

Summary of Activities (Quarter 3)

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Overview

Our *PyMOL Fellowship* Project is to establish high-level interfaces based on *PyMOL* framework¹ called *PyMOL-PUB* (called *PyMOL-advance* previously). Its repository is now set out in <https://github.com/BGI-SynBio/PyMOL-PUB>. These high-level interfaces effectively establish the channel from structure data to publication-quality figures. As shown in Figure 1, they can help bioinformaticians, algorithm scientists and computer engineers to create figures for their manuscripts in a simpler and more rapid way.

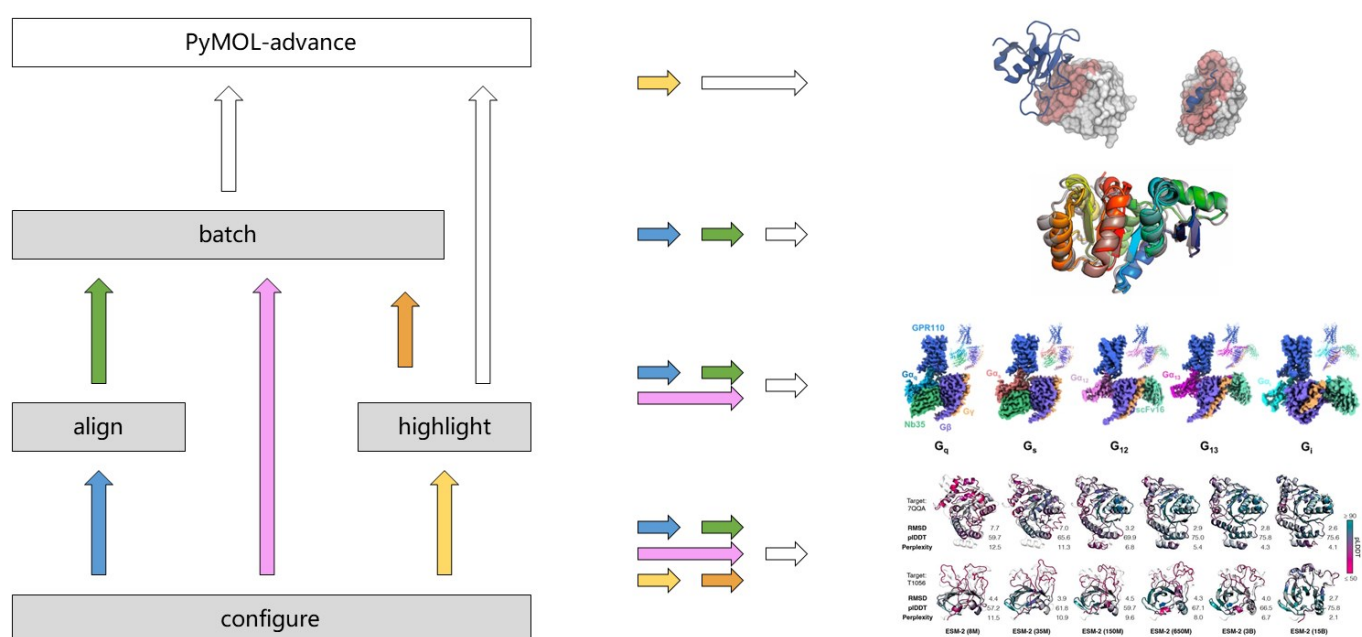


Figure 1. core requirement architecture and target cases²⁻⁵.

As we mentioned in the proposal, we need to optimize the structures visualization module and construct more valuable cases in our third quarter. Besides, we need to complete a project introduction website and provide use methods of the established interfaces.

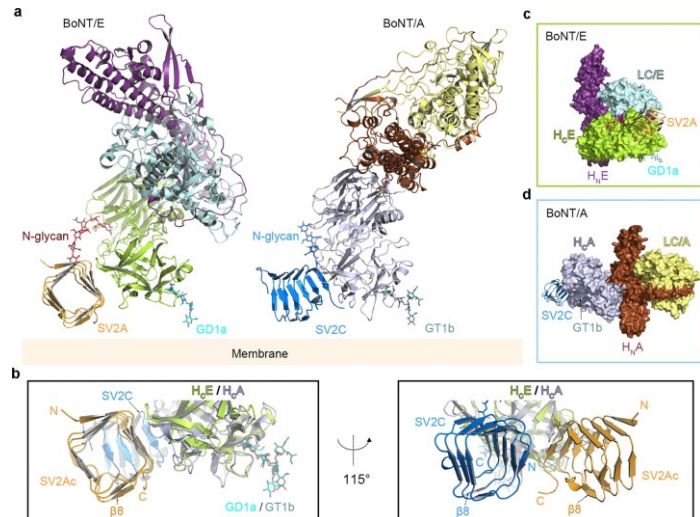
Quarterly Goal

- 1. optimize the structures visualization module:** To improve the practicability and reliability of the structures visualization module, we consider adding a structure focus function and more structure rendering options to StructureImage class.
- 2. construct more valuable cases:** To demonstrate how to use the interface and how to achieve specific painting goals, we consider reproducing valuable figures based on *PyMOL-PUB* and compare them to those published in academic articles.
- 3. complete a project introduction website:** To explain the design specifications for the project, we create a web document, based on the ReadtheDocs, to exhibit the code architecture and interface parameter information of *PyMOL-PUB*.

Solutions

- Function adjustment:** Focus the visual on the structure content that needs to be zoomed by use “set_zoom” function. The “closed_surface” and “independent_color” parameters are added to the “set_shape” function to control the creation of the closed surface and render the structure more flexibly. Integrate the widget icon drawing code into the “layout.py” and build the “obtain_widget_icon” interface to obtain the widget icon based on the predetermined setting.
- case implementation:** We collected an integrated figure from the publication shown in Table 1. Upon comparing our sample figure to this published academic article, we find that our design is strikingly similar, and only requires a few lines of code. Moreover, this case includes the operations of partial area coloring, structure alignment, batch visualization, local scaling, conformational rotation, and multiple sub-graph merging, which can effectively demonstrate the capacity of *PyMOL-PUB* to draw complex structural figures.

Table 1. Collected case.

case	figure	feature	reference
1		<ul style="list-style-type: none"> ● Partial area coloring; ● Structure alignment information; ● Batch visualization; ● Local scaling; ● Conformational rotation; ● Multiple sub-graph merging. 	6

The figure built using *PyMOL-PUB* have a high quality similar to the original one published in top journals (see Figure 2).

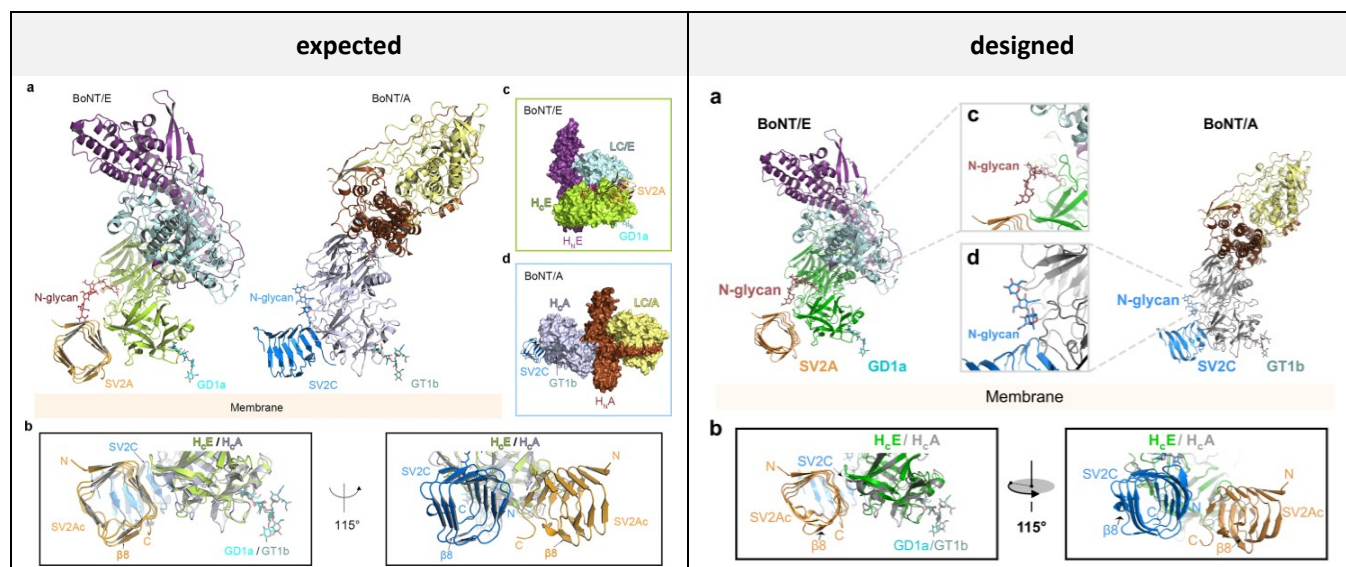


Figure 2. The comparable case.

- 3. Documentation of *PyMOL-PUB*:** In order to better explain the functional design and usage of *PyMOL-PUB*, we have completed various documents, which include the README for each code module and the project introduction website at <https://pymol-pub.readthedocs.io/en/latest/>. In addition, we have completed a manuscript to promote *PyMOL-PUB* that has been submitted to the *Bioinformatics* Journal and is currently with reviewers. We paste the submitted user manual into the following text to further clarify our workload.

Remaining Issues

- 1. Easy-to-use features:** We have distributed our extension to several users to gather their feedback. However, some users are not skilled in programming with Python, and they are hoping to have alternative methods of interaction such as command lines. Further amplifying the influence of *PyMOL* and this extension is valuable, so we plan to conduct research and make improvements to this aspect of the software in the coming two quarters. The current dilemma is that a small number of feedback samples make it difficult for us to clearly infer the progress direction. We are uncertain about whether we should adopt *PyMOL GUI*, develop a command line interface, or even integrate it into subsequent versions of *PyMOL*. Besides, we are also unsure if incorporating machine learning would be beneficial in reducing the need for manual intervention. We may work together to conduct a user survey for broader users to deepen our judgment on further research and development.

Next Quarter

The next quarter should include two contents in order: promoting a user survey and programming the easy-to-use feature. Although our previous plan was to develop configuration schemes, this may change due to the choices of larger-scale users. In essence, our aim is to make *PyMOL-PUB* accessible to users who may have less experience in programming.

Reference

- 1 DeLano, W. L. Pymol: An open-source molecular graphics tool. *CCP4 Newsl. Protein Crystallogr* **40**, 82-92 (2002).
- 2 Corbi-Verge, C. & Kim, P. M. Motif mediated protein-protein interactions as drug targets. *Cell Communication and Signaling* **14**, 1-12 (2016).
- 3 Yang, J. *et al.* Improved protein structure prediction using predicted interresidue orientations. *Proceedings of the National Academy of Sciences* **117**, 1496-1503 (2020).
- 4 Zhu, X. *et al.* Structural basis of adhesion GPCR GPR110 activation by stalk peptide and G-proteins coupling. *Nature Communications* **13**, 5513 (2022).
- 5 Lin, Z. *et al.* Language models of protein sequences at the scale of evolution enable accurate structure prediction. *BioRxiv* (2022).
- 6 Liu, Z. *et al.* Structural basis for botulinum neurotoxin e recognition of synaptic vesicle protein 2. *Nature Communications* **14**, 2338 (2023).