2C), 34.0, 66.2, 123.1 (2C), 127.8, 129.0 (2C), 152.2, 177.2; HRMS (ESI): \(m/z\) [M+Na\(^+\)] calcd. for C\(_{13}\)H\(_{18}\)O\(_3\)Na: 245.1154; found: 245.1155.

4-hydroxy-3,5-dimethylbenzyl cyclohexanecarboxylate (3m): Pale brown solid, mp 54–55 °C, 0.09 g (36%); \(^1\)H NMR (400 MHz, CDCl\(_3\), ppm), \(\delta\) 1.18–1.93 (m, 10H), 2.24 (s, 6H), 2.28–2.35 (m, 1H), 4.67 (br s, 1H), 4.96 (s, 2H), 6.97 (s, 2H); \(^1\)C NMR (100 MHz, CDCl\(_3\), ppm), \(\delta\) 15.9 (2C), 25.5 (2C), 25.8, 29.0 (2C), 43.3, 66.0, 123.1 (2C), 127.8, 129.0 (2C), 152.2, 176.2; HRMS (ESI): \(m/z\) [M+Na\(^+\)] calcd. for C\(_{16}\)H\(_{22}\)O\(_3\)Na: 285.1467; found: 285.1461.
4-hydroxy-3-methoxy-5-methylbenzyl benzoate (4b): White solid, mp 75–76 °C, 0.18 g (68%); $^1$H NMR (400 MHz, CDCl$_3$, ppm), $\delta$ 2.27 (s, 3H), 3.90 (s, 3H), 5.25 (s, 2H), 5.73 (br s, 1H), 6.82–6.88 (m, 2H), 7.41–7.45 (m, 2H), 7.53–7.57 (m, 1H), 8.05–8.07 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm), $\delta$ 15.4, 56.1, 66.9, 108.9, 123.8, 123.9, 126.8, 128.4 (2C), 129.7 (2C), 130.3, 133.0, 143.9, 146.2, 166.6; HRMS (ESI): $m/z$ [M+Na$^+$] calcd. for C$_{16}$H$_{16}$O$_4$Na: 295.0946; found: 295.0938.

4-hydroxy-3,5-dimethoxybenzyl benzoate (4c): Yellow solid, mp 79–82 °C, 0.18 g (61%); $^1$H NMR (400 MHz, CDCl$_3$, ppm), $\delta$ 3.91 (s, 6H), 5.27 (s, 2H), 5.56 (br s, 1H), 6.70 (s, 2H), 7.42–7.47 (m, 2H), 7.54–7.58 (m, 1H), 8.03–8.09 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm), $\delta$ 56.4 (2C), 67.3, 105.6 (2C), 127.0, 128.4 (2C), 129.7 (2C), 130.2, 133.1, 134.9, 147.0, 166.6; HRMS (ESI): $m/z$ [M+Na$^+$] calcd. for C$_{16}$H$_{16}$O$_5$Na: 311.0895; found: 311.0893.

3-(tert-butyl)-4-hydroxy-5-methylbenzyl benzoate (4d): Yellow oil, 0.17 g (57%); $^1$H NMR (400 MHz, CDCl$_3$, ppm), $\delta$ 1.43 (s, 9H), 2.27 (s, 3H), 4.84 (br s, 1H), 5.25 (s, 2H), 7.12 (d, $J$ = 1.6 Hz, 1H), 7.23 (d, $J$ = 1.6 Hz, 1H), 7.41–7.45 (m, 2H), 7.53–7.57 (m, 1H), 8.04–8.09 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$, ppm), $\delta$ 16.0, 29.7 (3C), 34.6, 67.2, 123.2, 125.9, 127.2, 128.3 (2C), 129.2, 129.7 (2C), 130.4, 132.9, 135.8, 152.9, 166.6; HRMS (ESI): $m/z$ [M+Na$^+$] calcd. for C$_{19}$H$_{22}$O$_3$Na: 321.1467; found: 321.1459.

3,5-di-tert-butyl-4-hydroxybenzyl benzoate (4e): Orange solid, mp
80–82 °C, 0.12 g (36%); ¹H NMR (400 MHz, CDCl₃, ppm), δ 1.46 (s, 18H), 5.27 (s, 2H), 5.29 (br s, 1H), 7.27 (s, 2H), 7.40–7.47 (m, 2H), 7.51–7.58 (m, 1H), 8.05–8.11 (m, 2H); ¹³C NMR (100 MHz, CDCl₃, ppm), δ 30.3 (6C), 34.3 (2C), 67.6, 125.8 (2C), 126.6, 128.3 (2C), 129.7 (2C), 130.5, 132.9, 136.0, 154.0, 166.7; HRMS (ESI): m/z [M+Na⁺] calcd. for C₂₂H₂₈O₃Na: 363.1936; found: 363.1935.

4. Copies of Spectra
Elemental Composition Report

Multiple Mass Analysis: 26 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron ions
147 formula(s) evaluated with 26 results within limits (up to 1000 closest results for each mass)
Elements Used:
C: 0-16 H: 0-16 O: 0-3

Minimum: 3.00  Maximum: 100.00
-1.5

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<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
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</tr>
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<tbody>
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<td>256.1100</td>
<td>12.51</td>
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<td>2.5</td>
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</tbody>
</table>
Elemental Composition Report

Multiple Mass Analysis: 22 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
136 formula(e) evaluated with 22 results within limits (up to 1000 closest results for each mass)
Elements Used:
C: 0.17  H: 0.18  O: 0.3

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<td>6.29</td>
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<td>0.4</td>
<td>5.0</td>
<td>0.2</td>
<td>C17H18O3</td>
</tr>
</tbody>
</table>

3b

3c

[Chemical structures and mass spectra graphs]
Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = - 1.5, max = 100.0
Element prediction: Off
Number of isotopic peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron ions
11 formula(s) evaluated with 1 result within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-17  H: 0-50  O: 0-4  Na: 0-1

YF-JI

JYF-Z2N-3 12 (0.168) Cm (7:12)

ECUST Institute of Fine Chem

10-Apr-2015
15:01:54
1: TOF MS/MS+
3.06e+003

Minimum: 303.2089
Maximum: 309.1107

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  i-FIT (Norm) Formula
309.1107  309.1103  0.4  1.3  8.5  49.2  0.0  C17 H18 O4 Na
## Elemental Composition Report

**Multiple Mass Analysis: 38 mass(es) processed**

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electronic ions
663 formula(e) evaluated with 52 results within limits (up to 1000 closest results for each mass)

Elements Used:
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- H: 0-15
- O: 0-3
- 35Cl: 0-1
- 37Cl: 0-1

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<th>Mass</th>
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<td>2.2</td>
<td>C16 H15 O3 35Cl</td>
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</tbody>
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![Chemical Structure Image](image-url)
### Elemental Composition Report

**Multiple Mass Analysis: 15 mass(es) processed**

- **Tolerance:** 5.0 mDa / **DBE:** min = -1.5, max = 50.0
- **Element prediction:** Off

**Monoisotopic Mass, Odd and Even Electron Ions**

164 formula(e) evaluated with 26 results within limits (up to 1000 closest results for each mass)

**Elements Used:**
- C: 0-16
- H: 0-15
- O: 0-3
- F: 0-1

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<th>Mass</th>
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Elemental Composition Report

Multiple Mass Analysis: 46 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
375 formula(s) evaluated with 52 results within limits (up to 1000 closest results for each mass)
Elements Used:
C: 0-16    H: 0-15    N: 0-1    O: 0-5

Minimum: 1.50    Maximum: 100.00    R.A. 5.0    10.0 -1.5    50.0

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3g
Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM /
DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
15 formulas evaluated with 1 result(s) within limits (up to 1 best isotopic matches for each mass)
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YFY-ZNN-16 (0.402) Cm (46.6)

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Elemental Composition Report

Multiple Mass Analysis: 23 mass(es) processed
Tolerance = 5.0 mDa
DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron ions
117 formula(e) evaluated with 23 results within limits (up to 1000 closest results for each mass)
Elements Used:
C: 0-12  H: 0-14  O: 0-3

Minimum: 3.00
Maximum: 100.00  5.0  10.0  50.0

Mass  RA  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
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Elemental Composition Report

Multiple Mass Analysis: 22 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
108 formula(s) evaluated with 22 results within limits (up to 1000 closest results for each mass)
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C: 0-11   H: 0-14   O: 0-3

Minimum: 3.00   Maximum: 100.00
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<th>Calc. Mass</th>
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<td>7.13</td>
<td>194.0943</td>
<td>0.1</td>
<td>0.5</td>
<td>5.0</td>
<td>3.0</td>
<td>C11 H14 O3</td>
</tr>
</tbody>
</table>

---

3k
**Elemental Composition Report**

**Multiple Mass Analysis: 27 mass(es) processed**
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron ions
151 formula(e) evaluated with 27 results within limits (up to 1000 closest results for each mass)

Elements Used:
C: 0-12  H: 0-16  O: 0-3

Minimum:  3.00  5.0  10.0  -1.5
Maximum:  100.00  10.0  50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>RA</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>208.1098</td>
<td>13.09</td>
<td>208.1099</td>
<td>-0.1</td>
<td>-0.5</td>
<td>5.0</td>
<td>1.3</td>
<td>C12 H16 O3</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM  /  DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 2

Monoisotopic Mass, Even Electron Ions
38 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0.22  H: 0.50  O: 0.5  Na: 0.1

Minimum:  -1.5
Maximum:   300.0  50.0  100.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DEB</th>
<th>I-FIT</th>
<th>I-FIT (Theo)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>245.1155</td>
<td>245.1154</td>
<td>0.1</td>
<td>0.4</td>
<td>4.5</td>
<td>5.7</td>
<td>0.0</td>
<td>Cl3 H18 O3 Na</td>
</tr>
</tbody>
</table>

3m
### Elemental Composition Report

**Single Mass Analysis**

- **Tolerance**: 50.0 PPM
- **DBE**: min = -1.5, max = 100.0
- **Element prediction**: Off
- **Number of isotope peaks used for I-FIT**: 2

**Monoisotopic Mass, Even Electron Ions**

45 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)

**Elements Used:**

- C: 0-22
- H: 0-50
- O: 0-5
- Na: 0-1

**Instrument:** YF-JL

**Operator:** ECUST Institute of Fine Chem

**Date:** 15-Apr-2018 20:49:32

**Method:** TOF MS ESI-

**Retention Time:** 8.23m

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>i-FIT (Shore)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>285.1461</td>
<td>285.1467</td>
<td>-0.6</td>
<td>-2.1</td>
<td>5.5</td>
<td>18.6</td>
<td>0.0</td>
<td>C16 H22 O3 Na</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 2

Monoisotopic Mass, Even Electron ions
14 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:
C: 0-17  H: 0-50  O: 0-4  N: 0-1

CYP-227/12-51 (0.416) Cm (45.51)

ECUST Institute of Fine Chem
16-Apr-2015
1: TOF MS EQ-
1.87e+003

Minimum: 500.0 50.0 -1.5
Maximum: 100.0

Mass  Calc. Mass mDa PPM DBE i-FIT i-FIT (Stoich) Formula

295.0938 295.0946 -0.8 -2.7 8.5 25.9 0.0 C\textsubscript{16} H\textsubscript{16} O\textsubscript{4} N

4c

![Chemical Structure Image]

![Mass Spectrogram Image]
**Elemental Composition Report**

**Single Mass Analysis**
- Tolerance = 50.0 PPM  /  DBE: min = -1.5, max = 100.0
- Element prediction: Off
- Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

**Elements Used:**
- C: 0-17  H: 0-50  O: 0-5  Na: 0-1

**Instrument:**
- VY-JI  ECUST Institute of Fine Chem

**Date:**
- 16-Apr-2015  10:28:12
- 1: TOF MS ES+
  4.86hH003

**Ions:**
- JYF-ZZ210-32 (0.290) Cm (29.33)

**Mass Table:**

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>i-FIT (d16)</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>311.0893</td>
<td>311.0895</td>
<td>-0.2</td>
<td>-0.6</td>
<td>8.5</td>
<td>27.8</td>
<td>0.0</td>
<td>C16 H16 O5 Na</td>
</tr>
</tbody>
</table>
Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monooctopletic Mass, Even Electron ions
22 formula(s) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:
C: 0-19  H: 0-50  O: 0-5  Na: 0-1

YFJl  ECDST Institute of Fine Chem
JYF-ZZ94 27 (0.250) Cm (27-42)
16-Apr-2015
10:40:46
1. TOF MS/ES+ 4.98e+083

Minimum: 321.1459
Maximum: 321.1467

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  i-FIT (kcal mol⁻¹) Formula
321.1459  321.1467  -0.8  -2.5  8.5  38.9  0.0  C19 H22 O3 Na
Elemental Composition Report

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 2

Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-50 O: 0-5 Na: 0-1

VF-JJ

ECUST Institute of Fine Chem

JYF-Z2H-15 14 (0.179) Cm (12.19)

16-Apr-2015
20:44:06
1: TOF MS ES+
4.74e1003

Minimum:
Maximum:

Mass   Calc. Mass   mDa   PPM   DBE   I-FIT   I-FIT (Sturm) Formula
363.1935   363.1936   -0.1   -0.3   0.5   10.0  0.0  C25 H20 O3 Na
5. References