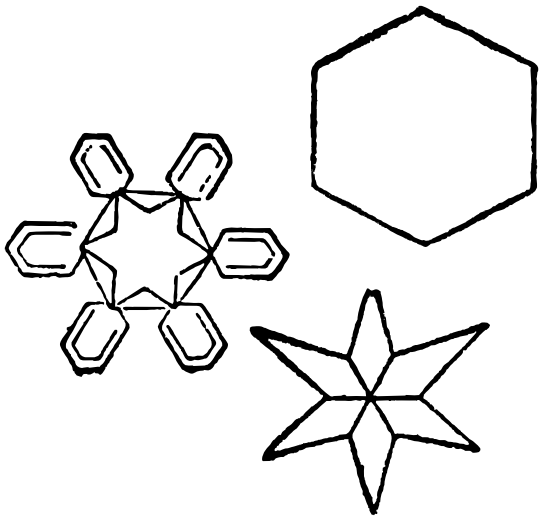
CIRCE
Crystal Engineering

Experimental cocrystal, polymorph and salt screening
Thermal stability studies
Physicochemical characterization

Experimental cocrystal, polymorph and salt screening

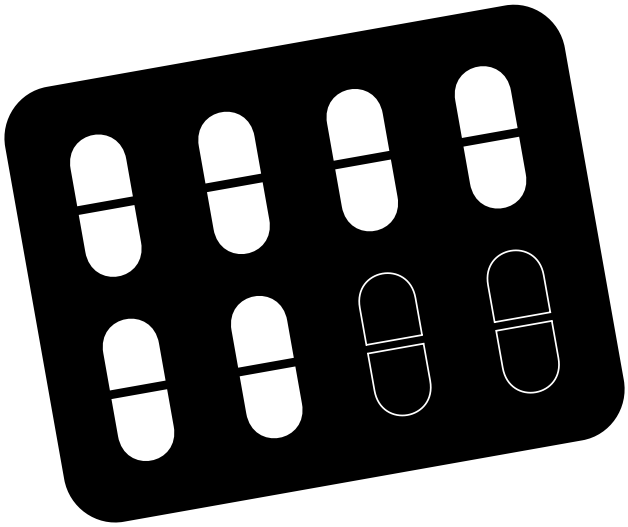
Although our hallmark are the virtual prediction technologies, CIRCE possess extensive facilities and capabilities to carry out experimental screening to search for new cocrystals, polymorphs and salts. The facilities are equipped with the state-of-the-art instruments necessary to perform experimental screening and the technical staff has an extensive and proven experience in the field.



We offer to companies wishing to work with us and take advantage of our expertise in the field of cocrystals two different kind of contracts: the standard experimental cocrystal screening or the virtually predicted one. Salts and polymorphs screening are also available.

Thermal stability studies

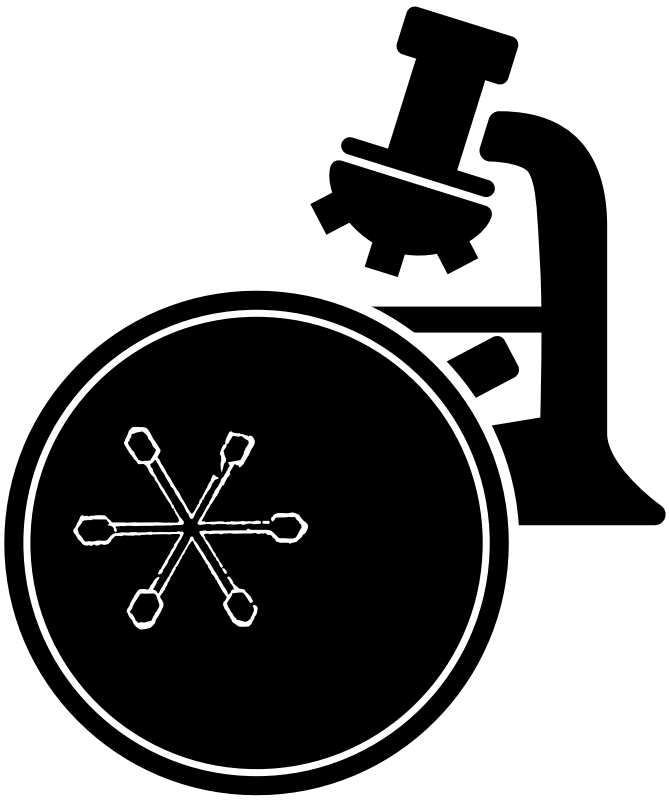
CIRCE has the convenient facilities, devices and technical staff to perform the necessary experiments to evaluate the stability of a particular crystal form. These studies are long-term studies carried out in chambers with controlled temperature and humidity conditions to determine the best packaging and storing conditions and to ensure good viability and stability of the product along time. These experiments are conducted accordingly with the ICH guidance and partner desires.



For the evaluation of the thermal stability, X-ray Diffraction and/or calorimetric techniques are routinely used.

Physicochemical characterization

One of the most important steps to do when searching for a new crystal form is the appropriate physicochemical characterization of all the solids obtained during the screening process which will enables us to discover new forms. Once a new cocrystal, polymorph or salt is produced a full characterization of it is necessary in order to ensure its novelty.



The expertise and facilities of CIRCE allow to perform accurate characterizations of those new cocrystals, polymorphs or salts, as well as raw materials, APIs and drug products developed by or for the pharmaceutical and the agrochemical industries.

Our facilities have the technical staff and are equipped with the state-of-the-art instruments and devices necessary to carry out a precise characterization of the physicochemical properties.

These include:

Crystallography: To know the three dimensional structure of a new crystal form and to discern between an existing form and a new one, crystallography techniques are essential. With this purpose, Single Crystal and Powder X-Ray Diffraction are available for our partners.

Calorimetric techniques: Differential Scanning Calorimetry and Thermogravimetry are techniques which can provide useful thermal information of a new crystal form, including melting point, thermal stability, polymorphic transformations, Loss on Drying Test, etc.

Thermomicroscopy: Hot-stage microscopy give important information about the presence of solvent in a new form together with its thermal stability and can be an additional technique for in situ formation of cocrystals through the “Kofler hot stage contact method”.

Spectroscopic techniques: Analytical techniques to measure purity and composition, are also available in CIRCE. These include NMR and FTIR.

Center for Intelligent Research in Crystal Engineering (CIRCE)

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