Supporting Information

Efficient Synthesis of Carboxylic Esters via Palladium(II)-Catalyzed Direct Alkoxy carbonylation of Arenes with CO and Alcohols

Bin Liu,*a and Bing-Feng Shi,*a,b

a Department of Chemistry, Zhejiang University, Hangzhou 310027, China
b State Key Laboratory of Bioorganic & Natural Products Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Science, Shanghai 200032, China.
Fax: 0086-571-87951895.
E-mail: bfshi@zju.edu.cn.

Table of Contents

S1
General Information

S2
Experimental Procedure

S2-3
Optimization of Reaction Conditions

S2-3
General Procedure for carbonylation of 1 with CO and Alcohol

S3
Characterization Data of Products

S4-S6
NMR Analysis of Products

S7-S17
HRMS Analysis of Products

S18-S22
A: General Information and Starting Materials

**General Information.** Dioxane was dried by sodium and freshly distilled. The other materials and solvents were purchased from Aladdin and other commercial suppliers and used without additional purification. NMR spectra were recorded on a Brüker Avance operating for $^1$H NMR at 400 MHz, and $^{13}$C NMR at 100 MHz using TMS as internal standard. Chemical shifts were given relative to CDCl$_3$(7.26 ppm for $^1$H NMR, 77.16 ppm for $^{13}$C NMR). Data are represented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz). Mass spectroscopy data of the products were collected on an HRMS-TOF instrument or a low-resolution MS instrument using EI ionization. All substrates were prepared according to the following literature.$^1$

B: General Procedure for carbonylation of 1 with CO and Alcohol

\[
\begin{align*}
\text{1a} & \quad \text{10 mol\% Pd(OAc)$_2$} \\
& \quad \text{oxidant, additive} \\
& \quad \text{CO:O$_2$ (4:1, 1 atm)} \\
& \quad 1,4-	ext{dioxane, } T, 8 \text{ h} \\
\rightarrow & \quad \text{2a} \\
& \quad \text{2a}
\end{align*}
\]

A mixture of substrate 1 (0.2 mmol), Pd(OAc)$_2$ (10 mmol %), CuBr$_2$ (0.2 mmol), NaOAc (0.3 mmol), alcohol (3.0 mmol) and Dioxane (2.0 mL) in a 50 mL Schlenk tube (purged with CO:O$_2$ = 4:1) was heated at 100 °C for 24 hours. The reaction mixture was cooled to rt, and concentrated in vacuo. The residue was purified by chromatography on silica gel to afford the desired product 2.

---

C: Characterization Data of Products

Pentyl 2-(pyridin-2-yl)benzoate (2a). Yellow oil. Spectral data were consistent with literature values.\(^2\) \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 8.65 \, (d, \, J = 4.0 \, Hz, \, 1H), \, 7.85 \, (d, \, J = 8.0 \, Hz, \, 1H), \, 7.76 \, (d, \, J = 8.0 \, Hz, \, 1H), \, 7.57-7.56 \, (m, \, 2H), \, 7.46 \, (t, \, J = 8.0 \, Hz, \, 2H), \, 7.28 \, (d, \, J = 8.0 \, Hz, \, 1H), \, 4.08 \, (t, \, J = 6.0 \, Hz, \, 2H), \, 1.45-1.38 \, (m, \, 2H),\)
\(1.24-1.21 \, (m, \, 2H), \, 1.12-1.06 \, (m, \, 2H), \, 0.84 \, (t, \, J = 8.0 \, Hz, \, 3H)\).

Pentyl 4-methyl-2-(pyridin-2-yl)benzoate (2b). \(\delta 8.64 \, (d, \, J = 4.8 \, Hz, \, 1H), \, 7.77 \, (d, \, J = 7.6 \, Hz, \, 1H), \, 7.72 \, (d, \, J = 7.6 \, Hz, \, 1H), \, 7.41 \, (d, \, J = 7.6 \, Hz, \, 1H), \, 7.34 \, (s, \, 1H), \, 7.27 \, (d, \, J = 7.6 \, Hz, \, 2H), \, 4.04 \, (t, \, J = 6.8 \, Hz, \, 2H), \, 2.43 \, (s, \, 3H), \, 1.41-1.35 \, (m, \, 2H), \, 1.25-1.19 \, (m, \, 2H), \, 1.11-1.04 \, (m, \, 2H), \, 0.83 \, (t, \, J = 7.2 \, Hz, \, 3H)\). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta 168.6, \, 159.2, \, 149.0, \, 141.6, \, 141.2, \, 135.9, \, 130.7, \, 130.1, \, 128.9, \, 123.0, \, 121.9, \, 55.0, \, 28.0, \, 22.3, \, 21.4, \, 13.9\). HRMS (EI-TOF) calc. for C\(_{18}\)H\(_{21}\)NO\(_2\) (M\(^+\)): 283.1572, found: 283.1573.

Pentyl 5-methyl-2-(pyridin-2-yl)benzoate (2c). Oil. Spectral data were consistent with literature values.\(^2\) \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 8.62 \, (d, \, J = 4.4 \, Hz, \, 2H), \, 7.73 \, (t, \, J = 7.2 \, Hz, \, 2H), \, 7.62 \, (s, \, 1H), \, 7.44 \, (d, \, J = 7.6 \, Hz, \, 2H), \, 7.35 \, (d, \, J = 7.6 \, Hz, \, 1H), \, 7.24-7.20 \, (m, \, 1H), \, 4.05 \, (t, \, J = 7.6 \, Hz, \, 2H), \, 2.43 \, (s, \, 3H), \, 1.43-1.35 \, (m, \, 2H), \, 1.23-1.16 \, (m, \, 2H), \, 1.09-1.02 \, (m, \, 2H), \, 0.82 \, (t, \, J = 7.6 \, Hz, \, 3H)\).

4-Methyl 1-pentyl 2-(pyridin-2-yl)terephthalate (2d). Yellow Oil. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 8.65 \, (d, \, J = \)}

4.8 Hz, 1H), 8.24 (d, J = 1.6 Hz, 1H), 8.12 (dd, J1 = 1.2 Hz, J2 = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.78 (dt, J1 = 1.6 Hz, J2 = 7.8 Hz, 1H), 7.55 (d, J = 8.0 Hz, 1H), 7.31-7.27 (m, 1H), 4.10 (t, J = 6.6 Hz, 2H), 3.95 (s, 3H), 1.47-1.40 (m, 2H), 1.24-1.18 (m, 2H), 1.13-1.07 (m, 2H), 0.84 (t, J = 7.4 Hz, 3H), 13C NMR (100 MHz, CDCl3): δ 168.6, 166.2, 157.8, 149.3, 140.9, 136.6, 136.2, 132.3, 129.9, 122.8, 122.6, 65.7, 52.6, 28.1, 28.0, 22.4, 14.0. HRMS (EI-TOF) calc. for C19H21NO4 (M+): 327.1471, found: 327.1470

Pentyl 4-methoxy-2-(pyridin-2-yl)benzoate (2e). Oil. 1H NMR (400 MHz, CDCl3):

δ 8.65 (d, J = 4.0 Hz, 1H), 7.90 (d, J = 8.4 Hz, 1H), 7.73 (dt, J1 = 8.0 Hz, J2 = 2.6 Hz, 1H), 7.39 (d, J = 7.6 Hz, 1H), 7.29-7.27 (m, 1H), 6.99-6.96 (m, 2H), 4.08 (t, J = 6.8 Hz, 2H), 3.88 (s, 3H), 1.39-1.35 (m, 2H), 1.26-1.20 (m, 2H), 1.14-1.08 (m, 2H), 0.85 (t, J = 7.2 Hz, 3H), 13C NMR (100 MHz, CDCl3): δ 167.8, 161.7, 159.3, 148.9, 143.7, 135.9, 132.3, 123.1, 122.0, 115.4, 113.6, 64.8, 55.5, 28.0, 27.9, 22.2, 13.9. HRMS (EI-TOF) calc. for C18H21NO3 (M+): 299.1521, found: 299.1522.

Pentyl 4-chloro-2-(pyridin-2-yl)benzoate (2f). Oil. 1H NMR (400 MHz, CDCl3):

δ 8.64 (d, J = 4.4 Hz, 1H), 7.80-7.77 (m, 1H), 7.74 (dd, J1 = 7.6 Hz, J2 = 1.6 Hz, 1H), 7.53 (d, J = 2.0 Hz, 1H), 7.45 (d, J = 2.0 Hz, 1H), 7.42 (d, J = 2.0 Hz, 1H), 7.30-7.28 (m, 1H), 4.05 (t, J = 6.6 Hz, 2H), 1.43-1.36 (m, 2H), 1.25-1.19 (m, 2H), 1.11-1.03 (m, 2H), 0.83 (t, J = 7.2 Hz, 3H), 13C NMR (100 MHz, CDCl3): δ 167.9, 157.6, 149.2, 142.7, 137.2, 136.3, 131.3, 130.0, 128.3, 122.8, 122.4, 65.4, 27.9, 22.2, 13.9. HRMS (EI-TOF) calc. for C17H18ClNO2 (M+): 303.1026, found: 303.1025.
Pentyl 3-(pyridin-2-yl)-2-naphthoate (2g). Oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 8.76 (d, $J = 4.8$ Hz, 1H), 8.37 (s, 1 H), 8.00 (s, 1H), 7.95 (d, $J = 7.6$ Hz, 1H), 7.90 (d, $J = 7.6$ Hz, 1H), 7.78 (t, $J = 7.6$ Hz, 1H), 7.60-7.54 (m, 3H), 7.28-7.27 (m, 1H), 4.12 (t, $J = 6.4$ Hz, 2H), 1.48-1.41 (m, 2H), 1.27-1.19 (m, 2H), 1.15-1.07 (m, 2H), 0.84 (t, $J = 7.6$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$): δ 168.9, 159.0, 149.0, 137.4, 136.2, 134.1, 132.2, 130.8, 129.5, 128.0, 127.1, 122.8, 121.8, 65.3, 28.0, 27.9, 22.3, 13.9. HRMS (EI-TOF) calc. for C$_{21}$H$_{21}$NO$_2$ (M$^+$): 319.1572, found: 319.1570.

Pentyl benzo[h]quinoline-10-carboxylate (2h). Oil. $^1$H NMR (400 MHz, CDCl$_3$): δ 8.89 (dd, $J_1 = 6.8$ Hz, $J_2 = 2.0$ Hz, 1H), 8.15 (dd, $J_1 = 8.0$ Hz, $J_2 = 1.2$ Hz, 1H), 7.95 (dd, $J_1 = 6.8$ Hz, $J_2 = 2.0$ Hz, 1H), 7.81 (d, $J = 8.8$ Hz, 1H), 7.71-7.67 (m, 3H), 7.50 (dd, $J_1 = 8.0$ Hz, $J_2 = 4.4$ Hz, 1H), 4.53 (t, $J = 6.8$ Hz, 2H), 1.81-1.76 (m, 2H), 1.37-1.35 (m, 4H), 0.88 (t, $J = 6.8$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$): δ 175.2, 147.7, 145.0, 135.5, 133.9, 132.5, 129.2, 127.7, 126.9, 126.0, 121.9, 65.7, 28.2, 22.3, 13.9. HRMS (EI-TOF) calc. for C$_{19}$H$_{19}$NO$_2$ (M$^+$): 293.1416, found: 293.1414.

Pentyl 2-(pyridin-2-yl)thiophene-3-carboxylate (2i). Oil. Spectral data were consistent with literature values.$^2$ $^1$H NMR (400 MHz, CDCl$_3$): δ 8.64 (d, $J = 4.0$ Hz, 1H), 7.86 (d, $J = 8.0$ Hz, 1H), 7.73 (dt, $J_1 = 7.6$ Hz, $J_2 = 1.6$ Hz, 1H), 7.51 (d, $J = 5.2$ Hz, 1H), 7.35 (d, $J = 5.2$ Hz, 1H), 7.28-7.25 (m, 1H), 4.22 (t, $J = 6.4$ Hz, 2H), 1.65-1.60 (m, 2H), 1.30-1.23 (m, 2H), 0.89 (t, $J = 6.8$ Hz, 3H).

---

Pentyl 2-(4-fluoropyridin-2-yl)-4-methoxybenzoate (2j). Oil. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.49 (d, $J = 2.8$ Hz, 1H), 7.90 (d, $J = 8.8$ Hz, 1H), 7.44 (dt, $J_1 = 8.4$ Hz, $J_2 = 2.8$ Hz, 1H), 7.38 (dd, $J_1 = 8.8$ Hz, $J_2 = 4.4$ Hz, 1H), 6.98- 6.94 (m, 2H), 4.04 (t, $J = 6.6$ Hz, 2H), 3.87 (s, 3H), 1.47- 1.40 (m, 2H), 1.28- 1.20 (m, 2H), 1.17-1.09 (m, 2H), 0.86 (t, $J = 7.4$ Hz, 3H), $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 167.7, 161.9, 158.9 (d, $J_{C-F} = 250$ Hz), 155.6, 142.9, 137.1 (d, $J_{C-F} = 30$ Hz), 124.2 (d, $J_{C-F} = 10$ Hz), 123.1 (t, $J_{C-F} = 20$ Hz), 115.7, 113.8, 65.1, 55.7, 28.3, 28.2, 22.4, 14.0. HRMS (EI-TOF) calc. for C$_{18}$H$_{20}$FNO$_3$ (M$^+$): 317.1427, found: 317.1430.

Pentyl 2-(4-chloropyridin-2-yl)-4-methoxybenzoate (2k). Oil. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.59 (d, $J = 2.4$ Hz, 1H), 7.91 (d, $J = 8.4$ Hz, 1H), 7.70 (dd, $J_1 = 8.4$ Hz, $J_2 = 2.4$ Hz, 1H), 7.34 (d, $J = 8.4$ Hz, 1H), 6.97 (dd, $J_1 = 8.6$ Hz, $J_2 = 2.6$ Hz, 1H), 6.95- 6.94 (m, 1H), 4.05 (t, $J = 6.6$ Hz, 2H), 3.87 (s, 3H), 1.48-1.40 (m, 2H), 1.28-1.21 (m, 2H), 1.15-1.10 (m, 2H), 0.86 (t, $J = 7.2$ Hz, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 167.5, 161.8, 157.5, 147.8, 142.6, 135.7, 132.5, 130.7, 124.0, 123.0, 115.5, 113.8, 65.0, 55.6, 28.2, 28.0, 22.3, 13.9. HRMS (EI-TOF) calc. for C$_{18}$H$_{20}$ClNO$_3$ (M$^+$): 333.1132, found: 333.1133.

Pentyl 4-methoxy-2-(pyrimidin-2-yl)benzoate (2l). Oil. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.81 (d, $J = 4.8$ Hz, 2H), 7.81 (d, $J = 8.4$ Hz, 1H), 7.32 (d, $J = 2.8$ Hz, 1H), 7.27-7.24 (m, 1H), 7.01 (dt, $J_1 = 8.4$ Hz, $J_2 = 2.4$ Hz, 1H), 4.08 (t, $J = 6.6$ Hz, 2H), 3.89 (s, 3H), 1.47-1.43 (m, 2H), 1.29-1.22 (m, 2H), 1.19-1.12 (m, 2H), 0.85 (t, $J = 7.2$ Hz, 3H), $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 168.2, 166.7, 161.6, 156.8, 141.3, 137.6, 124.3, 119.1, 115.0, 114.8, 65.0, 55.6, 28.1, 28.0, 22.3, 13.9. HRMS (EI-TOF) calc. for C$_{17}$H$_{20}$N$_2$O$_3$ (M$^+$): 300.1474, found: 300.1472.
D: NMR Analysis of Products

Pentyl 2-(pyridin-2-yl)benzoate (2a)

Pentyl 4-methyl-2-(pyridin-2-yl)benzoate (2b)
Pentyl 5-methyl-2-(pyridin-2-yl)benzoate (2c)
4-Methyl 1-pentyl 2-(pyridin-2-yl)terephthalate (2d)
Pentyl 4-methoxy-2-(pyridin-2-yl)benzoate (2e)
Pentyl 4-chloro-2-(pyridin-2-yl)benzoate (2f)
Pentyl 3-(pyridin-2-yl)-2-naphthoate (2g)

\[
\text{Py} \\
\text{CO}_2\text{C}_5\text{H}_{11}
\]
Pentyl benzo[h]quinoline-10-carboxylate (2h)

\[
\text{C}_5\text{H}_{11}\text{O}_2\text{C}
\]
Pentyl 2-(pyridin-2-yl)thiophene-3-carboxylate (2i)

\[
\text{Py}
\]

\[
\text{CO}_2\text{C}_5\text{H}_{11}
\]

Pentyl 2-(4-fluoropyridin-2-yl)-4-methoxybenzoate (2j)
Pentyl 2-(4-chloropyridin-2-yl)-4-methoxybenzoate (2k)
Pentyl 4-methoxy-2-(pyrimidin-2-yl)benzoate (2l)
HRMS Analysis of Products

Pentyl 4-methyl-2-(pyridin-2-yl)benzoate (2b)

Elemental Composition Report

Tolerance = 1.4 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
40 formulae evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-300 N: 0-1 O: 0-4
i-PE 22-May-2012 GCT Premier Zhejiang University
ls-2-140.81(1.357)

<table>
<thead>
<tr>
<th>Mass</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>283.1573</td>
<td>283.1572</td>
<td>0.1</td>
<td>0.4</td>
<td>9.0</td>
<td>5547419.0</td>
<td>C18 H21 N O2</td>
</tr>
</tbody>
</table>

4-Methyl 1-pentyl 2-(pyridin-2-yl)terephthalate (2d)

Elemental Composition Report

Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
104 formulae evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-200 N: 0-3 O: 0-5
i-PE 6-5-5-121 (2.210) Cm (121:129)
TOF MS El+

<table>
<thead>
<tr>
<th>Mass</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>327.1470</td>
<td>327.1471</td>
<td>0.1</td>
<td>0.3</td>
<td>10.0</td>
<td>5546655.0</td>
<td>C19 H21 N O4</td>
</tr>
</tbody>
</table>
Pentyl 4-methoxy-2-(pyridin-2-yl)benzoate (2e)

Elemental Composition Report

Tolerance = 1.0 mDa  /  DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
73 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100  H: 0-300  N: 0-2  O: 0-6
22-May-2012 GCT Premier Zhejiang University
b-2-135-3 5.525 (3.543)

Minimum: 1.0  0.8  -1.5
Maximum: 50.0

Mass    Calc. Mass  mDa  PPM  DBE  I-FIT  Formula
299.1522 299.1521  0.1  0.3  9.0  5546210.0  C18 H21 N O3

Pentyl 4-chloro-2-(pyridin-2-yl)benzoate (2f)

Elemental Composition Report

Tolerance = 1.4 mDa  /  DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-100  H: 0-300  N: 0-1  O: 0-4  Cl: 1-1
22-May-2012 GCT Premier Zhejiang University
b-2-135-3 1.55 (2.04)

Minimum: 1.4  0.6  -1.5
Maximum: 50.0

Mass    Calc. Mass  mDa  PPM  DBE  I-FIT  Formula
303.1025 303.1028  0.1  -0.3  9.0  5546501.5  C17 H18 N O2 Cl
Pentyl 3-(pyridin-2-yl)-2-naphthoate (2g)

Elemental Composition Report

Tolerance = 1.4 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
45 formulae evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:
C: 0-100 H: 0-300 N: 0-1 O: 0-4
22-May-2020 CT/Instrument: Zhejiang University
ib-2-154-1 151 (2.52)

Minimum:
Maximum:

Mass Calc. Mass mDa PPM DBE i-FIT Formula
319.1570 319.1572 -0.2 -0.6 12.0 5547881.0 C21 H21 N O2

Pentyl benzo[h]quinoline-10-carboxylate (2h)

Elemental Composition Report

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
138 formulae evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:
C: 0-100 H: 0-300 N: 0-5 O: 0-5
22-May-2020 CT/Instrument: Zhejiang University
ib-2-52 130 (2.93)

Minimum:
Maximum:

Mass Calc. Mass mDa PPM DBE i-FIT Formula
293.1414 293.1410 -0.2 -0.7 11.0 5547778.0 C19 H19 N O2
Pentyl 2-(4-fluoropyridin-2-yl)-4-methoxybenzoate (2j).

**Elemental Composition Report**

**Tolerance = 1.4 mDa / DBE: min = -1.5, max = 50.0**  
Element prediction: Off

**Monoisotopic Mass, Odd and Even Electron Ions**  
39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

**Elements Used:**  
C: 0-100  H: 0-300  N: 0-1  O: 0-4  F: 1-1

22-May-2012/GCT Premier Zhejiang University  
H-2.154.1 118 (1.960)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>317.1430</td>
<td>317.1427</td>
<td>0.3</td>
<td>0.9</td>
<td>9.0</td>
<td>5546907.5</td>
<td>Cl8 H20 N O3 F</td>
</tr>
</tbody>
</table>

Pentyl 2-(4-chloropyridin-2-yl)-4-methoxybenzoate (2k)

**Elemental Composition Report**

**Tolerance = 1.4 mDa / DBE: min = -1.5, max = 50.0**  
Element prediction: Off

**Monoisotopic Mass, Odd and Even Electron Ions**  
335 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

**Elements Used:**  
C: 0-100  H: 0-300  N: 0-5  O: 0-5  Cl: 1-1

22-May-2012/GCT Premier Zhejiang University  
H-2.154.2 107 (2.767)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>333.1133</td>
<td>333.1132</td>
<td>0.1</td>
<td>0.3</td>
<td>9.0</td>
<td>5546243.5</td>
<td>Cl8 H20 N O3 Cl</td>
</tr>
</tbody>
</table>
Pentyl 4-methoxy-2-(pyrimidin-2-yl)benzoate (2l)

**Elemental Composition Report**

Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
94 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:
C: 0-100  H: 0-200  N: 0-3  O: 0-5

**TICF MS EI+**

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-PIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>300.1472</td>
<td>300.1474</td>
<td>-0.2</td>
<td>-0.7</td>
<td>9.0</td>
<td>5548996.5</td>
<td>C17 H20 N2 O3</td>
</tr>
</tbody>
</table>