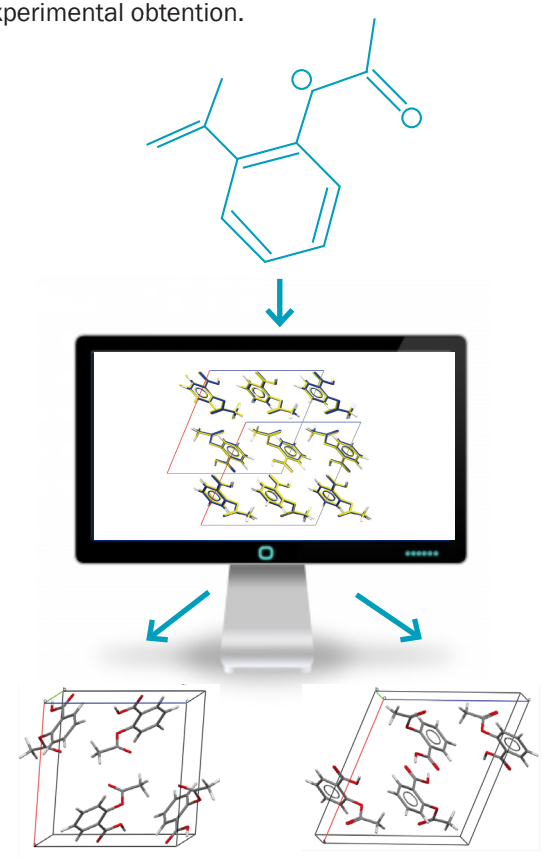
The computational prediction (In silico screening) of polymorphs is a high impact field for the materials, chemical and pharmaceutical companies. It is a preliminary step in the quest for crystal polymorphs, where one identifies how likely the crystal of interest can present polymorphism and which structure and properties could present the most likely polymorphs.

A computational study allows to identify the most likely crystal structures, which agree in most cases with the thermodynamically most stable structures. The in-silico screening screening of the possible competitive structures can also suggest metastable forms or solvate formation (that is, patentable alternative forms), previous to their experimental obtention.



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PreCrystal

Prediction of Crystal

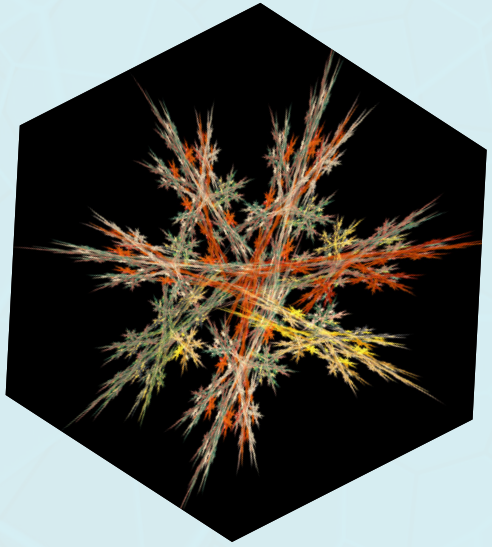
ANALYSIS AND PREDICITOM OF CRYSTAL STRUCTURES OF TECHNOLOGICA RELEVANCE

(pharmaceuticalcompounds, dyes, semiconductors...)

GEM² Grup d'Estructura de Materials Moleculars
Grupo de Estructura de Materiales Moleculares
Molecular Materials Structure Group

Red de Referencia en Química Teórica y Computacional

PreCrystal is a service offered by the GEM2 (Grupo de Estructura de Materiales Moleculares) de la Universitat de Barcelona to research groups at university and chemical companies. The GEM2 research group has developed a powerful computational tool to predict and optimize crystal structures, named PixCryPar. This is a highly efficient computer program capable of predicting the most likely crystalline structure of a molecule or co-crystal. The main basis for a reliable prediction is a proper description of the intermolecular interactions found in the crystal. PixCryPar describes them by means of a new generation of intermolecular potentials (pixel potentials), where the ab initio calculated molecular density in a volume is
condensed in a pixel). The energy associated to a crystal structure is then expressed as a sum over these pixels. At the end of the analysis, the most stable crystal structures are ordered according to their energy. In silico polymorph prediction is the new and reliable alternative to have a preliminar screening, thus minimizing expensive trial-and-error experimental tests.



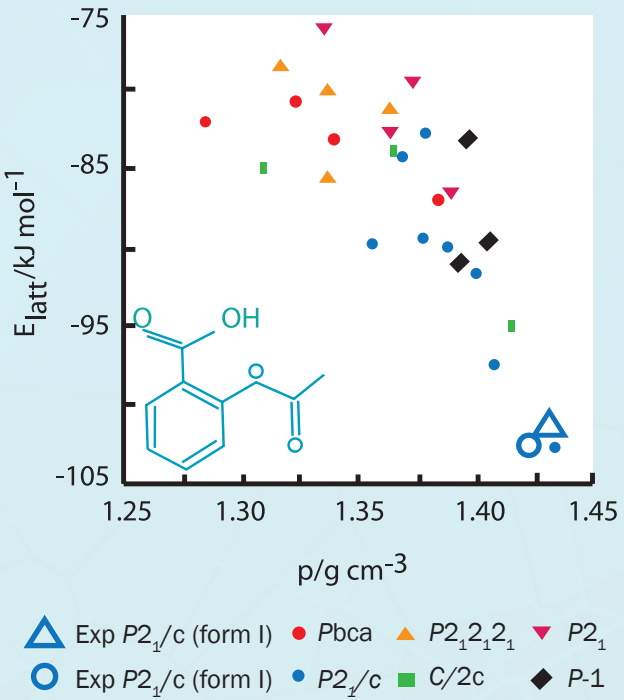
Addressed to:

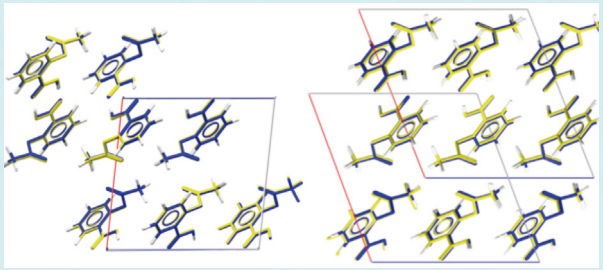
- Pharmaceutical companies
- Chemical companies
- Material companies
- University research groups

What we can do?

- Predict and properly characterize crystal polymorphs, finding new potentially patentable forms.
- Investigate their technological properties (optical, magnetic and electric properties).
- Determine the possible formation of a cocrystal and salts.
- Study the energetic stability of the crystal structure of APIs and excipients relative to the formation of API-excipient co-crystals.

Energy ranking for the all possible crystal structures calculated for aspirin using PIXCRYPAR. Calculated structures for △ form-I and ○ form-II (empty symbols correspond to the experimental structures).





Superposition of the form-I and form-II for the predicted aspirin (PIXCRYPAR) with the experimental ones.