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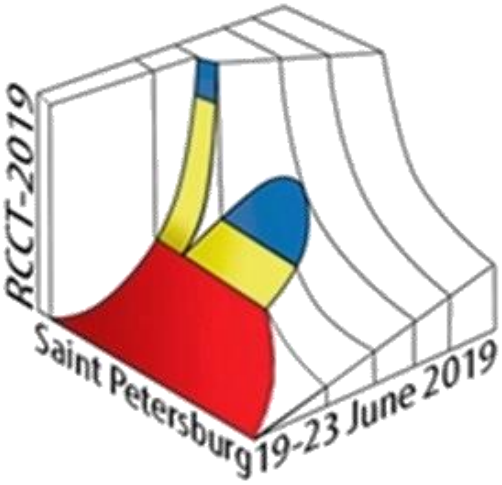

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BOOK OF ABSTRACTS

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Screening of Conformational Diversity of Molecules of Biologically Active Compouds Based on Nuclear Overhauser Effect Spectroscopy

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Depending on conditions, crystallization of polymorphs from solution can be either kinetically or thermodynamically controlled. In the latter case, the obtained polymorph is independent of the nature of the solvent. It was shown [1] that even in cases when the choice of the solvent seems to be crucial, this can be in fact a minor factor related to the concentration achieved in the chosen solvent rather than a specific effect of solvent–solute interaction. Therefore, it is necessary to determine solubility curves and the width of the metastable zone in order to control the crystallization process of a polymorph. A very important factor, however, is very rarely taken into account today: namely, the influence of a molecule's conformational state on the crystallization process. Spatial structures of the molecule was shown to be a key factor in the nucleation, regarding both kinetics [2,3] and thermodynamics of the process [4]. In this work we propose a method of screening of the conformational state depending on the pressure and temperature, based on nuclear Overhauser effect spectroscopy. This approach can provide unique information on structural characteristics of small molecules in subcritical and supercritical states.

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