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Picolinic acid solubility, aggregation and crystallization studies

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Crystallization is a method to obtain solids from solution that has been around for a long time. However, it remains unclear how molecules aggregate in solution and form a crystal. Many variables can affect the crystallization outcome and the appearance of polymorphs, for instance, the temperature and the solvent used in the crystallization. In order to synthesize only the desired solid, of a given compound, it is crucial to study the existence of polymorphism and what are the exact conditions in which we are able to obtain the pretended crystalline structure [1].

The study of a family of compounds with systematic variations in the molecular structure could help uncover the molecular mechanisms throughout crystallization. Therefore, picolinic acid (Fig. 1), an isomer of nicotinic acid, and the hydroxynicotinic acids, which have been thoroughly studied in our group [2,3], could constitute models for such study. This family of compounds have known biological relevance, namely picolinic acid, is used to chelate several metals, in particular zinc and chromium and these specific chelates are sold as alimentary supplements [4]. In this work some early results on both the solubility (obtained through the gravimetric method) and solid state structure (by means of PXRD) of picolinic acid, at different temperatures, in three polar solvents: water, ethanol (both protic solvents) and acetonitrile (aprotic solvent) will be presented. These results show us that picolinic acid is very soluble in water (for $T \approx 293$ K, $C_{PA} \approx 862.5$ g·kg^{-1}), way less soluble in ethanol ($C_{PA} \approx 57.1$ g·kg^{-1}) and even less in acetonitrile ($C_{PA} \approx 17.0$ g·kg^{-1}). Moreover, its solubility increases with temperature, as expected.

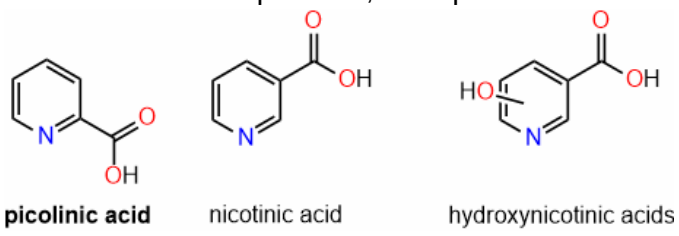

Figure 1. Molecular structures of picolinic, nicotinic and hydroxynicotinic acids.

Acknowledgements
This work was supported by Fundação para a Ciência e a Tecnologia (FCT), Portugal through Projects PTDC/QUI-OUT/28401/2017 (LISBOA-01-0145-FEDER-028401), UIDB/00100/2020 and UIDP/00100/2020.

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