Supporting Information

Cocrystals of zileuton with enhanced physical stability

Xin Chen,ab Duanxiu Li,a Chun Luo,a Jinqiu Wang,c Zongwu Deng,a Hailu Zhang*a

a Laboratory of Magnetic Resonance Spectroscopy and Imaging, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, Suzhou 215123, P.R. China.
b School of Pharmacy, Xi’an Jiaotong University, Shaanxi 710061, P.R. China.
c Crystal Pharmatech, Suzhou Industrial Park, Suzhou 215123, P.R. China.

*Corresponding author:
Tel: +86-512-62872713, Fax: +86-512-62603079, E-mail: hlzhang2008@sinano.ac.cn.

SI1
Fig. S1 Experimental and simulated powder XRD patterns of ZIL form A (a and b), ZIL form H (c and d), ZIL-NIC (e and f), and ZIL-ISO (g and h).
Fig. S2 TG curve of ZIL form H.
Fig. S3 Powder XRD patterns of ZIL form A (a), ZIL form H (b), and form H after dehydration (c).
Fig. S4 Dissolution profiles of ZIL form A (■), ZIL form H (●), ZIL-NIC (▲), and ZIL-ISO (▼) in HCl aqueous solution (pH 1.2) at 37 °C.
Fig. S5 Powder XRD patterns of ZIL form A (a), ZIL form H (b), ZIL-NIC (c), and ZIL-ISO (d) after dissolution experiments. Simulated powder XRD patterns of ZIL form H (e).
Fig. S6 DVS curve of ZIL form A. Square symbols represent moisture sorption and roundness symbols represent moisture desorption.
Fig. S7 Powder XRD patterns of ZIL form A (a and b) before and after equilibrating at 95% RH/25°C for 3 h. Simulated powder XRD pattern of ZIL form H (c).
Fig. S8 Powder XRD patterns of ZIL form A (a-c), ZIL-NIC (d and e), and ZIL-ISO (f and g) before and after equilibrating at 75% RH/40°C for different periods. Simulated powder XRD patterns of ZIL form H (h).
Table. S1 pH values before and after dissolution experiment.

<table>
<thead>
<tr>
<th>Name</th>
<th>ZIL form A</th>
<th>ZIL form H</th>
<th>ZIL-NIC</th>
<th>ZIL-ISO</th>
</tr>
</thead>
<tbody>
<tr>
<td>before</td>
<td>1.2</td>
<td>1.2</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>after</td>
<td>1.06</td>
<td>1.08</td>
<td>1.06</td>
<td>1.12</td>
</tr>
</tbody>
</table>