Supplementary Information for

Polymorphism of the β,γ-hydroxylactone derived from indomethacin

Nikoletta B. Báthori* and Clive L. Oliver*

Crystal Engineering Research Unit, Department of Chemistry, Cape Peninsula University of Technology, P.O. Box 652, Cape Town, 8000, South Africa. E-mail: bathorin@cput.ac.za; Fax: +27 21 460 8354

Centre for Supramolecular Chemistry Research, Department of Chemistry, University of Cape Town, South Africa. E-mail: clive.oliver@uct.ac.za; Fax: +27 21 650 5419; Tel: +27 21 650 3830

1. Powder X-ray diffraction patterns of the two polymorphs and the in situ prepared form I in bulk.

![Figure 1S](image-url)

Figure 1S In situ preparation of Form I. Generated powder X-ray patterns of form II (blue), form I (red) and bulk material produced to obtain significant amount of the metastable form (black).
2. Differential Scanning Calorimetry

![Differential Scanning Calorimetry Graph]

Figure 2S Melting points of γ-Indomethacin, and form I and II.

Form I
- Ton = 194.08°C
- Tm = 203.02°C
- Heat of fusion = 43.85 J/g

Form II
- Ton = 219.16°C
- Tm = 224.48°C
- Heat of fusion = 137.37 J/g

Indomethacin
- Ton = 159.59°C
- Tm = 160.88°C
3. **Computational chemistry details.**

Applied basis set: B3LYP/6-31G**

<table>
<thead>
<tr>
<th>Colour</th>
<th>Molecule</th>
<th>Energy / kJ mol⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Red</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>Orange</td>
<td>0.73</td>
</tr>
<tr>
<td>3</td>
<td>Cyan</td>
<td>10.20</td>
</tr>
<tr>
<td>4</td>
<td>Green</td>
<td>9.63</td>
</tr>
<tr>
<td>5</td>
<td>Magenta</td>
<td>11.88</td>
</tr>
<tr>
<td>6</td>
<td>Dark gray</td>
<td>12.61</td>
</tr>
<tr>
<td>7</td>
<td>Light green</td>
<td>19.78</td>
</tr>
<tr>
<td>8</td>
<td>Pink</td>
<td>19.39</td>
</tr>
<tr>
<td>Crystal structure</td>
<td>Black</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 3S Overlay of the possible conformers.
4. **Hydrogen bond pattern and intermolecular potentials in form I and II.**

Figure 4S Packing diagrams are showing the hydrogen bond pattern in form I (left) and form II (right). Molecules are coloured by symmetry equivalence are showing the two types of centro-symmetrical dimers (A and B) and the calculated intermolecular potentials (kJ mol⁻¹) between the related molecules.
5. Hirshfeld surfaces and fingerprint plots for molecules

![Hirshfeld surfaces and fingerprint plots for molecules in form I and II.](image)

Figure 5S Hirshfeld surfaces and fingerprint plots of molecules in form I and II.
6. Hirshfeld surfaces and fingerprint plots for dimers

![Hirshfeld surfaces and fingerprint plots for dimers in form I and II.](image)

Figure 6S Hirshfeld surfaces and fingerprint plots of dimers in form I and II.