MS34-P09 | AFFINITY PREDICTIONS FOR COCRYSTALS' DESIGN: COMPUTATIONAL VS. EXPERIMENTAL RESULTS.

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Lately, in order to enhance aqueous solubility, dissolution rate, hygroscopicity or bioavailability of poorly water soluble pharmaceutical molecules, the design of functional molecular materials using cocrystallization has attracted increasing interest. Cocrystals are multicomponent materials composed of neutral chemical species present in the same crystal lattice in a certain stoichiometric ratio and assembled via weak interactions such as van der Waals, hydrogen, halogen or π-π. Pharmaceutical cocrystals usually refer to the combination of two APIs (active pharmaceutical ingredients) or one API and another small molecule that form a homogeneous crystalline single-phase system. Cocrystallization can be obtained by many techniques such as crystallization from solution, neat and liquid-assisted grinding, among many others. Using those techniques is usually considered a time consuming approach as it requires the experimental screening of a large number of chemicals. In the present study, calculations have been performed to estimate energetic affinity between an API and a large set of small organic molecules of pharmaceutical interests. Computational results were directly compared to the experimental ones, including all the literature data. Thus, the validity of the computational tool aiming to shorten the cocrystal design has been assessed.

This project has received funding from the Interreg 2 Seas programme 2014-2020 co-funded by the European Regional Development Fund under subsidy contract 2S01-059_IMODE.