

Accepted Manuscript

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PII: S0928-0987(18)30097-6

DOI: doi:[10.1016/j.ejps.2018.02.020](https://doi.org/10.1016/j.ejps.2018.02.020)

Reference: PHASCI 4417

To appear in: *European Journal of Pharmaceutical Sciences*

Received date: 8 November 2017

Revised date: 4 February 2018

Accepted date: 19 February 2018

Please cite this article as: Ilma Nugrahani, Dwi Utami, Slamet Ibrahim, Yuda Prasetya Nugraha, Hidehiro Uekusa , Zwitterionic cocrystal of diclofenac and l-proline: Structure determination, solubility, kinetics of cocrystallization, and stability study. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Phasci(2017), doi:[10.1016/j.ejps.2018.02.020](https://doi.org/10.1016/j.ejps.2018.02.020)

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Zwitterionic cocrystal of diclofenac and l-proline: Structure determination, solubility, kinetics of cocrystallization, and stability study

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Abstract

In recent decades, the design of cocrystals has developed significantly due to the unique characteristics and advantages of cocrystals, which help to improve the physicochemical properties of drugs, especially solubility. Zwitterions are attractive and interesting co-formers. However, the physicochemical properties of cocrystals with zwitterionic co-formers, i.e. zwitterionic cocrystals, have not been adequately evaluated. In this study, solid-state characterization of a newly developed zwitterionic cocrystal of diclofenac (DFA), a non-steroidal anti-inflammatory drug, and the amino acid L-proline (PRO) was performed using Fourier-transform infrared spectroscopy, differential scanning calorimetry, and powder X-ray diffraction (PXRD) analyses. In addition, the crystal structure of the cocrystal (DFA-PRO) was determined by single-crystal X-ray diffraction analysis, after which the zwitterionic structure was confirmed. The cocrystallization during co-grinding, which was investigated by PXRD, followed first-order kinetics. Furthermore, the solubility of the zwitterionic cocrystals was 7.5-times higher than that of the DFA crystals. The results indicate that the cocrystal is

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