Summary of Activities (Quarter 4)

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Overview

Our *PyMOL Fellowship* Project is to establish high-level interfaces based on the *PyMOL* framework[1] called *PyMOL-PUB*. Its repository is now set out at 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 create figures for their manuscripts in a simpler and more rapid way.
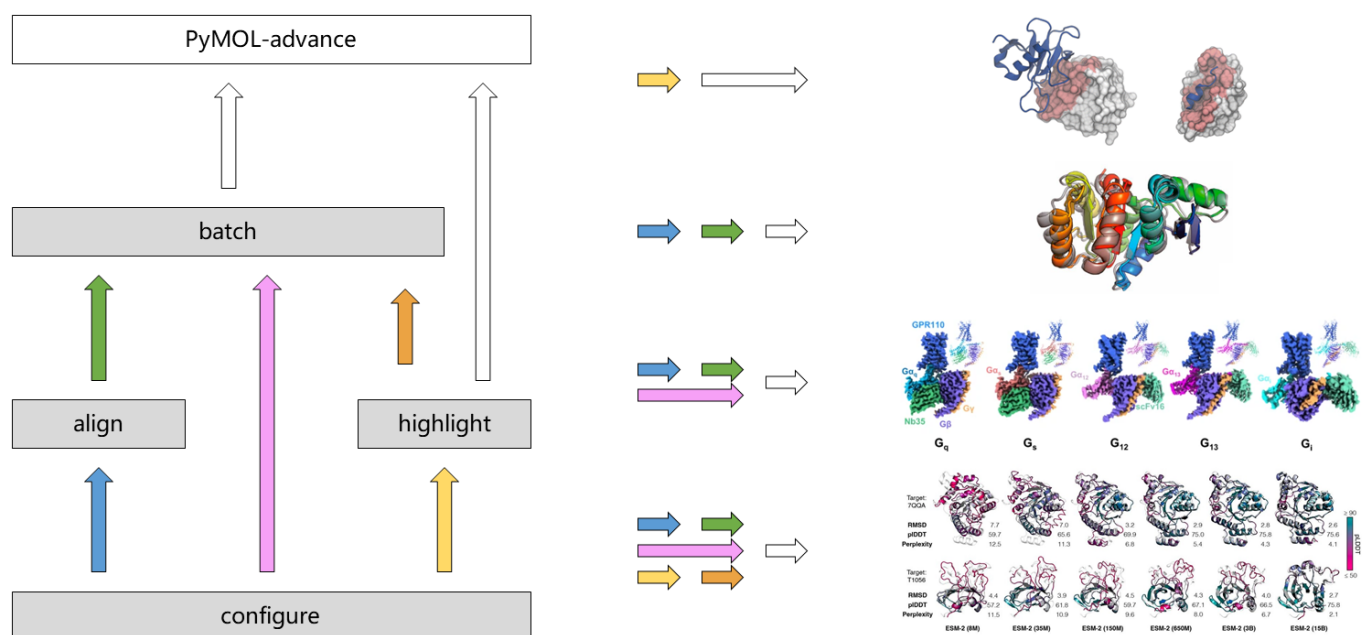

Figure 1. core requirement architecture and target cases[2-5].

As we mentioned in the proposal, we need to program the easy-to-use feature in our fourth quarter. Besides, we need to complete publication of a manuscript and provide detailed usage methods of the established interfaces.

Quarterly Goal

1. **program the easy-to-use feature:** To expand the usage of *PyMOL-PUB* tools, we consider developing a Graphical User Interface (GUI) based on the structure visualization modules.

2. **complete publication of a manuscript:** To promote the *PyMOL-PUB* project, we prepare a manuscript and hope to publish it in a journal so that more users can know and use *PyMOL-PUB*, and we can collect more users' feedback information.

3. **provide detailed usage methods:** To explain the design specifications and usage of this project, the content of the Technical Manual needs to be further updated to exhibit the code architecture, interface parameter information and usage guidelines of *PyMOL-PUB*.

Solutions

1. **GUI development:** Based on the basic drawing process in *PyMOL-PUB*, such as figure layout setting, structure file loading, element hiding, representation setting, conformational rotation and coloring adjustment, a process-oriented GUI was developed. *PyMOL-PUB*'s GUI helps users interact with the drawing process, who can experience convenient and fast image parameter input and layout setting strategies. The complete code for the GUI is shown in the "windows.py" file.

2. **manuscript published:** Currently, we have completed the publication of a manuscript related to the *PyMOL-PUB* tool, titled *Rapid generation of high-quality structure figures for publication with PyMOL-PUB*. The detailed content of the manuscript can be found at the *Bioinformatics* publication website (https://doi.org/10.1093/bioinformatics/btae139).

3. **Technical Manual update:** After the GUI development and drawing code updates in the fourth quarter, we have updated the corresponding content in the *PyMOL-PUB*'s Technical Manual. The main specific content is the update of the code architecture description and the addition of usage guidelines for the GUI. The Technical Manual is also displayed as *Supplementary data* in the published manuscript.

Remaining issues

As we mentioned in our publication, we may work together to disseminate the high-quality inputs and outputs based on PyMOL-PUB, like the gallery on the official website of Matplotlib, helping to further reduce the learning curve for beginners.

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).