Management of Reaction Data with the Open Reaction Database

https://open-reaction-database.org/
help@open-reaction-database.org

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ChemSpider Webinar Data Storage and Management
19th May 2026

The State of Reaction Data in the 21st Century

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The need for more & better reaction data

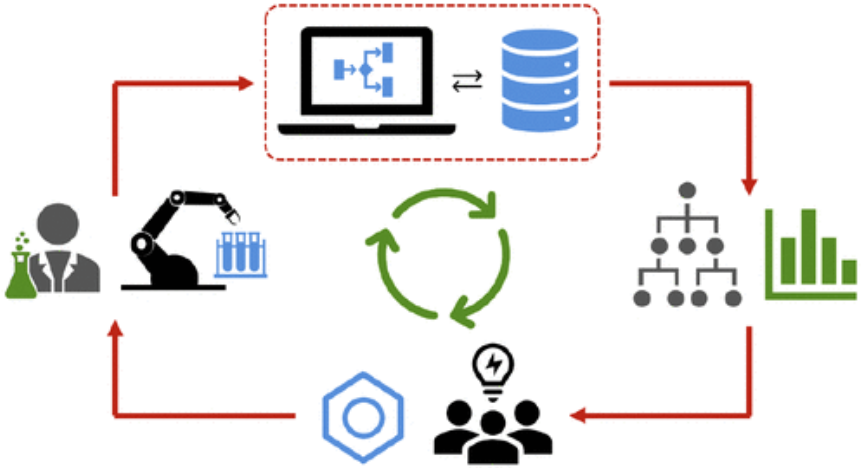
A growing chorus across the community calls for open, structured reaction data.

- **2019 —** *The digitization of organic synthesis* · Davies, *Nature*
- **2020 —** *Molecular Machine Learning: The Future of Synthetic Chemistry?* · Pflüger & Glorius, *Angew. Chem.*
- **2021 —** *Call for a Public Open Database of All Chemical Reactions* · Baldi, *J. Chem. Inf. Model.*
- **2023 —** *Data Sharing in Chemistry: A Case for Mandating Structured Reaction Data* · Mercado, Kearnes & Coley, *J. Chem. Inf. Model.*
- **2024 —** *AI for Retrosynthetic Planning Needs Both Data and Expert Knowledge* · Strieth-Kalthoff *et al., JACS*

The Open Reaction Database

- Building predictive models for chemistry relies on the availability of structured reaction data
- The ORD is an initiative to "support machine learning and related efforts in reaction prediction, chemical synthesis planning, and experiment design”

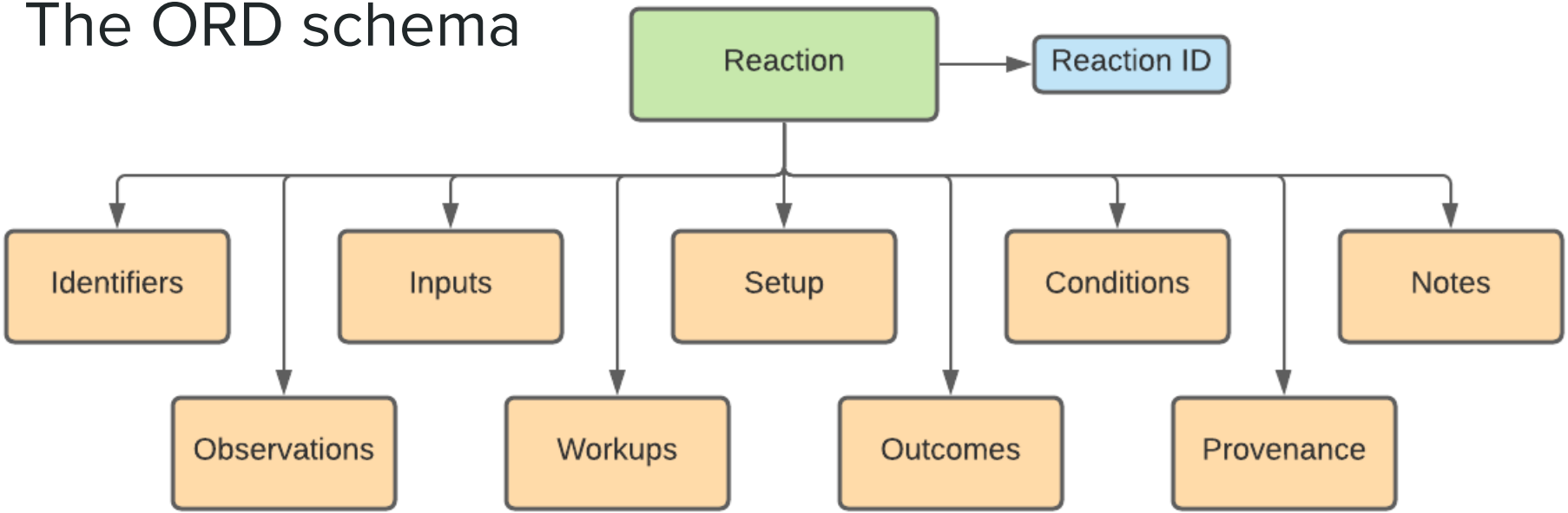
Experimenters



AI and Data Scientists

Kearnes et al. *JACS* **2021**, doi.org/10.1021/jacs.1c09820

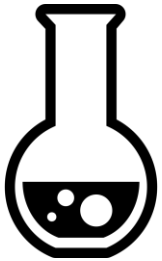
The ORD schema



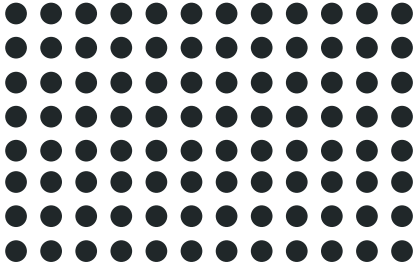
- Capture the most important aspects of reactions in a *structured* format.
- Allow additional details in a flexible, *unstructured* format.

Kearnes et al. *JACS* **2021**, doi.org/10.1021/jacs.1c09820

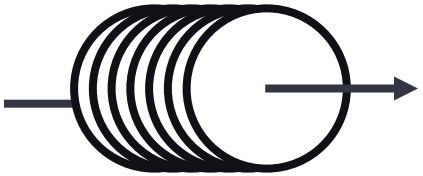
Traditional and Modern Synthesis



Batch Synthesis



Singleton or High-Throughput

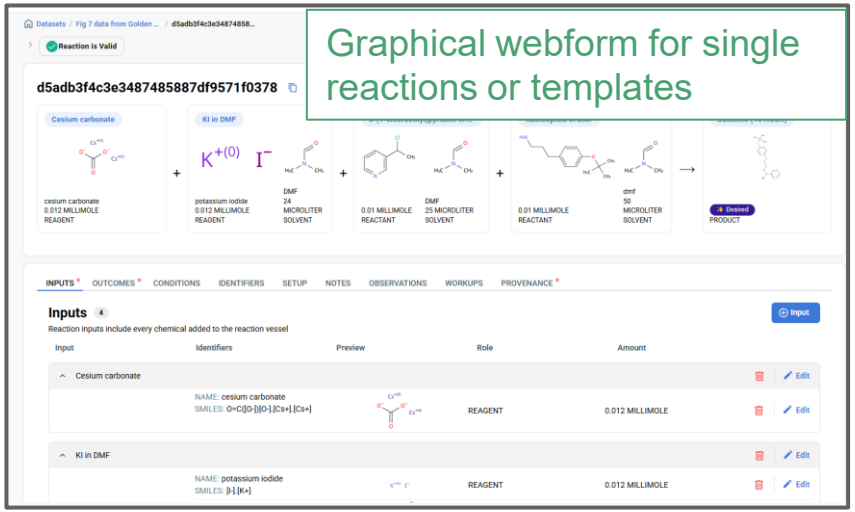


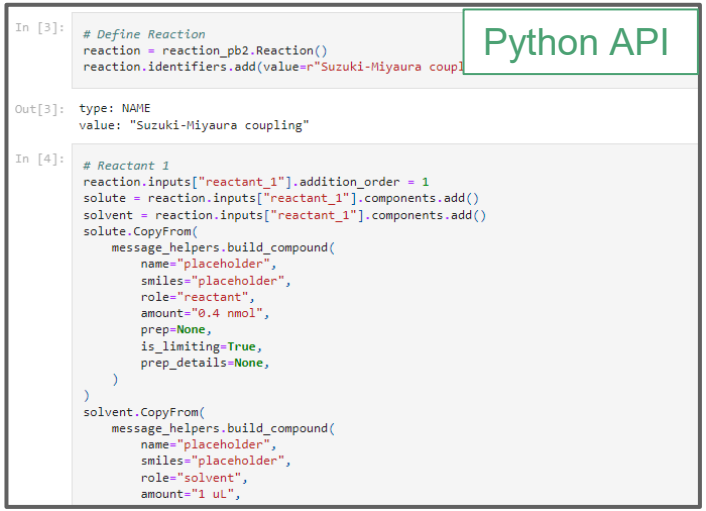
Flow Chemistry

Photochemistry

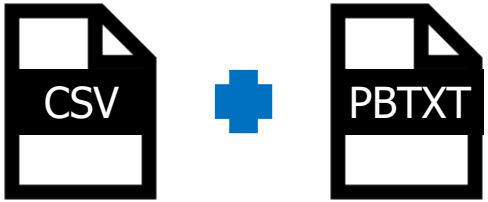
Electrochemistry

Data enumeration workflow





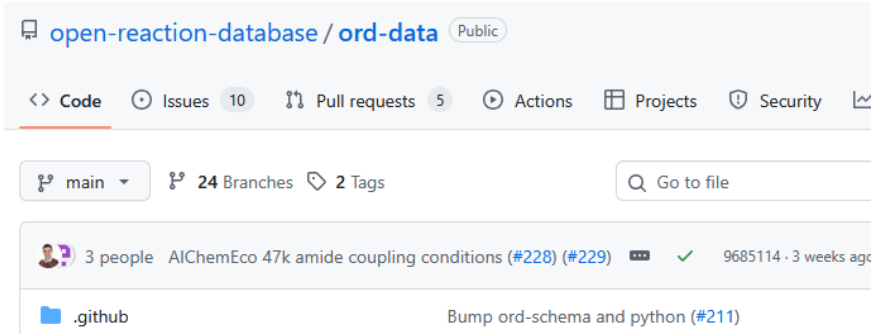
Dataset defined by iterating a template over a spreadsheet of Reactions and their changing parameters



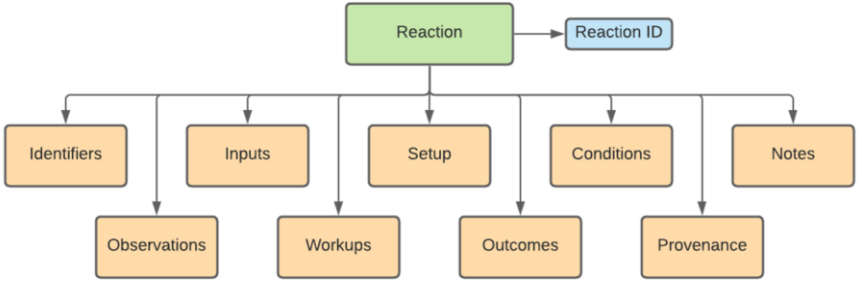
- HTE full factorial datasets
- Optimisation tables
- Substrate scope tables

ORD tools

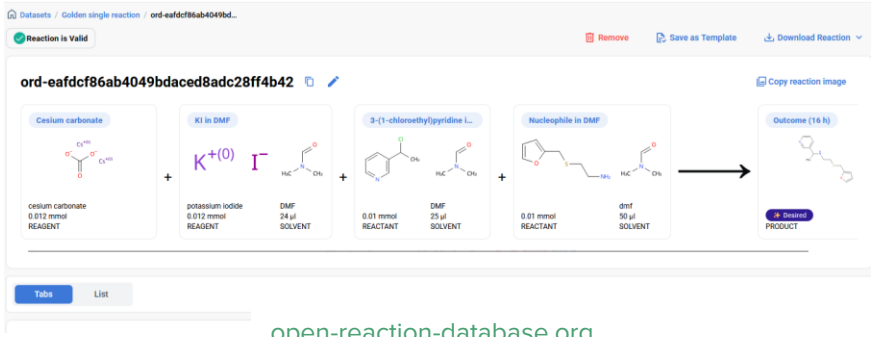
ord-data repository



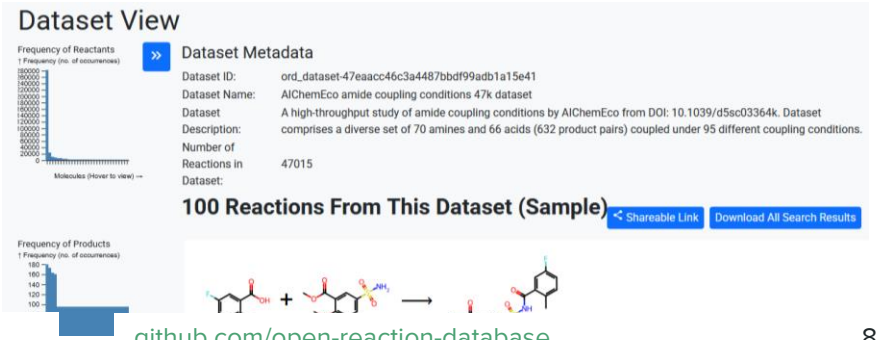
ord-schema package



ord-app reaction editor



ord-interface



open-reaction-database.org

github.com/open-reaction-database

Data stored as protocol buffers

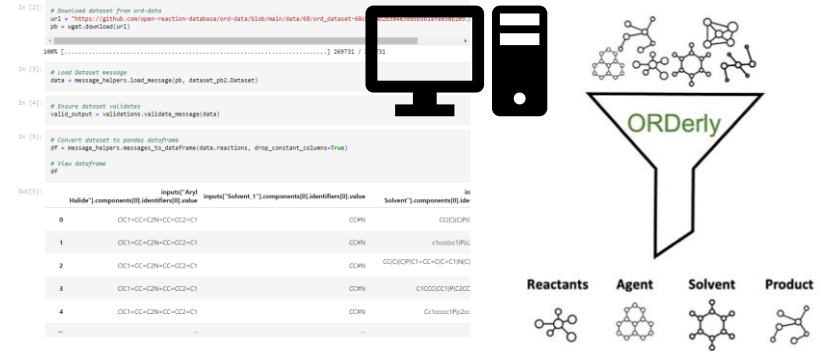
Exchangeable

ORD dataset

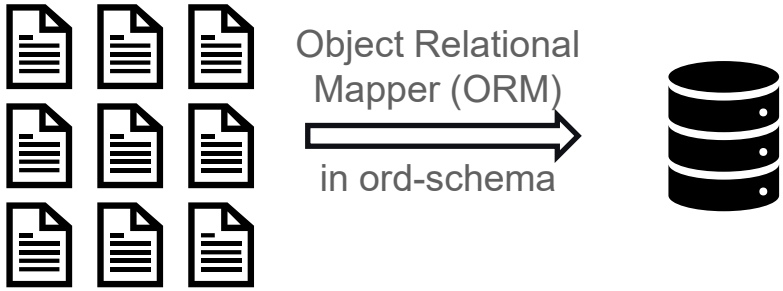
Extendable & Evolving

```
conditions {
  temperature {
    control {
      type: DRY_ALUMINUM_PLATE
      details: "additional free-text descriptions"    }
    setpoint {
      value: 80.0
      precision: 5.0
      units: CELSIUS
    } }}
```

Machine Actionable



Unpack datasets into a searchable database



collection of ORD datasets

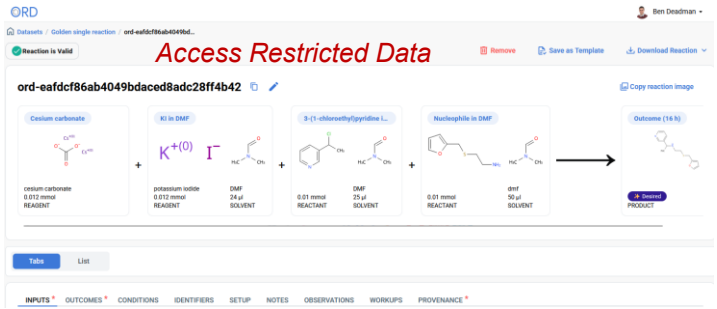
PostgreSQL database

Wigh et al. *J. Chem. Inf. Model.* **2024**, doi.org/10.1021/acs.jcim.4c00292

Open access policies

Software Vendors are also welcome to re-use ORD tools in their products under an Apache 2.0 license.

ord-app reaction editor
app.open-reaction-database.org



User initiated submission via GitHub

Public ORD Repository & Database

CC-BY-SA 4.0

optional release to public ORD

OR you can send your data to a private repository

Institutional or private repositories and/or reaction editors

Pool ORD formatted data from all repositories you have access to.

Some Quick Notices

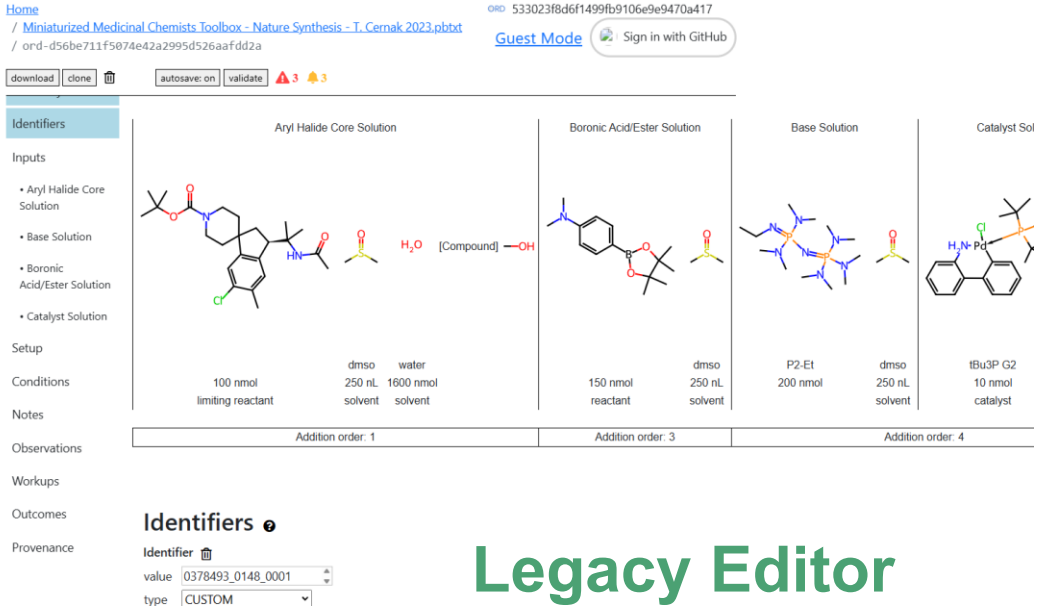
- **Dataset rewards —** $300 vouchers for eligible 2026 datasets
- **Legacy editor —** the old reaction editor is being retired

Dataset Rewards

- Receive a $300 Tremendous voucher for eligible datasets accepted in 2026
- Global participation
- 3 ways to get involved:
  - Pick from the Dataset Wishlist
  - Invited papers
  - Suggest a priority paper
- Terms and conditions apply

Closing the Legacy Reaction Editor

- New ORD Reaction Editor replaced the legacy editor in **July 2025**.
- Old editor still online at https://open-reaction-database.org/editor/dataset but will **shutdown after 31 July 2026.**
- Download your datasets if you want to keep them.



Acknowledgements

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ORDerly
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