PRESENTATION TITLE: *Accelerating Drug Discovery in Academia and Industry with Just a Few Clicks- Accessible Computational Workflows to Design Custom Experiments*

ABSTRACT: Several design and analysis tools are available to chemists for routine usage, like NMR, chromatography, and spectrometry. Computational tools are still under-utilized by bench chemists to design, rationalize, and analyze their everyday experiments. Molecular Forecaster believes that computer-aided molecular/drug design should be accessible, accurate, and ubiquitous in laboratories. Here, we present our fully integrated and fully automated modular workflows; any chemist can test their molecules with a few clicks. For example, before stepping up to the bench, you could simulate the synthesis of a reagent required to catalyze a separate chemical reaction used to design a series of drug candidates. You could then compute accurate depictions of these products binding to your protein target and of their metabolic liabilities to cytochrome P450s.