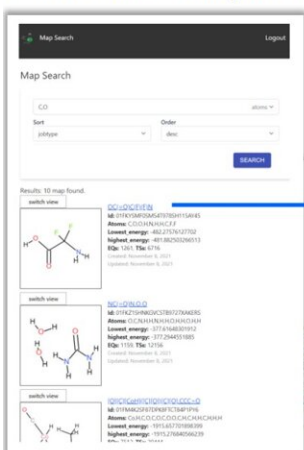


# A user-friendly platform for virtual exploration of chemical reactions

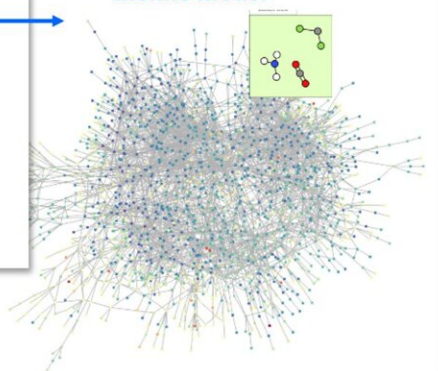
July 3 2023

Search for reaction path network

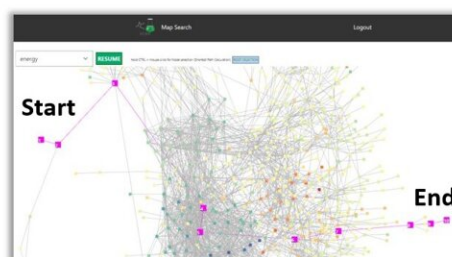


Network visualization

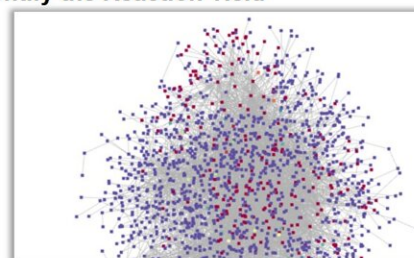
Mouse over to display atomic model



Shortest Path Calculator



Identify the Reaction Yield



**SCAN-GUI: Data analyses and data visualization for scientists**

Searching Chemical Action and Network (SCAN) has a graphical user interface (GUI) that can be used for data analyses and data visualization. Credit: Keisuke Takahashi

A new online platform to explore computationally calculated chemical reaction pathways has been released, allowing for in-depth understanding and design of chemical reactions.

Advances in [computational chemistry](#) have lead to the discovery of new

reaction pathways for the synthesis of high-value compounds. Computational chemistry generates much data, and the process of organizing and visualizing this data is vital to be able to utilize it for future research.

A team of researchers from Hokkaido University, led by Professor Keisuke Takahashi at the Faculty of Chemistry and Professor Satoshi Maeda at the Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), have developed a centralized, interactive, and user-friendly platform, Searching Chemical Action and Network (SCAN), to explore reaction pathways generated by computational chemistry. Their research was published in the journal *Digital Discovery*.

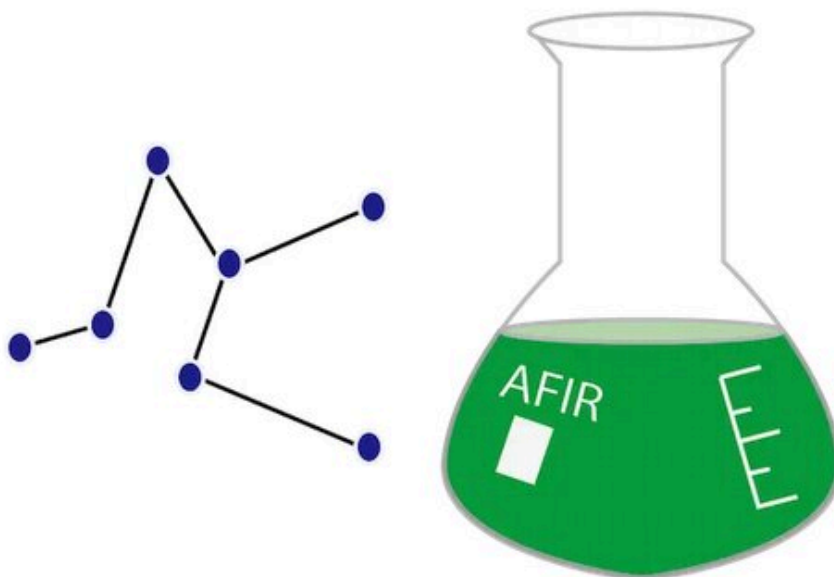
"From a computational viewpoint, [chemical reactions](#) can be considered as extremely complex networks that consist of numerous molecular interactions," explains Takahashi. "Many tools have been developed to calculate these networks, such as the AFIR method we use at WPI-ICReDD. However, tools to explore these calculated networks are also needed, which led us to the current study."



Map Search

Useful Links

Login



# SCAN

Searching Chemical Actions and Networks

Get Started

Available Resources:

14 maps

84434 EQs

219784 edges

The homepage of Searching Chemical Action and Network (SCAN), the newly released platform. Credit: [scan.sci.hokudai.ac.jp/](http://scan.sci.hokudai.ac.jp/)

Broadly, all the raw data from AFIR calculations form a "data lake." This data is then subjected to a pre-processing step, creating a "data warehouse." Finally, the "data mart" accesses and retrieves data from the data warehouse and provides tools to visualize, analyze, and share the retrieved data.

"The pre-processing step is crucial," Maeda elaborates. "The raw data from AFIR contains an immense amount of information, from which the key data required for the SCAN platform must be extracted. This key data is sufficient to allow the creation of an interactive reaction [pathway](#) map which can be searched and viewed."

SCAN is accessible on the internet at <https://scan.sci.hokudai.ac.jp/>. The [source code](#) for SCAN is also publicly available.

"We have developed SCAN with a user-friendly graphic [user interface](#)," concludes Takahashi. "Users can search and explore the chemical reaction path network generated by the first principle calculation (AFIR). It will aid in achieving a detailed understanding of complex chemical reaction pathways."

**More information:** Searching Chemical Action and Network (SCAN): Interactive Chemical Reaction Path Network Platform, *Digital Discovery* (2023). [DOI: 10.1039/D3DD00026E](https://doi.org/10.1039/D3DD00026E)

Provided by Hokkaido University

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