MINISTERIO
DE CIENCIA, INNOVACIÓN
Y UNIVERSIDADES

INSTITUTO DE
BIOMEDICINA DE
VALENCIA CSIC

PROPOSAL: MX-2351
BEAMLINE: ID23-2
DATE: 22-23 / 09 / 2021
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EXPERIMENT REPORT

At ID23-2, we collected three crystals of Arbitrium protein receptor from Bacillus subtilis Katmira phage in complex with DNA. The structure has been included in a scientific article that is currently in the 3rd revision round in Nature Communications: Gallego del Sol F, Quiles-Puchalt N, Brady A, Penadés JR, Marina A (2022) Insights into the mechanism of action of the arbitrium communication system in SPbeta phages.

We collected 15 crystals of three different recombinant constructs of antifungal protein B from Peniciclium expansum. Crystals diffracted to 1.2 A resolution and structures could be solved by molecular replacement using a previously solved model.

We diffracted 32 crystals of CheA protein in complex with various compounds. The collected data was used for the identification of binding modes of the compounds. In total, we found 4 compounds bound to the protein which we intend to modify further to improve their binding affinity. Overall, the obtained structures were used for rational drug design and will be published in the next 4-5 months.

In addition, we collected 43 datasets of human DHO protein bearing different pathogenic mutations, both free and in complex with different substrates/activators. The structures, solved by molecular replacement at 1.3-2.0 Å resolution, allowed us to explain the damaging effect of the mutations at the atomic level and to capture the protein in different conformational stages related to the catalytic cycle. These results will be the subject of a research article that we plan to submit in the next 6 months.

Furthermore, we screened for the first time, crystals of His-phosphotransferase protein Hpt from Chaetomium thermophilum. In total, we tested 32 crystals, and identified conditions were crystals diffracted to ~8 Å resolution. Thanks to this information, we expanded the crystallization conditions and obtained high-quality crystals that allowed us to determine the structure at 2.4 Å. A manuscript containing the Hpt structure will be prepared shortly.

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