

West-Life: A VRE for Structural Biology

Friday, 18 March 2016 10:50 (30 minutes)

The focus of structural biology is shifting from single macromolecules produced by simpler prokaryotic organisms, to the macromolecular machinery of higher organisms, including systems of central relevance for human health. Structural biologists are expert in one or more techniques. They now often need to use complementary techniques in which they are less expert. INSTRUCT supports them in using multiple experimental techniques, and visiting multiple experimental facilities, within a single project.

The Protein Data Bank is a public repository where final structures and (some) of the data leading to them are deposited. Nowadays journals require such a deposition as a precondition of publication. However, metadata are often incomplete.

West-Life will pilot an infrastructure for storing and processing data that supports the growing use of combined techniques. There are some technique-specific pipelines for data analysis and structure determination but little is available in terms of automated pipelines to handle integrated datasets. Integrated management of structural biology data from different techniques is lacking altogether.

West-Life will integrate the data management facilities and services (e.g. from WeNMR) that already exist, and enable the provision of new ones. The resulting integration will provide users with an overview of the experiments performed at the different research infrastructures visited, and links to the different data stores. It will extend existing facilities for processing this data. As processing is performed, it will automatically capture metadata reflecting the history of the project. The effort will use existing metadata standards, and integrate with them new domain-specific metadata terms.

West-Life will provide the application level services specific to use cases in structural biology, enabling structural biologists to get the benefit of the generic services developed by EUDAT and the EGL.

Summary

West-Life is a H2020 Virtual Research Environment project that will provide the application level services specific to use cases in structural biology, covering all experimental techniques (e.g. Xray, cryo-EM, NMR, SAXS), enabling structural biologists to get the benefit of the generic services developed by EUDAT and the EGL.

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Session Classification: Biomedicine & Life Science Session II

Track Classification: Virtual Research Environment (including Middleware, tools, services, workflow, ... etc.)