Expert Feedback from Dr. Lin

As the user feedback is important to the development of autonomous tools for wet-lab. I wish to obtain some comments from first-hand chemistry researcher. Therefore, I invited Dr. Lin, a PhD in Organic Chemistry from the University of Oxford and a close friend of mine, to share the following thoughts after trying out the system:

Feedback: The assistant is quite handy for quickly looking up molecular properties like logP, TPSA, or finding similar compounds based on structure. The way it brings together tools like PubChem, RDKit, SmallWorld, and PDB under one roof is genuinely helpful, especially for fast screening.

In a research setting though, we often rely on literature sources like **Google Scholar** or **SciFinder** to get insights into mechanisms, conditions, or biological relevance—things that structured data alone can't capture. That said, the integration of Google Patents is a good step for exploring commercial potential and keeping an eye on IP landscape. If future versions could pull in academic literature or even reaction data, that would really bring it closer to how researchers think and work in practice. — *Lin*

Comments: we can potentially develop the tool to integrate Scholar search and other research tools, so that the they can support chemical research whilst the Patent can reflect the commercial values of chemicals. — *Xi Chen*

My Learning and Thinking Reflection

Working on this chemistry assistant has been a great learning journey. I started by trying to figure out how to avoid hallucinations from the language model—where it might make up data. Instead of letting the model guess, I designed a system where it plans what needs to be known and uses real tools to get accurate answers.

One of the most interesting parts was understanding how different identifiers—like PDB IDs, molecular formulas, chemical names, and SMILES—connect to each other. I didn't expect PDB entries to be so complex, often linking to multiple components. That pushed me to think more carefully about how to extract and normalize information.

I also realized how different types of data serve different needs: patents are great for seeing if something might have commercial value, while papers and literature are still the go-to for scientific understanding. That distinction really shaped how I thought about future directions for the system.

— *Xi Chen*