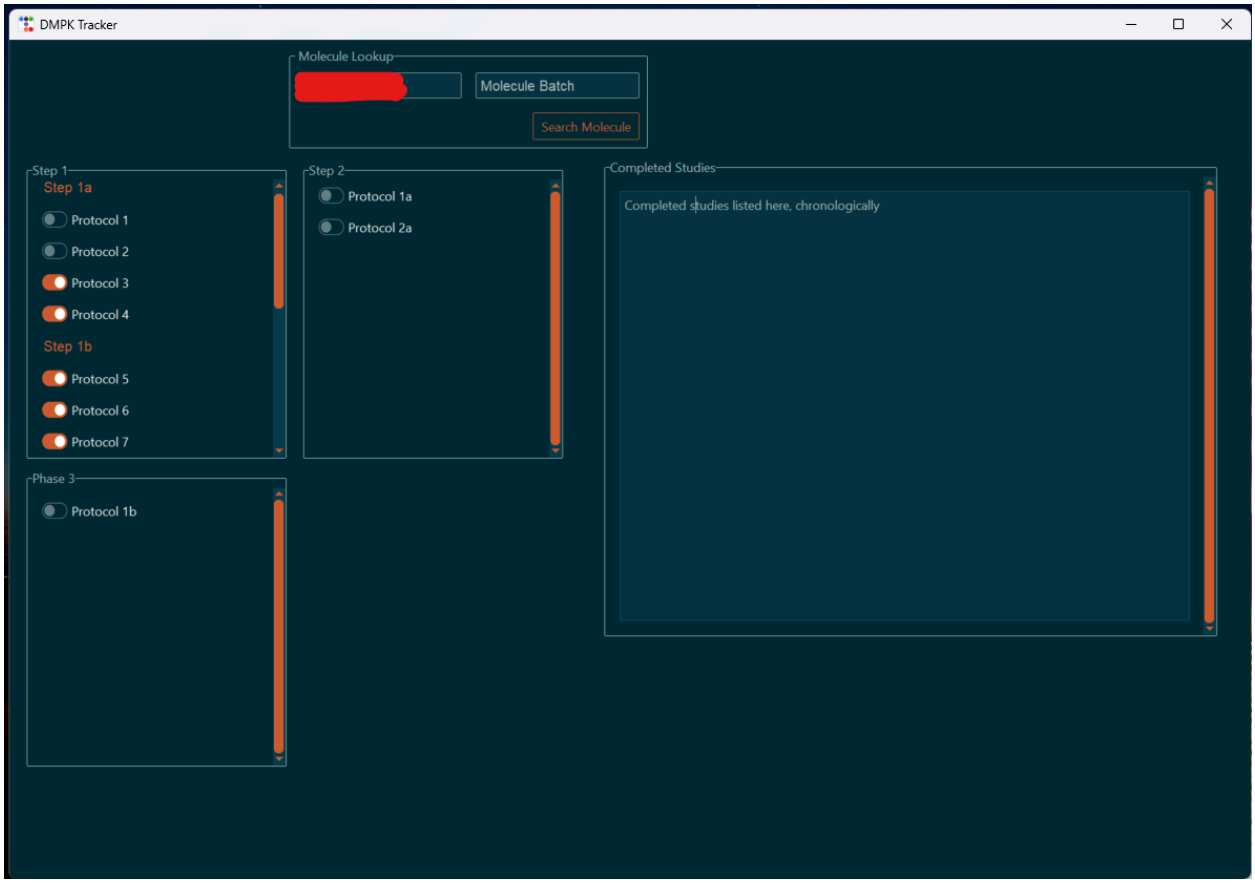
Introduction -

In the realm of small molecule discovery, companies often sift through or generate thousands of molecules before selecting a lead candidate for clinical trials. Assessing the potency and tolerability of these compounds is a data-intensive task, posing a significant challenge to efficient tracking. While many companies turn to commercial databases dedicated to storing the outcomes of these studies, these databases often lack configurability. Their user interfaces are typically inflexible and do not permit user adaptation.

DMPK studies are time-consuming and financially demanding endeavors. To minimize financial risks, companies evaluating numerous compounds must establish a systematic flow-scheme that dictates the sequence of studies based on their priorities for a 'successful' molecule. For instance, a company might decide that 'Molecule-1001' must demonstrate tolerable results in CYP450 induction, LM toxicity, and Nerve Binding Affinity before progressing to Phase 2 DMPK studies. Study databases may display which studies have been uploaded for a particular compound, but they seldom empower users to design a system as described above.

This program was built with this issue in mind. Users can input the name of a molecule of their choice, It then queries the API of a database and retrieves the completed protocols that are associated with that molecule. Importantly, it allows the end user to configure their own display, customizing it to accommodate any flow scheme they desire. Below is an *example image of this program in action:



*Note: This GUI has been altered to preserve sensitive confidential information. The molecule name in the search engine has also been blocked out for the same reason.

Under The Hood -

This program was built using Python scripting, in combination with tkinter, and ttkbootstrap. Tkinter is a standard toolkit for GUI development in Python, making it easy to build desktop applications with interactive elements. Likewise, ttkbootstrap is a Python package that enhances Tkinter by incorporating the popular Bootstrap feel. It brings modern and visually appealing styling options to Tkinter.

The source code of this project has been altered to remove sensitive, confidential information. The skeleton structure of the program is well documented and easily modified to fit user needs. There are three main parts: 1) the search engine, which connects to the API, 2) the frames which house the DMPK studies of your choice. These study names have been changed to “protocol _”, but should be updated to match whatever name they have in the DMPK database, 3) the dictionary at the end of the program which has a key:value pair that feeds back into the functions, update_checkboxes(). Every protocol needs to be entered into the dictionary so that the state of checkboxes can be changed. When Querying the database, a string of protocol names associated with that molecule should be returned, and then compared to the dictionary. If there is a match, the corresponding checkbox is toggled on.