Analysis of the Experimental Resolution of (+/-) Ibuprofen (PART III)

Refer to the Web page listed below
http://chemconnections.org/organic/chem226/Labs/opt-rotation/ibupro-resolution-09.html

Separation Scheme:

1) Complete the following Table.

**Experimental Optical Rotation Data:**

<table>
<thead>
<tr>
<th>Cell path length = 10.0 cm</th>
<th>Temperature = 25 °C</th>
<th>$\lambda = 589 \text{ nm}$ (sodium D)</th>
<th>solvent = ethanol</th>
<th>$\alpha_{\text{solvent}} = 0^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mass (g)</td>
<td>Volume (mL)</td>
<td>$\alpha$</td>
<td>[(\alpha)] (calc.)</td>
</tr>
<tr>
<td><em>Ibuprofen A</em></td>
<td>0.99</td>
<td>5.00</td>
<td>+10.85°</td>
<td></td>
</tr>
<tr>
<td><em>Ibuprofen B</em></td>
<td>0.76</td>
<td>5.00</td>
<td>-7.45°</td>
<td></td>
</tr>
</tbody>
</table>

**Calculations:**

\[ [\alpha]_A = \quad \quad [\alpha]_B = \]

Using the literature values for pure $d$- ibuprofen, $[\alpha] = +59^\circ$ and pure $l$- ibuprofen, $[\alpha] = -57^\circ$, complete the following table for ibuprofen A and B. Show your calculations for optical purity and enantiomeric excess.

<table>
<thead>
<tr>
<th></th>
<th>optical purity</th>
<th>% R-</th>
<th>% S-</th>
<th>enantiomeric excess: (%) indicate $d$- or $l$-</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Ibuprofen A</em></td>
<td>\</td>
<td>\</td>
<td>\</td>
<td>\</td>
</tr>
<tr>
<td><em>Ibuprofen B</em></td>
<td>\</td>
<td>\</td>
<td>\</td>
<td>\</td>
</tr>
</tbody>
</table>
Calculations:
Optical Purity & Enantiomeric Excess A

Optical Purity B & Enantiomeric Excess B

2) Complete the structures indicating stereochemistry for the two diastereomeric salts:

![Structure 1: Soluble (aq)](image1)

![Structure 2: Insoluble (aq)](image2)

3) Complete the drawings indicating stereochemistry for ibuprofen A and ibuprofen B.

![Ibuprofen A](image3)

![Ibuprofen B](image4)

4) The published experimental procedure for resolving \(d,l\)-ibuprofen was not reproducible and required many changes. A collection of reliable procedures, which have been tested at least once for reproducibility, are published in *Organic Syntheses*. Using the Cumulative Index for Volumes I-V cite one of two available tested procedures for the resolution of \(d,l\)-\(\alpha\)-phenylethylamine. Draw the 3-d structure for the S-stereoisomer, and explain if you can tell if it rotates polarized light to left or right or not.