COFUND – Project : Advanced scientific visualization of membrane proteins and their assemblies

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Industrial Partner: Pale Blue (https://pale.blue/)

Intra-Labex partners: Undefined at this point; a/several membrane protein study systems may be chosen with the goal to make better sense of existing structural data and integrate heterogeneous datasets

Labex-theme: mostly 2 (study the structures of membrane proteins) but possibly also 3 (multi-scale integrated structural biology approaches)

Short description:

The host lab has been developing original tools for visualization [1] and analysis [2] of (membrane) protein structures and assemblies, which have been ported into advanced environments such as virtual reality headsets and display walls. The Unitymol tool is now routinely used at several sites of the UCB Biopharma company. The company Pale Blue has expressed interest in exploring our approaches further, in particular in an industrial context (see also support letter for the Cofund project).

Here, we specifically intend to apply and improve these approaches for the study of membrane proteins and their assemblies, which are more complex than the use cases we have focused on so far [3]. We have ideal conditions for this at IBPC, because several groups produce and analyze state of the art structural datasets, and we have advanced visualization equipment available. We plan in particular to add a more comprehensive support for the variety of structural data nowadays available, in particular cryo-EM data sets, which have only been marginally implemented so far (previous focus was on Xray crystallographic data). We have demonstrated the utility of such approaches recently for exploring SARS-COVID-related structural data [4].

The industrial viewpoint would attempt to inject additional components of drug design tools for interesting membrane protein targets. It will be a particular area of application with novel ideas on the representation and exploration of the chemical space for a given system and for the leveraging of human intuition in the process.
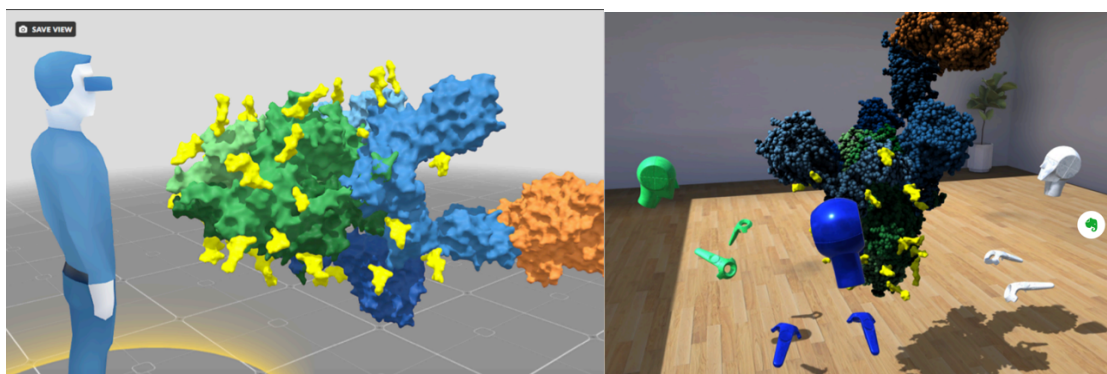
[1] Lv et al., PLOS One (2013), 8(3): e57990
[2] Taly, Expert Opin Drug Discov (2013), 8, 1285-1296
[3] Brandner, et al. Mitochondrion (2019), 49, 234-244.
Esmenjaud, et al. (2019). The EMBO journal, 38(2), e99894.
[4] Martinez & Baaden, Acta Cryst D (2021), D77, 746-754