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Towards Autonomous Robotic Systems

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RoboChemTaxy: A Taxonomy of Robotic Manipulation for Chemistry Lab Automation

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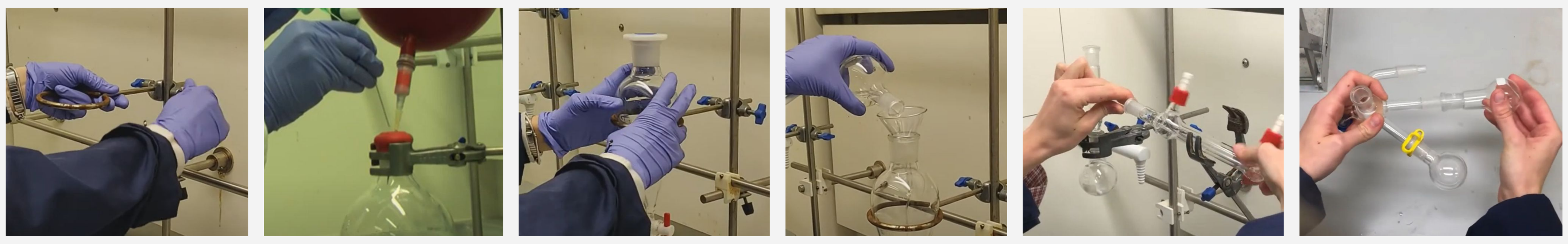
Motivation

- Chemistry automation has long been a goal for increasing experimental throughput, safety, and reproducibility. Traditional systems, however, are often highly task-specific—relying on custom hardware and fixed workflows, making them **difficult to generalize** across experiments or labs.
- Recently, robotic arms have emerged as a flexible alternative, capable of mimicking human manipulation and adapting to a wide range of chemical tasks. Yet most researches still focus on isolated case studies or specific pipelines, lacking a **systematic analysis** of how these systems are structured.
- This taxonomy addresses that gap by **categorizing and analyzing robotic chemists manipulations**, aiming to guide future development with clearer design principles and shared vocabulary.
- Furthermore, it aligns with the emerging **Model Context Protocol (MCP)** paradigm, enabling **a unified interface** from large language model (LLM) planning to low-level robot execution. This **bridges symbolic reasoning and physical action** in a modular and reusable way.

Taxonomy



core experimental skills taught to undergraduate chemistry major,
78 videos from "Chemistry Teaching Labs – University of York" YouTube channel

Force Sensitivity	**Control Directness**	**Motion Pattern**
Required precision in applied force	Direct or mediated object interaction	Single or repetitive movement
✔️: piercing ❌: placing	✔️: twisting ❌: pouring	✔️: dipping ❌: stirring

Three key dimensions derived from videos capture **essential patterns** for robotic manipulation in chemistry. We then define **four manipulation categories**, each with distinct variations with details shown in diagram on the right.

This taxonomy supports **benchmarking**, **skill decomposition**, and serves as a foundation for **learning from demonstration** (LfD) pipelines. This taxonomy highlights **fundamental manipulation challenges** currently underexplored in robotics. By formalizing these patterns, we aim to guide future research toward more generalizable and capable robotic chemists.

Positioning

Precise placement of objects by overcoming minor resistance to reach a desired pose.

- **Static Positioning** — Place without reorienting
- **Insertive Positioning** — Fit into constraint
- **Rotational Positioning** — Adjust orientation

Coupling

Joining or separating objects using controlled force to overcome resistance or deformation.

- **Forced Coupling** — Linear push/pull
- **Penetrative Coupling** — Force to pierce a barrier
- **Rotational Coupling** — Rotate with torque
- **Elastic Coupling** — Temporarily deform material

Tooling

Indirect manipulation of materials using tools or mediated forces such as gravity or pressure.

- **Squirting** — Apply pressure to dispense
- **Pouring** — Tilt to guide liquid flow
- **Dropping** — Fall into place by gravity
- **Scooping** — Gather powders with a tool
- **Dipping** — Submerge in liquid to collect

Agitating

Repetitive or periodic motion used to mix, clean, or interact with materials.

- **Swirling** — Gentle circular motion
- **Shaking** — Vigorous motion to mix
- **Twisting** — Axial rotation to spread
- **Stirring** — Use of a tool to blend
- **Wiping** — Dragging tool across surface

Natural Language Control

🧑‍🔬 **Chemist** — Natural Language — 🤔 **LLMs** — Taks Planning Functional Calls — **MCP Server**

- The **Model Context Protocol (MCP)** provides a standardized interface between LLMs and external tools, enabling **seamless communication** between high-level task planners and low-level robots control. MCP is **model-agnostic** — supporting integration with different or customized domain specific LLMs.
- Built on our taxonomy, manipulation steps can be composed into **modular macros**, which act as reusable tools provided by the **MCP server**. LLMs can orchestrate complex experimental procedures by invoking these macros through **function-calling**.
- Laboratories can easily **customize or extend** these macros to fit their specific workflows. New skills can even be taught through **one-shot demonstrations,** eliminating the need for manual programming and improving adaptability across labs.

MCP Server

🛠️**Setting up Separating funnel**
- **Static Positioning** Clamp
- **Twisting** Clasp Screw
- **Insertive Positioning** Separating Funnel

Pouring X ml Liquid
- **Static Positioning** Cylinder
- **Pouring**🔁 Flask containing liquid
- **Pouring** Cylinder with liquid

🧑‍🔬**User Defining / One-shot Learning -> Macros**

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