XRayLab: an X-ray diffraction facility for the International Space Station dedicated to the study of space-grown crystals

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The International Space Station (ISS) is a great technical achievement, designed as a flexible laboratory able to support science in a wide range of disciplines. Unfortunately, to make use of the ISS is still unappealing to a large number of potential users, due to the burden of complex rules and long procedures associated with developing and operating equipment on board the Station. The policy of the European Space Agency (ESA) about the utilization of the Columbus module changed recently, opening to the possibility of accessing the ISS on a commercial basis. This will allow for the establishment of new commercial services supporting the performance of additional science and technological research and development.

One of the most interesting aspects is related to the possible biological advancements coming from the study of space-grown protein crystals. One of the initiatives under preparation, with the support[1] of the European Union (EU), is centred on the XRayLab facility and aims at boosting the research in various fields, thanks to the singular effect of the microgravity on crystals' quality, associated with the unprecedented capability of performing in situ X-ray diffraction (XRD) measurements.

A promising application of this crystallography technique targets protein-pharmaceutical compounds molecular complexes crystallized in orbit, with the objective of:

elucidating rigid protein atomic structures and configurations

identifying protein-ligand docking relationships (structure-activity relationships)

High quality crystals will grow in the microgravity environment guaranteed by the ISS, in a dedicated experimental microfluidic setting called the PharmaCard (Figure 1). The XRD measurements will be performed in situ, by means of this novel XRD instrument, to avoid deterioration of the protein crystals when exposed to the re-entry and ground transport stress environment. The acquired data, consisting of the XRD pattern images, will be either downlinked or stored in data storage media that will then be downloaded to ground for computational analysis and structural determination.

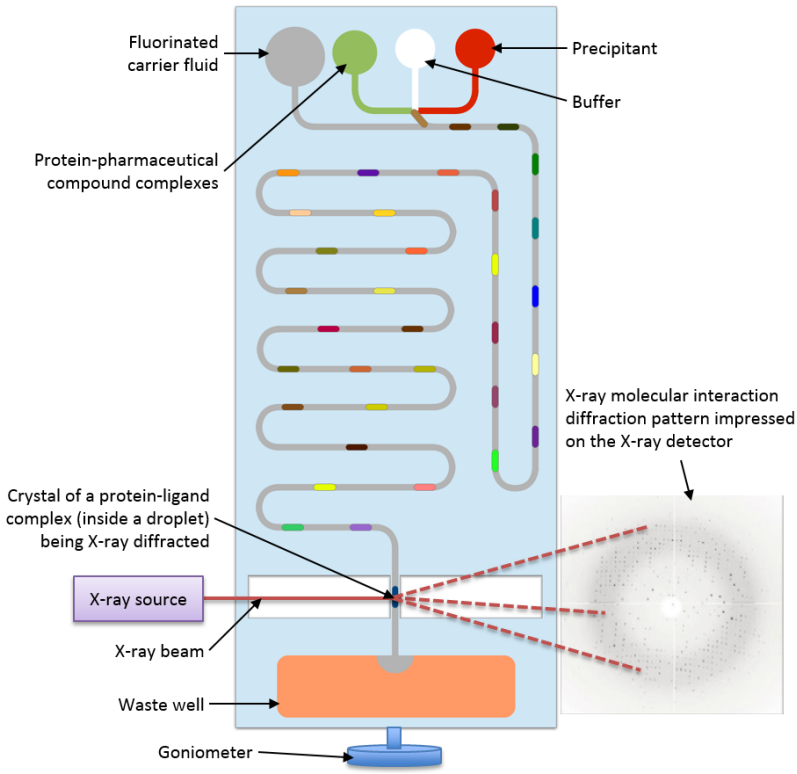

Figure 1 PharmaCard and XRD (concept)

The utilization of the PharmaCard inside the XRayLab facility will target applications in the sectors of ligand-based and structure-based drug design and development.

In addition, the use of an XRD facility and of microfluidics in space may have other interesting applications for crystallography investigations of biological and synthetic molecules.

Crystallization is such a universal process that humans cannot safely explore and understand space without a deep knowledge of how molecules join themselves under microgravity to form crystals, from nano- to metre-size scale[2].

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1. J.M. García Ruiz, F. Otálora, in Answers to a questionnaire on the PharmaLab experimental facility for Space Applications Services (Dec. 2015)