Conformational and enantiotropic polymorphism of a 1:1 cocrystal involving ethenzamide and ethylmalonic acid

Srinivasulu Aitipamula,*a Pui Shan Chow,a and Reginald B.H. Tan*,a,b

*aInstitute of Chemical and Engineering Sciences, A*STAR (Agency for Science, Technology and Research), 1, Pesek Road, Jurong Island, Singapore, 627833. Tel: (65) 6796 3858, Fax: (65) 6316 6183.

Email: srinivasulu_aitipamula@ices.a-star.edu.sg

bDepartment of Chemical & Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117576.

Email: reginald_tan@ices.a-star.edu.sg

Electronic Supplementary Information

Contents

Table S1. Comparison of torsion angles in different conformers of EMA molecule.

Figures. S1-S2 Hot-stage experiments on Forms I and II of EA•EMA cocrystal.

Figure S3 ORTEP diagram of EA•EMA cocrystal Form I

Figure S4 ORTEP diagram of EA•EMA cocrystal Form I

Figure S5 TGA traces of Forms I and II of EA•EMA cocrystal.

Figure S6 Comparison of PXRD patterns of the powders obtained in the slurry and extended grinding experiments.
Table S1. Comparison of torsion angles in EMA molecules.

<table>
<thead>
<tr>
<th>Torsion angle (τ)</th>
<th>Form I</th>
<th>Form II</th>
</tr>
</thead>
<tbody>
<tr>
<td>τ₁</td>
<td>57.15(17)</td>
<td>122.24(19)</td>
</tr>
<tr>
<td>τ₂</td>
<td>-67.01(16)</td>
<td>-112.15(19)</td>
</tr>
<tr>
<td>τ₃</td>
<td>-123.15(13)</td>
<td>-57.3(2)</td>
</tr>
<tr>
<td>τ₄</td>
<td>112.70(13)</td>
<td>68.32(19)</td>
</tr>
</tbody>
</table>

Figure S1. Hot-stage microscopy experiments on EA•EMA cocrystal Form I.
Figure S2. Hot-stage microscopy experiments on EA•EMA cocrystal Form II.

Figure S3. ORTEP diagram for Form I of the EA•EMA cocrystal showing the atom numbering. Thermal ellipsoids were drawn at 50 % probability.
**Figure S4** ORTEP diagram for Form II of the EA•EMA cocrystal showing the atom numbering. Thermal ellipsoids were drawn at 50 % probability.

**Figure S5** TGA traces of Forms I and II of EA•EMA cocrystal.
Figure S6. Comparison of PXRD patterns of (a) Form II, (b) Form I, sample obtained from (c) slurry experiment on a 1:1 physical mixture of Form I and II, (d) slurry experiment on Form I, (e) NG on Form I, 30 min, (f) NG on Form I, 60 min, (g) NG on Form II, 30 min, (h) NG on Form II, 60 min. Notice that Form I converts to Form II in slurry experiment and extended grinding.