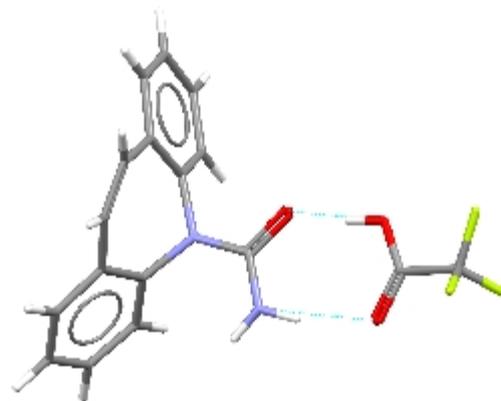
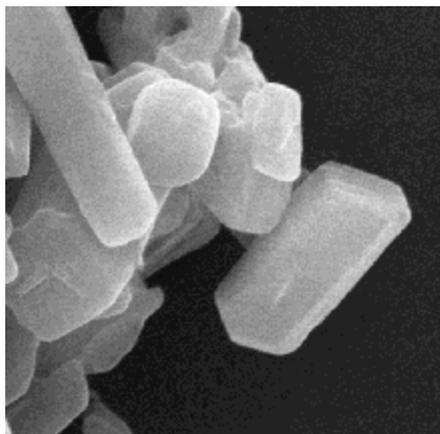


CIRCE
COCRYSTAL
SCREENING
(CCS)

COCRYSTAL SCREENING

Cocrystals can improve API's properties and can extend the intellectual property.

A cocrystal is a crystalline material formed by an API (Active Pharmaceutical Ingredient) and a coformer or a second API that can **improve the physicochemical properties** of the original API and that is considered as a new formulation of the aforementioned API (FDA, 2012). **This entails a big impact on the pharmaceutical industry because each new solid form can be patented.**



CIRCE offers virtual and experimental cocrystal screening services and helps your company to solve your problems related to your APIs.

These supramolecular compounds are formed by stoichiometric amounts of an API and a coformer with which it does not form a salt through ionic bonds, but a complex through non covalent interactions.

For this reason, in CIRCE we offer a new and unique virtual cocrystal prediction service that determines what coformers are more likely to cocrystallize with an API. This new high-speed computational system substitute the slow and complex traditional screening assays based only on experimentation.



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

Our technology: CIRCE COCRYSTAL SCREENING (CCS)

**CIRCE system:
exclusive and
validated.**

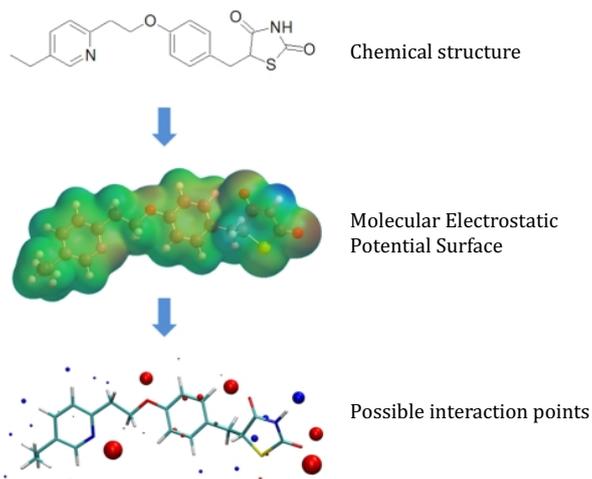
**CIRCE offers virtual
and experimental
cocrystal screening
services:
faster
more efficient
safer
better cost/benefit**

**Fast evaluation of
data bases with
2500 possible
coformers with
excellent results.**

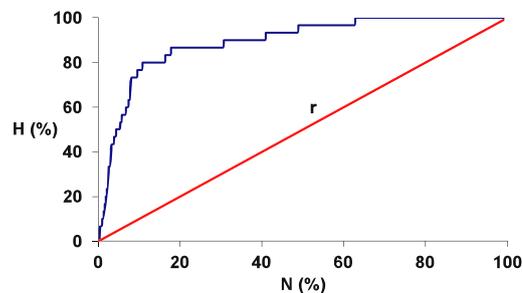
This new and exclusive co-crystal prediction system has been validated for different APIs and it has been proved that there is a very good correlation between both the cocrystallization experimental data and the theoretical probabilities offered by the predictive software.

This new and unique computational methodology allows to discover new cocrystals with a higher ratio of success compared with the classical methods, expending less time and less associated costs.

We use a selection from around 2500 coformers belonging to the lists of molecules considered as safe for humans, versus the 30-40 that usually are used in a traditional experimental screening. With our technology, we can reduce to 1% the number of coformers to test, with an 80% of probability to discover a new co-crystal.



CIRCE's computational technology determines for each API and its possible coformer, through the Molecular Electrostatic Potential Surface those interaction points more likely to establish intermolecular interactions.



Caffeine is chosen as a model because is one of the most cocrystallized compound in the Cambridge Crystallographic Data Center (CCDC) data base. The 80% of the experimental observed cocrystals are inside the 20% of the best predicted coformers. The red line represents probability of finding a hit as a result of random.

“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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