Supporting information

Lipase Catalyzed Green Synthesis of Enantiopure Atenolol
Bharat Prasad Dwivedee, Saptarshi Ghosh, Jayeeta Bhaumik, Linga Banoth and Uttam Chand Banerjee*

1. $^1$H NMR Spectra of (RS)-2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide

![NMR Spectra Image]
2. $^1$H NMR Spectra of (RS)-1-(4-(2-amino-2-oxoethyl)phenoxy)-3-chloropropan-2-yl acetate
3. $^1$H NMR Spectra of atenolol

<table>
<thead>
<tr>
<th>Analysis Info</th>
<th>Mass Spectrum List Report</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analysis Name</td>
<td>D:\Data\Dr. UCB\at-\z_A,1,01_743.d</td>
</tr>
<tr>
<td>Method</td>
<td>HIGH FLOW DIRECT INJECTION LOW MASS.m</td>
</tr>
<tr>
<td>Sample Name</td>
<td>at-\z</td>
</tr>
<tr>
<td>Comment</td>
<td></td>
</tr>
<tr>
<td>Source Type</td>
<td>ESI</td>
</tr>
<tr>
<td>Focus</td>
<td>Not active</td>
</tr>
<tr>
<td>Scan Begin</td>
<td>50 m/z</td>
</tr>
<tr>
<td>Scan End</td>
<td>600 m/z</td>
</tr>
<tr>
<td>Set Nebulizer</td>
<td></td>
</tr>
<tr>
<td>Set Dry Gas</td>
<td></td>
</tr>
<tr>
<td>Set Divert Valve</td>
<td></td>
</tr>
</tbody>
</table>

![Mass Spectrum Graph]

**Intens.**

248.1765

-MS, 5.5mm #327
5. Mass spectra of atenolol
6. HPLC chromatogram of (RS)-2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide

7. Chromatogram of enantiopure alcohol.
   a) (S)-(2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide)

   b) Chromatogram of (R)-(2-(4-(3-chloro-2-hydroxypropoxy)phenyl)acetamide)
8. Chromatogram of (RS)-1-(4-(2-amino-2-oxoethyl) phenoxy)-3-chloropropan-2-yl acetate

9. Selective HPLC chromatograms from lipase screening

*Candida antarctica* Lipase-A CLEA (maximum enantioselectivity observed)

*Candida cylindracea* (non selective)
*Candida rugosa (62316) (non selectivity)*

![Graph](image1)

*AMANO (non selectivity)*

![Graph](image2)

*Porcine pancreas lipase (no reactivity)*

![Graph](image3)
10. Selective HPLC chromatograms of solvent screening

Toluene (enantioselective)

Acetonitrile (no reactivity)

TBME (non selective)
Benzene (non selective)

11. HPLC chromatogram at optimized time period (18 h).

12. HPLC chromatogram using best acyl donor (Vinyl acetate)
13. HPLC chromatogram at optimized temperature (30 °C)

14. HPLC chromatogram at optimized enzyme concentration (15 mg/ml).

15. HPLC chromatogram at the optimized substrate concentration (20 mM)