

# Robotic Drug Discovery

An Automated **Design** and **Synthesis** System  
to Boost SAR Investigations

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# Automated Compound Design & Automated Compound Synthesis: Research Automation for Functionalized Molecules

Goal: Unmanned system for computational design and robotic synthesis 24 hours a day, 365 days a year  
 Autonomous research of drug candidates with cycles of hypothesis testing approach in the real world  
 Identification of potent compounds comparable to a clinical candidate in the test run

**Analysis of Synthesis Paths for Designed Conditions**



**Retro-synthesis**

Photo: Nakamura Choukou Co.,Ltd.



**Synthesis**

**Multi-channel Flow Reactor Integrated with Preparative Chromatography**

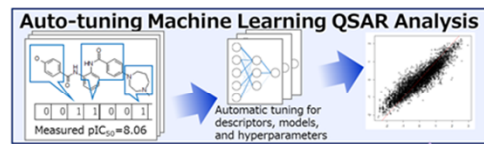
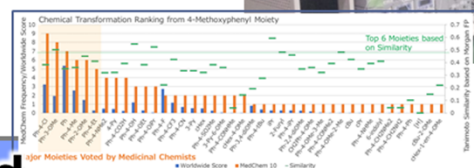
**Various Assays in Real World**

**1<sup>st</sup> Screening**

**Additional Assays**

**Design Based on Big Data Analysis in Medicinal Chemistry**

**Compound Design**



**Quantitative Profile Analysis with Machine Learning Technology**

**Library Screening**

**Profile Analysis**