



**SEMINAIRE Chimie Physique Microbiologie
pour les Matériaux et l'Environnement**

présenté par :

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**« Structural investigations of cocrystals by (macro)molecules
crystallography »**

**Mardi 5 mars 2024
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Salle de Conférences
LCPME 405 rue de Vandoeuvre
54600 Villers-lès-Nancy

R é s u m é

Cocrystal are multicomponent crystalline systems that can be found under different forms and can provide useful structural information, both in the fields of protein crystallography and small molecules crystallography.

In the present general presentation, selected examples of structural investigations of cocrystals by (macro)molecules crystallography performed at UNamur will be discussed.

In the field of protein crystallography, crystal structures of proteins cocrystallized with ligands allow a better understanding of the catalytic mechanisms of enzymes, their dynamics and open the way to structure-based drug design approaches. This will be illustrated on structures of cocrystals of indoleamine dioxygenase and phosphoserine phosphatases.

In the field of small molecules crystallography, cocrystallization is an interesting way to modulate the physico-chemical properties of solids. Examples of this crystal engineering approach applied to original cocrystals of molecules of pharmaceutical interest and on thermo-photo chromic compounds will be discussed.

The selected examples will, hopefully, stress the importance of cocrystals (in a broad sense) in solid state chemistry.