Chemicals and Instrumentation for water-solubility determination

All reagents used for analysis were of analytical reagent grade (Merck). A multielement solution of Ag, Al, As, Ba, Be, Bi, Ca, Cd, Co, Cr, Cs, Cu, Fe, Ga, In, K, Li, Mg, Mn, Na, Ni, Pb, Rb, Se, Sr, Tl, V, U, and Zn (100 mg/L, Merck) was used to prepare the calibration standards.
The analytical batch consisted of a set of calibration standards, which were analyzed at the beginning of the run, samples and a minimum of three procedural blanks.
A midrange calibration standard was measured at the end of each analytical run, to assess instrumental drift throughout the run. An eight-point calibration curve covering the range of 0.1-2000 μg/L was used for quantitative analysis. Standard solutions were prepared by diluting the multielement solutions cited above.
Aqueous solutions were prepared using ultrapure water, with a resistivity of 18.2MΩ cm, obtained from a Milli-Q plus system (Millipore, Bedford, MA). All glassware, polyethylene flasks, and tubes involved in sample preparation and measurement were cleaned with nitric acid (2%, v/v) overnight, rinsed with ultrapure water, and dried.
The determination of the element of interest was carried out utilizing an Elan DRC-e ICP-MS instrument (Perkin-Elmer SCIEX, Canada).
The sample delivery system consisted of a Perkin-Elmer autosampler model AS-93 Plus with a peristaltic pump and a cross-flow nebulizer with a Scott type spray chamber. Samples were introduced by means of a quartz nebulizer. The ICP torch was a standard torch (Fassel type torch) with a platinum injector. A solution containing Rh, Mg, Pb, Ba, and Ce (10 μg/L) was used to optimize the instrument in terms of sensitivity, resolution, and mass calibration.

Results obtained:

1 water-Solubility = 245 μM **1a** water-Solubility = 673 μM

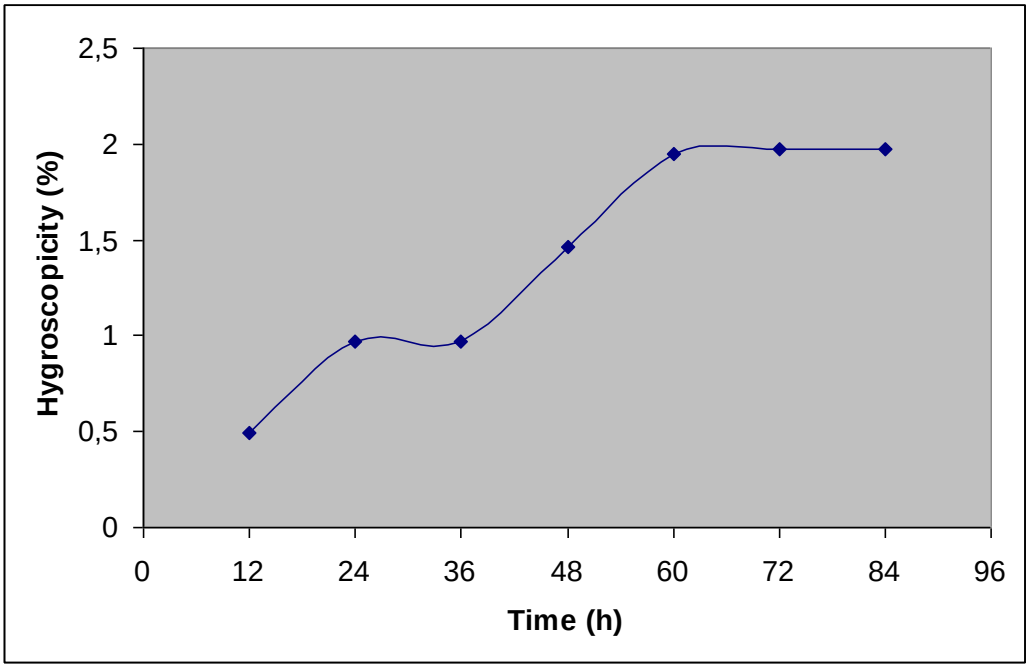

Figure S1 Hygroscopicity of **1a** at 25 °C and 85% RH.

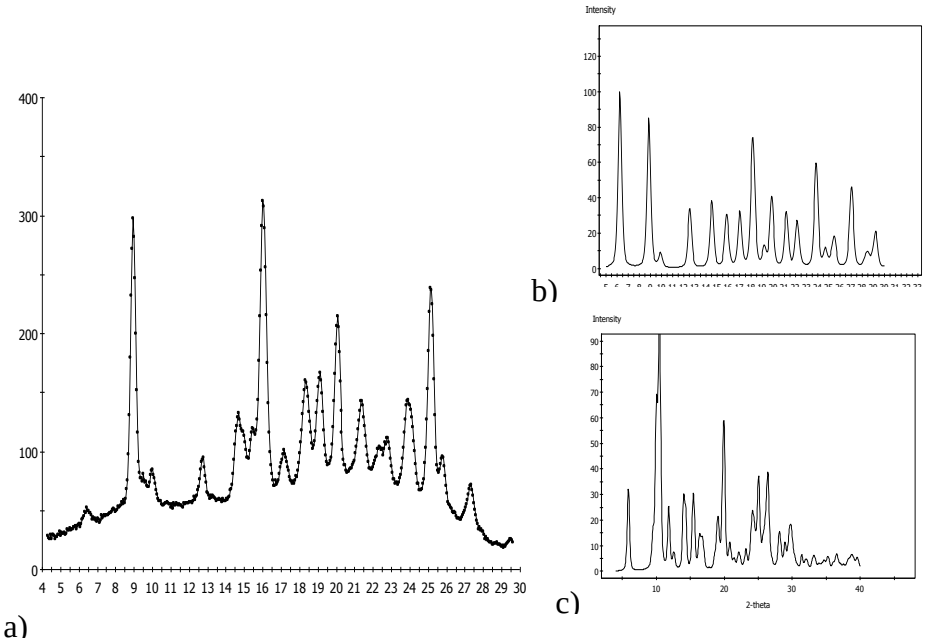

Figure S2 Powder patter of the crystalline powder obtained by grinding complex **2** and saccharine (a), compared with the diffractograms calculated from single crystal analysis of **2** (b) and **2a** (c).