Outlook

An AI tutor to help students visualize biomolecules with Jmol

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Hi,

As part of my sabbatical, I built a custom GPT that is supposed to help students create and troubleshoot Jmol scripts. I put it in the GPTstore (https://chatgpt.com/g/g-67ef4a0925d48191a63120240716bf95-jmol-jane), but it will be turned off in two days because I will stop paying for the premium service.

For posterity, I made two videos of the interactions, the first where I model a hard-working student, and the second where I model a lazy student not interested in learning. I am using the strange video format because I found no good way to get a PDF of a GPT dialog.

The materials the custom GPT has available are centered around biomolecules, so the large part of the Jmol functionality useful for small molecules and inorganic solids is not addressed. It is using "few-shot learning" - instead of providing the entire manual, I gave it half a dozen annotated scripts, together with a workflow and a cheat sheet. The cheat sheet was developed through a dialog with another AI, Claude, which "came up" with the chosen format (general syntax, explanation, example). The annotated scripts are based on Jmol scenes from Proteopedia.

The performance of the system is oddly bimodal. Sometimes it works great, and sometimes it fails spectacularly. However, having quality control from the user (by pasting the script into Jmol Simple) helps to spot the failures, and troubleshooting is a good learning strategy (for the student, not for the AI who forgets the conversation right away).

Here are some things Jmol Jane was good at in my experience:

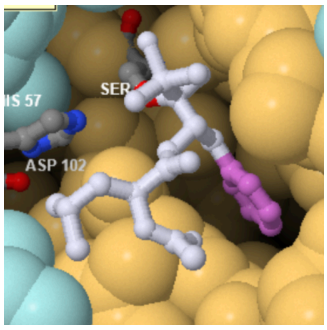
1) Syntax - almost every script runs without crashing
2) Following the examples of defining a subset of atoms first, and then using that named set in the figures
3) Responding to suggestions for improvement

Here are some of Jmol Jane's weak spots:

1) Saying that it looked something up when really it was hallucinated
2) Interpreting images (but see my anecdote below)
3) Orienting the 3D scene (the user can do this and report on the result of "show moveto" to incorporate the first view into the script)
4) Making sure the user contributes sufficiently to the conversation (the GPT tutor is much to verbose, even when instructed otherwise)

Finally, I want to share an anecdote (from the second video) that surprised me. I asked for an overall view of hemoglobin. The first try was zoomed in too much. The second try, properly zoomed, did not show a tetramer. I uploaded the image and said, "I thought this is a tetramer". The bot replied something like "Oh, it shows as a dimer" (not sure whether this was from image analysis or from figuring out the technical problem in the script) and changed the script to load biomolecule 1. I am puzzled how it figured that out - the example scripts did have one instance of "filter biomolecule 2", but the cheat sheet did not mention this topic, which everyone will eventually stumble over. Because the custom GPT is based on an LLM trained on almost the entire internet, it is not clear when this background data surfaces, and when the GTP utilizes the provided specific training material.

If you want to play with the tutor in the next two days, here is the link again: https://chatgpt.com/g/g-67ef4a0925d48191a63120240716bf95-jmol-jane



ChatGPT - Jmol Jane

Structural biology tutor for Jmol scripting.

chatgpt.com

Best,
Karsten