CIRCE
Crystal Engineering

CIRCE POLYMORPH SCREENING (CPS)

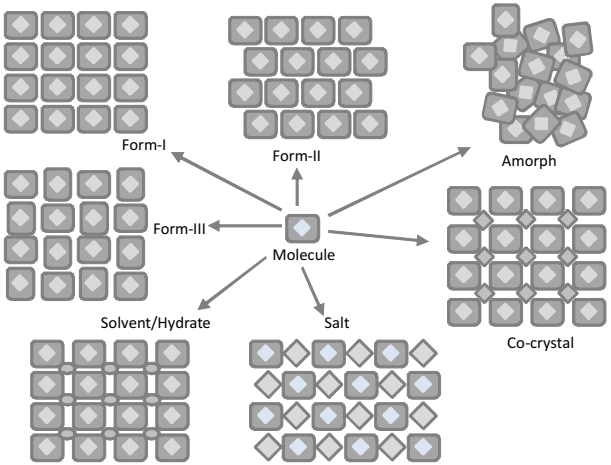
circecrystal.com

POLYMORPH SCREENING

The knowledge of the polymorphism is essential prior to the launch of a new API to the market

Polymorphism describes all the possible solid-state forms in which an API can exist; from the amorphous to the different crystal forms. Different polymorphs of a single API can present different physicochemical properties that affect their bioavailability and, therefore, their bioequivalence and also their intellectual property. For this reason, the pharmaceutical companies design strategies in order to know and patent all the possible polymorphs of a single API to avoid commercial conflicts of interest.

Polymorphic studies are necessary to design R&D strategies



CIRCE's prediction system reduces costs and time during the development of new drugs

In this sense, CIRCE has developed a polymorph prediction tool in order to identify the most thermodynamically stable polymorphs. This novel approach is a very useful guide for a more efficient experimental screening, reducing costs and time.

We provide Pharma companies with ***optimal drugs***, ***new IP*** *and* ***longer protected revenues***.

Our technology:
CIRCE POLYMORPH SCREENING (CPS)

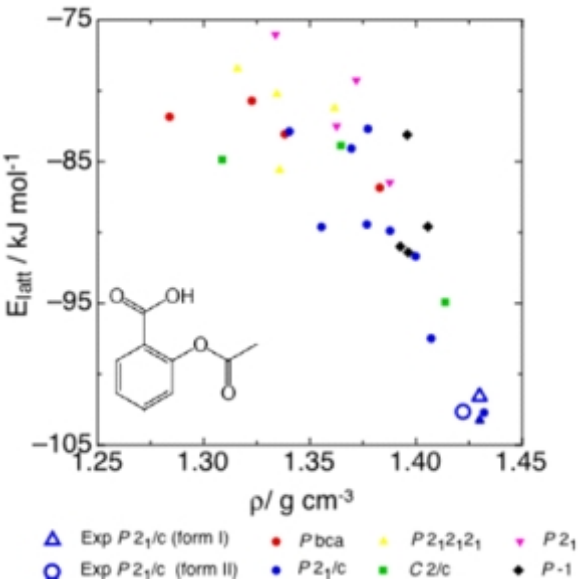
CIRCE's computational method predicts the structure and energy of any molecular crystal just from the chemical structure

Our polymorph prediction tool defines intermolecular energies computed by using the semi-classical Pixel intermolecular potential. Such approach describes the interaction energy between two molecules as the sum of the exchange-repulsion, electrostatic induction, charge transfer and dispersion components. We have transformed this approach into a parallel computer code that can predict the structure and energy of any molecular crystal, In order to comply with the assay, the geometry of the molecule is just required.

CIRCE has validated this method, studying the polimorphism of the Aspirin, a very well described case in literature. Our computational method has been able to predict the two polimorphs of aspirin, these two appearing to be almost isoenergetic. Up to now, our virtual polimorph screening technology is the only method able to predict the second polimorph of Aspirin.

Our computational method is able to predict the second polymorph of Aspirin

Energy-density distribution of all crystalline forms calculated for aspirin. The two experimental polymorphs (empty blue triangle and circle) are located close to the theoretical form-I and form-II points predicted by the CIRCE's technology.



“to maximize and protect the value of the pharmaceutical drugs”

In CIRCE we contribute to maximize the value of the R&D projects of our partners providing:

- The API crystalline form that presents the best physicochemical and pharmacological properties. We can choose the candidates with the best properties to hit the market from a wide variety of alternative structures such as polymorphs, salts or cocrystals.

- An adequate IP defensive position based on a much extended and consequently stronger patent portfolio of the product. Since we can find – and protect – the most likely crystalline forms of the API, we difficult the competitor's access to market through alternative polymorphs or cocrystals.

- A higher return on investment while accessing the market with a stronger IP protection and the expertise to extend patents.

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