3DBionotes Covid-19 Edition

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3DBionotes-WS, an ELIXIR recommended interoperability resource, is a set of web services that provides multiple annotations oriented to structural biology analysis. It can be accessed through a website interface that features a fully interactive 3D viewer for macromolecular structures and functional, genomic, proteomic and structural feature annotations.

Motivated by COVID-19 pandemic, we present a new section (*https://3dbionotes.cnb.csic.es/ws/covid19*) dedicated to SARS-CoV-2 viral protein structures that have been provided by X-ray crystallography, cryo-EM, NMR and various modelling and structural predictions approaches. The aim of this section is collecting and providing centralized access to all available structural information on the SARS-CoV-2 viral proteins, as well as other related viruses or interacting molecules. In addition, when validation and quality information is available from PDB-REDO [1] and the Coronavirus Structural Task Force [2], special tags are incorporated for every entry, pointing to the re-refined models.

Among the new annotations added are functional mappings for ligand binding sites and protein-protein interaction sites. Functional mapping annotations allow to locate the residues that are likely to constitute binding sites between SARS-CoV-2 proteins and other viral or human proteins [3] and for multiple candidate inhibitors already identified for SARS and MERS homologous proteins. Of particular interest are ligands tested in large-scale studies searching for potential drugs, like the one performed against the SARS-CoV-2 main protease using the PanDDA method [4] at the Diamond synchrotron, Oxford (*https://www.diamond.ac.uk/covid-19/for-scientists/Main-protease-structure-and-XChem*).

Regarding the genomic context, SARS-CoV-2 variants compiled at the China National Center for Bioinformation (*https://bigd.big.ac.cn/ncov/variation*) have been summarized in a new annotation track. Also, some methods to evaluate the quality of cryo-EM maps and the fit to their atomic models was incorporated. These methods are deepRes [5], that analyse the map local resolution and FSC-Q [6] and map Q-score [7], that inform about the fit and resolvability of the built atomic model.

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