From Molecules to Crystals: An Experimental and Theoretical Overview

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Crystallization from solution is indisputably one of the oldest and most widely used purification methods. Despite this fact, our current understanding of the early stages of crystallization is still in its infancy, particularly for organic solids. The nature, rate, and mechanism of formation of crystal nuclei seem to dictate the structural and physical properties of crystallized substances. Understanding how molecules assemble in solution to yield crystals is not only a fundamental scientific question, but also a matter of technological interest, if tight control over polymorph, morphology, and size distribution of a precipitated material is in view.

In this work, a comprehensive study of the occurrence of polymorphism in 4'-hydroxyacetophenone [1,2] and paracetamol, by using theoretical and experimental methods will be presented. Focus will be placed on how the solvent influences molecular conformations and assembly towards the formation of well-organized crystal structures. This discussion will include results obtained from Molecular Dynamics simulations analyzed with the computer program AGGREGATES [3], that extracts information about the local organization of the molecules (Figure 1).

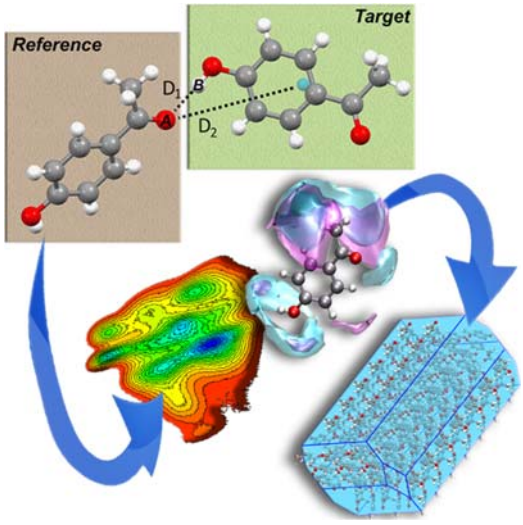

Figure 1. Schematic view of analysis results performed with the program AGGREGATES [3] to extract information about the organization of the molecules in Molecular Dynamics simulation results.

Acknowledgements
This work was supported by Fundação para a Ciência e a Tecnologia (FCT), Portugal (Projects UID/MULTI/00612/2013, UID/QUI/00100/2013, PTDC/QUI-OUT/28401/2017, LISBOA-01-0145-FEDER-028401). Post-Doctoral grants from FCT is gratefully acknowledged by Carlos Bernardes (SFRH/BPD/101505/2014).

References

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