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Evaluation of solvents' effect on solubility, intermolecular interaction energies and habit of ascorbic acid crystals (Article) [\(Open Access\)](#)

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Abstract

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Solubility of active pharmaceutical ingredient (API) in solvents is very important for drug development and manufacturing. Solubility data may provide further information such as thermochemical properties and intermolecular interactions that may lead to a better understanding of the formation of API crystals. In this study, solubility of ascorbic acid was determined by gravimetric method in four different commonly used polar protic solvents: water, methanol, ethanol and 2-propanol. The solubility of ascorbic acid crystal was also predicted using Conductor-like Screening Model – Realistic Solvent (COSMO-RS) approach. In this computational analysis, the generated ΔG values are based on the solubilities that were experimentally obtained to simulate the intermolecular forces. The intermolecular interaction data from COSMO-RS provide an insight into the relationship between the intermolecular interactions and its crystal habit across four different polar protic solvents. The habit of the crystals was then determined using light microscopy and scanning electron microscopy techniques, while the polymorphic form of the crystals was identified by X-ray powder diffraction and single X-ray diffraction techniques. The solubility and characterization data showed that the solvents with high polarity increased the solubility of ascorbic acid. The data also showed that different solvent polarity influenced the crystal habit, but did not change the crystal structure to form a new polymorph. © 2018 King Saud University

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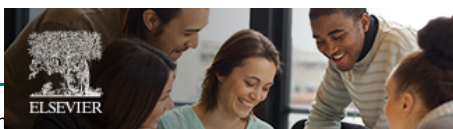
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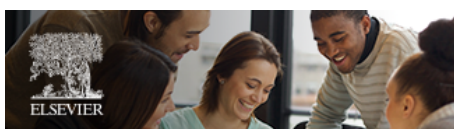
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