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Mitsui Chemicals, Inc.
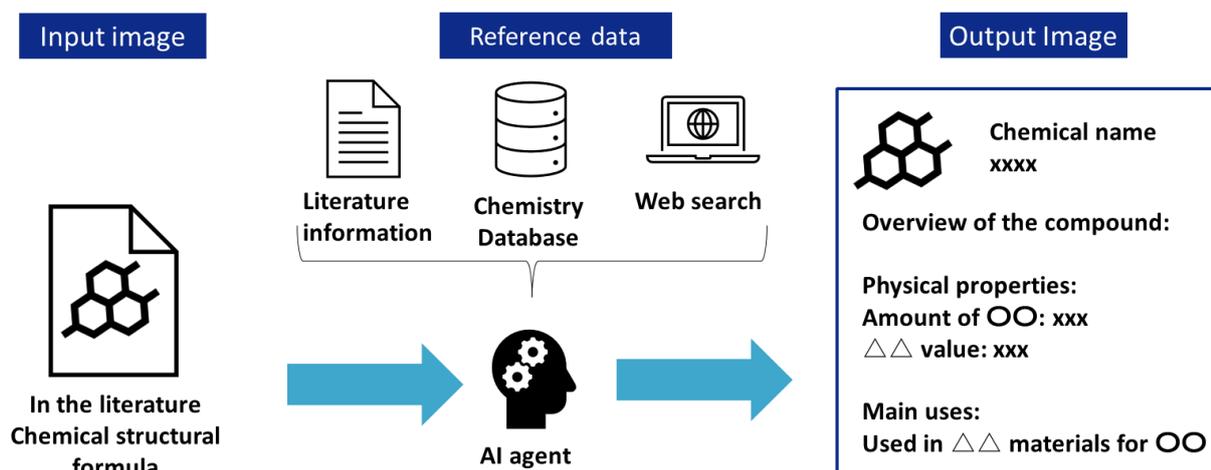
Mitsui Chemicals Develops AI Agent to Revolutionize Literature Reviews in R&D

Autonomously extracting compound information from chemical structural formulas to reduce literature review time by 80 percent or more

Mitsui Chemicals, Inc. (Tokyo: 4183; President & CEO: HASHIMOTO Osamu) today announced that it has developed its own AI agent that autonomously investigates and organizes information about compounds based on chemical structural formulas described in scientific literature and research reports, and has begun an in-house pilot trial of the AI agent. As initial verification confirmed that the agent could reduce the time spent by researchers on literature review by at least 80 percent, the company aims to complete the pilot trial before the end of fiscal 2025 and bring the AI agent into full-scale operation in fiscal 2026.

The investigation of compound information found in patent literature and academic papers is an essential part of chemical R&D. However, in the case of polymers and organic compounds with complex structures, it is difficult to accurately identify a compound's name from its structural formula alone. Until now, researchers have had to expend enormous time and effort in manually checking vast amounts of literature, piece by piece, to determine the correspondence between chemical structures and compound names. By combining the use of the newly developed AI agent with the chemical expertise of the company's researchers and engineers, Mitsui Chemicals has achieved the automation of advanced literature searches in a manner that was not possible using conventional methods.

This AI agent enables AI to read chemical structural formulas – something that had previously been unfeasible – and thereby allows AI agents to employ image and text information from literature in an integrated manner to autonomously identify and extract information about compounds. In addition to identifying compound

Input image

Reference data

Output Image

Literature information

Chemistry Database

Web search

In the literature Chemical structural formula

AI agent

Chemical name
xxxx

Overview of the compound:

Physical properties:
Amount of ○○: xxx
△△ value: xxx

Main uses:
Used in △△ materials for ○○

names, the AI agent can simultaneously obtain related information recorded in the literature, including uses, physical properties, manufacturing methods and experimental conditions. Furthermore, the agent generates more comprehensive compound information after consulting chemical databases and web search information if needed. It is also equipped with a report generation feature tailored to researchers' needs, which organizes the survey results into a format that supports subsequent analysis and decision-making.

Initial validation confirmed that literature reviews conducted using this AI agent reduced the time spent by researchers on investigation by at least 80 percent. Literature reviews that previously took about a month were shortened to a day or so, allowing researchers to spend more time focusing on creative R&D activities.

Mitsui Chemicals will continue utilizing cutting-edge digital technologies to address social challenges with the power of chemistry, and to contribute to a sustainable society through the creation of diverse value.