ChemCrow-Reaxys: An LLM-Powered Chemical Agentic Workflow Solution

The ChemCrow-Reaxys project aims to develop an advanced LLM-based agent system that leverages the comprehensive Reaxys chemistry database through its API. Building upon the successful ChemCrow framework [1], this system will assist chemists in complex tasks such as reaction planning, literature search, and compound property prediction while ensuring all recommendations are backed by peer-reviewed sources.
The development process will focus on creating specialized tools for structure search, property retrieval, and reaction condition optimization, while simultaneously building a robust benchmark suite to measure the system's performance. Key metrics will include prediction accuracy, API cost efficiency, synthesis planning success rates, and overall response time. The project will require approximately 4-6 months to complete, with deliverables including a working prototype, comprehensive benchmark results, and detailed documentation of the system's capabilities and limitations.

It will be at EPFL but in collaboration with Reaxys.

[1] https://www.nature.com/articles/s42256-024-00832-8

Contact :

Philippe Schwaller
Tenure-Track Assistant Professor

Laboratory of Artificial Chemical Intelligence | LIAC
Institute of Chemical Sciences and Engineering | ISIC
School of Basic Sciences | SB

philippe.schwaller@epfl.ch
schwallergroup.github.io