An Automated, Calibration-Free Platform for High-Throughput Reaction Screening and Data Analysis

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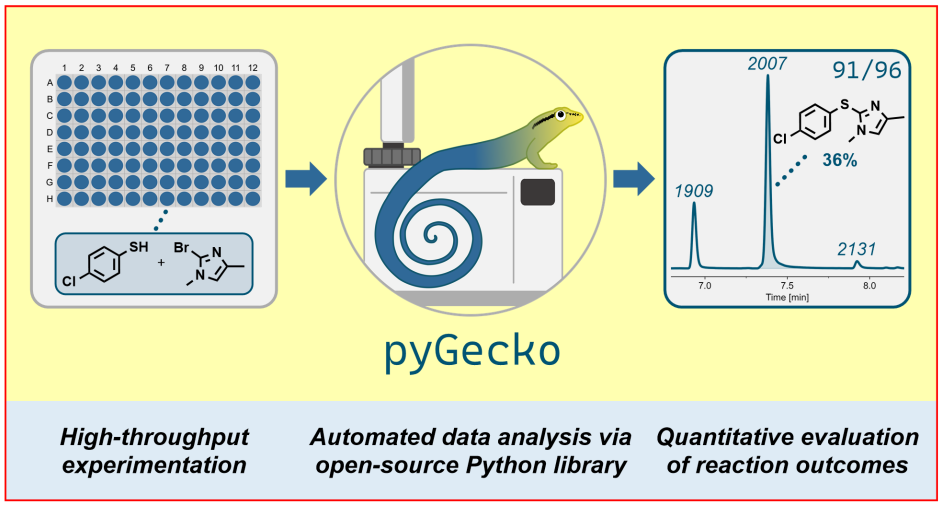

Figure 1: Workflow comprising automated reaction setup and workup, GC-MS and GC-FID analysis, and data processing via the open-source pyGecko library.

As AI-driven chemistry advances toward fully autonomous self-driving laboratories (SDLs), limited access to specialized instrumentation and efficient analysis of experimental data remain critical bottlenecks. Here, we address this challenge by introducing a semi-automated, high-throughput experimentation (HTE) workflow integrated with **pyGecko**, an open-source Python library for automated analysis of chromatographic data. This workflow eliminates the need for manual calibration by combining a flexible liquid-handling platform, GC-MS and GC-FID analysis, and automated data processing via pyGecko. This pyGecko library enables interpretation of measurements in the context of the experiment, including identification of internal standards and analytes based on retention times, molecular-ion or fragment masses, and spectral matching. Analytical outputs, together with chromatograms and spectra, are visualized and reported in standardized formats such as the Open Reaction Database (ORD) schema. The utility of the workflow is demonstrated through a scope evaluation of a site-selective thiolation of halogenated heteroarenes, and through a comparison of four cross-coupling protocols for challenging C–N bond formation. While fully functional as a stand-alone tool, this open-source framework is designed for seamless integration into closed-loop optimization workflows, enabling the next generation of accelerated chemical discovery.