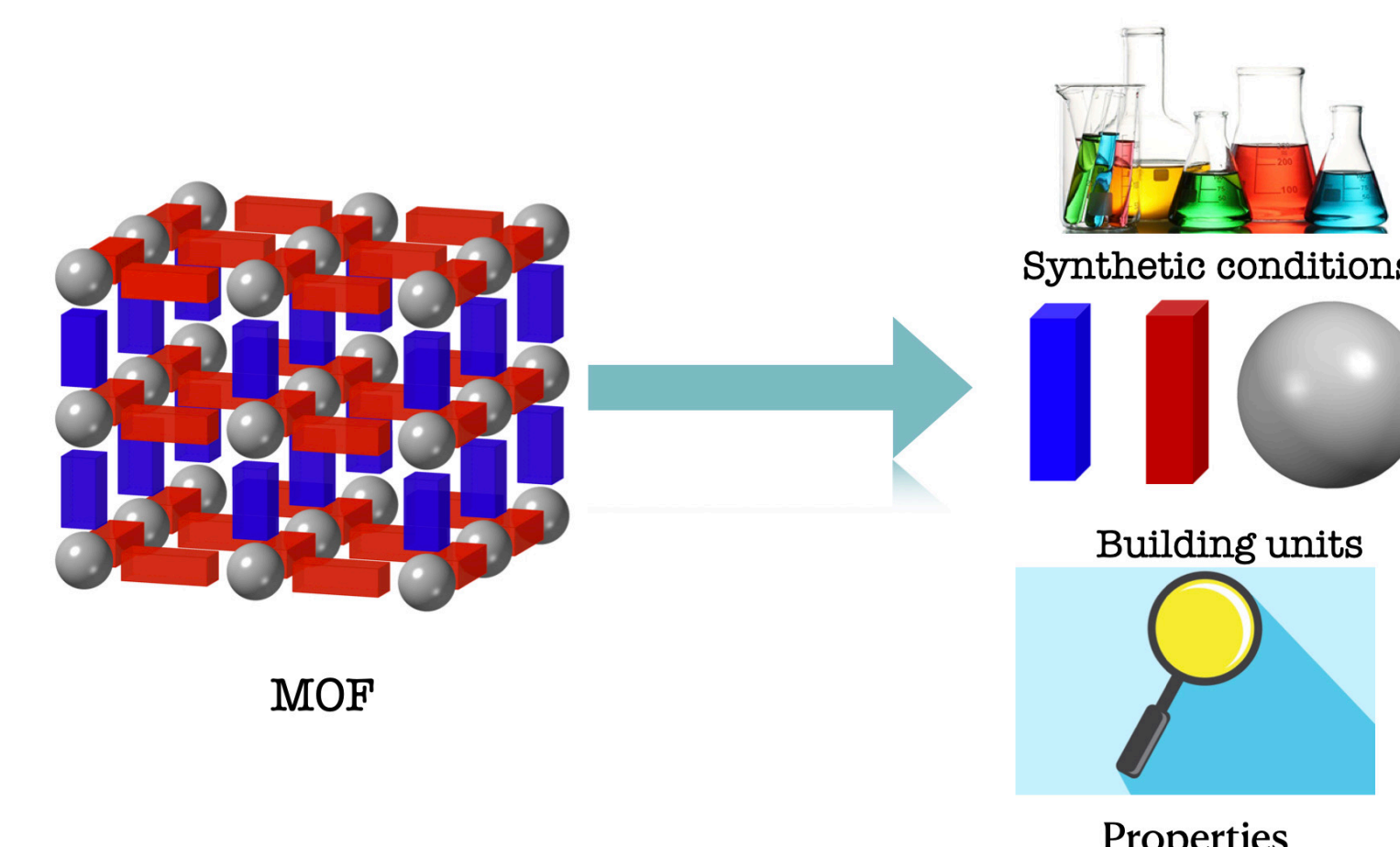
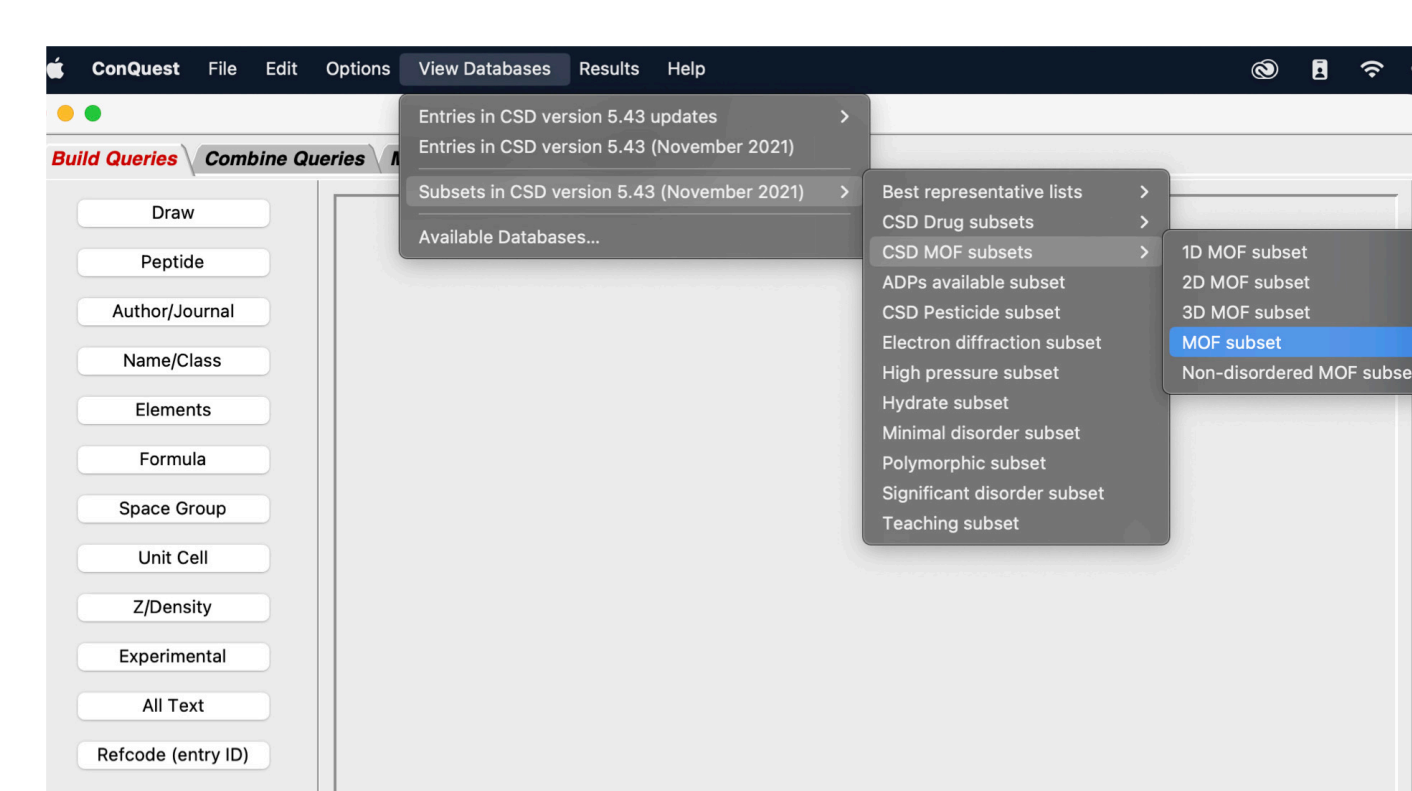


Summary

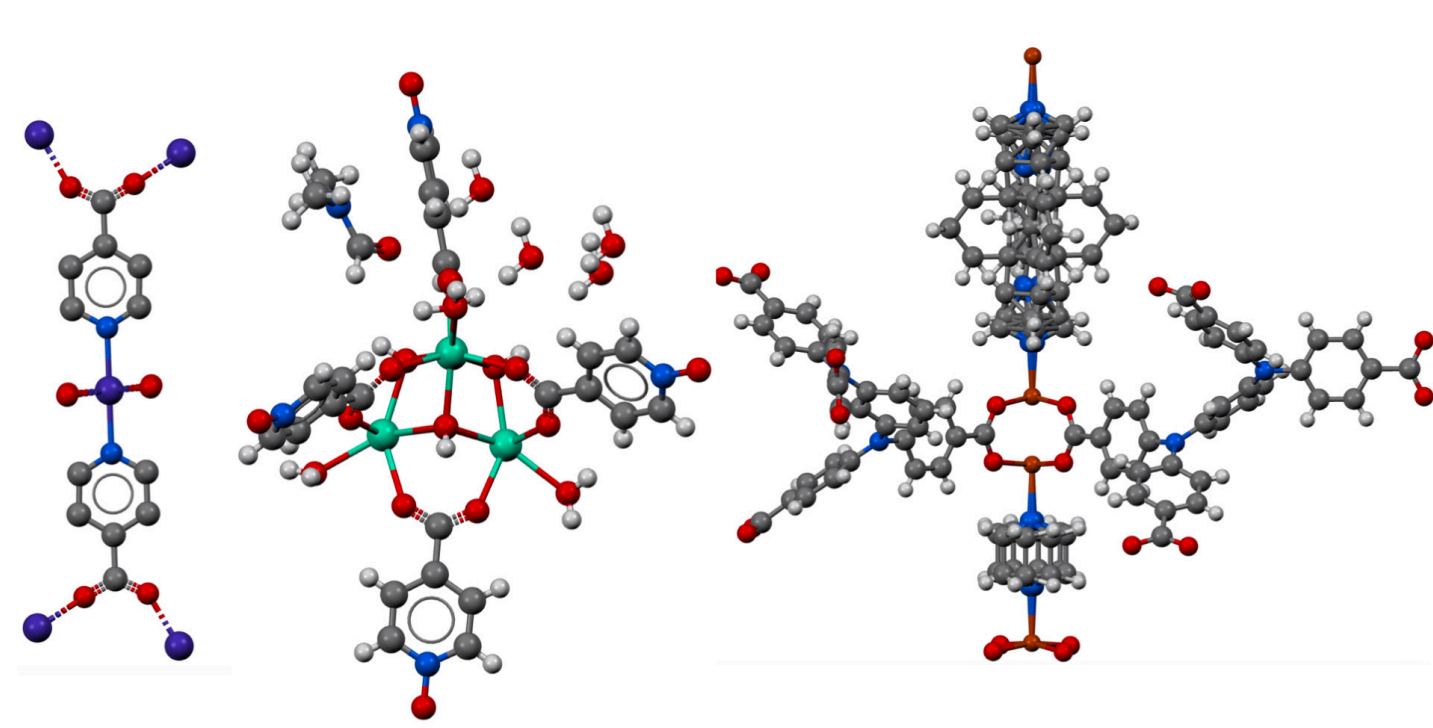
We have created a comprehensive, curated, and FAIR MOF database that maps the crystal structures of every MOF to their various properties. This database is our first step towards designing a robust model for predicting the synthesis conditions of MOFs. This tool will accelerate the discovery and synthesis of novel high-performing MOFs for targeted specific applications.



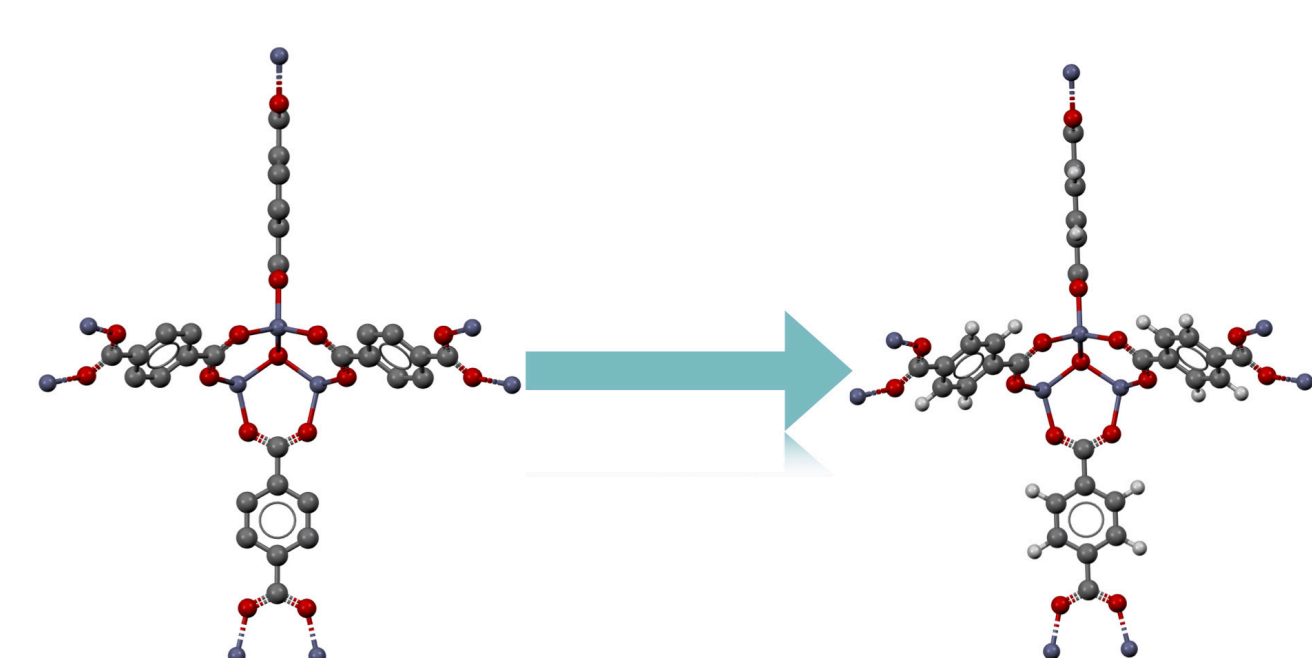
Structure, building units, and properties



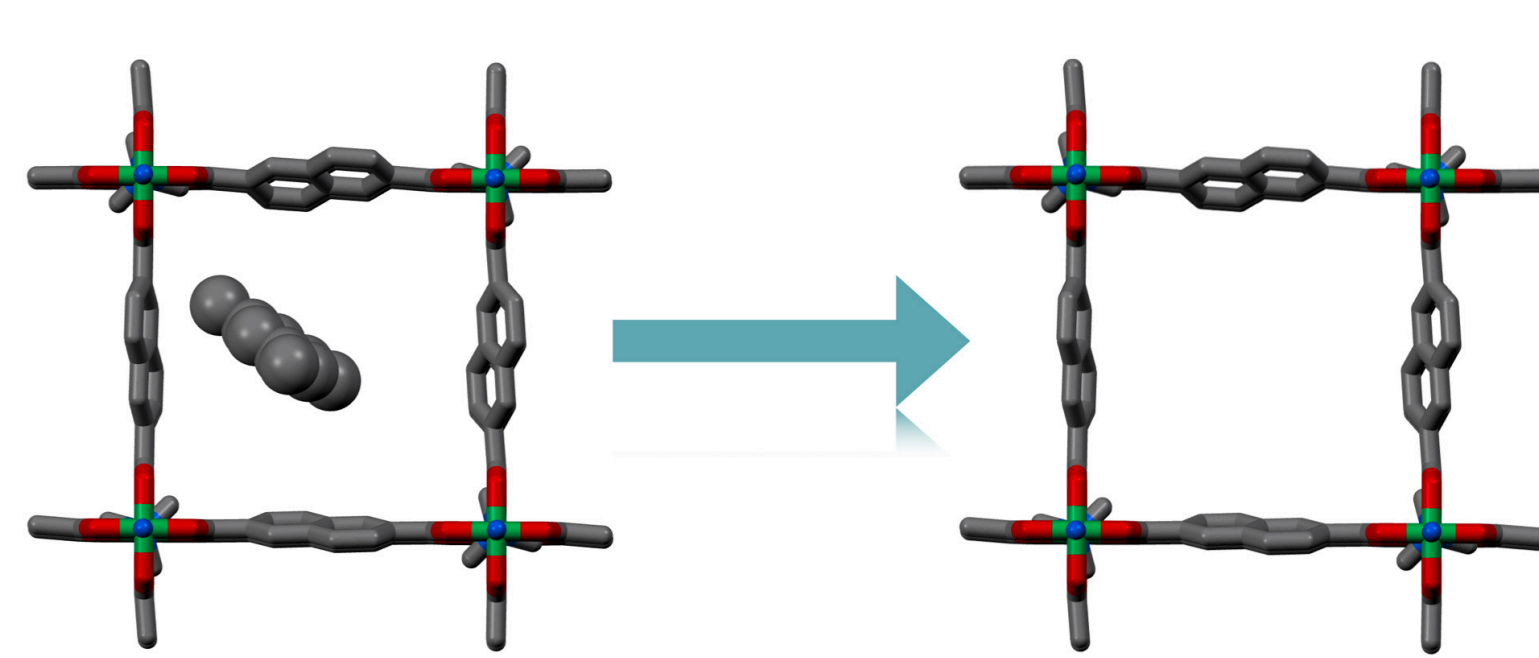
CSD MOF subset 2022



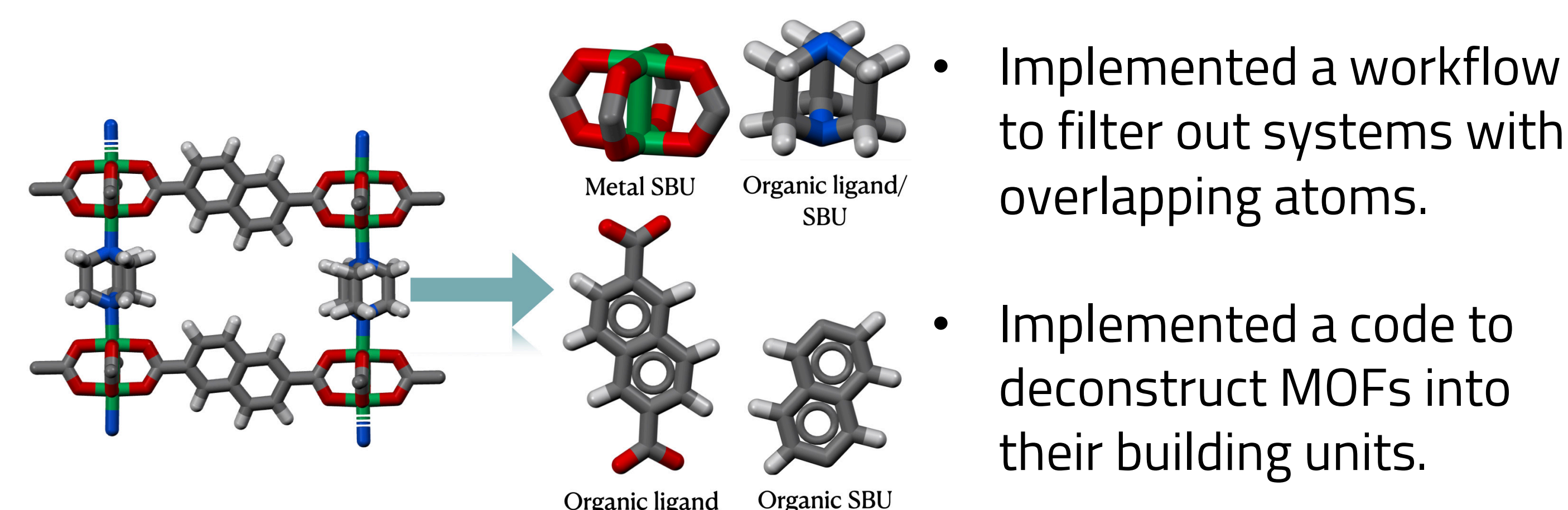
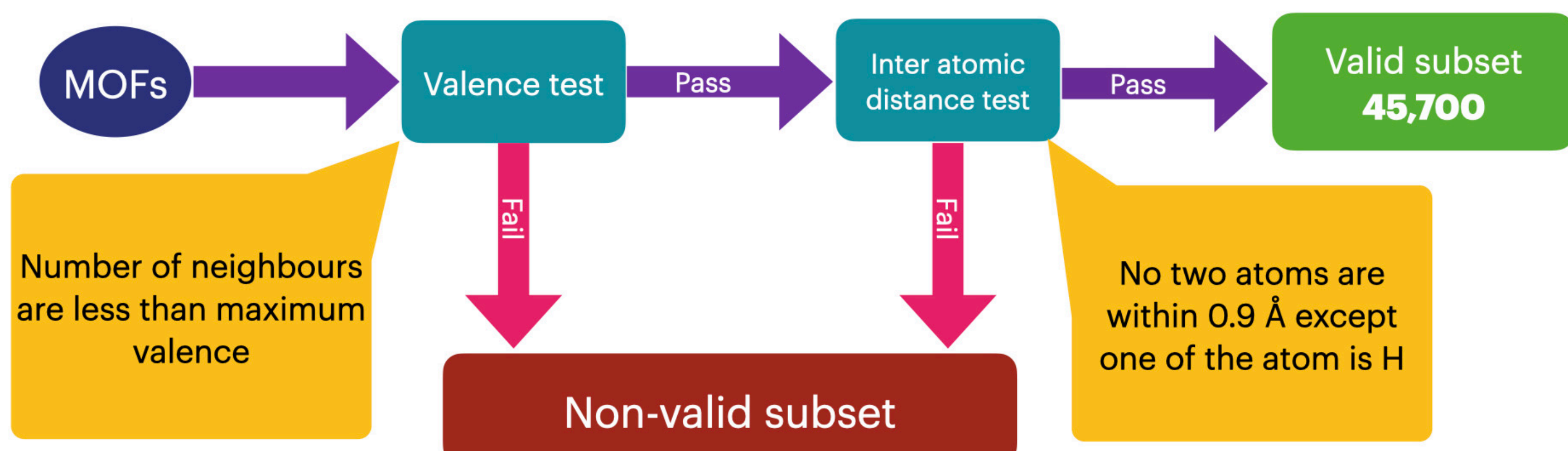
Three common errors in the CSD



Bond typing and adding missing hydrogen



Implemented code to remove unbound guest molecules

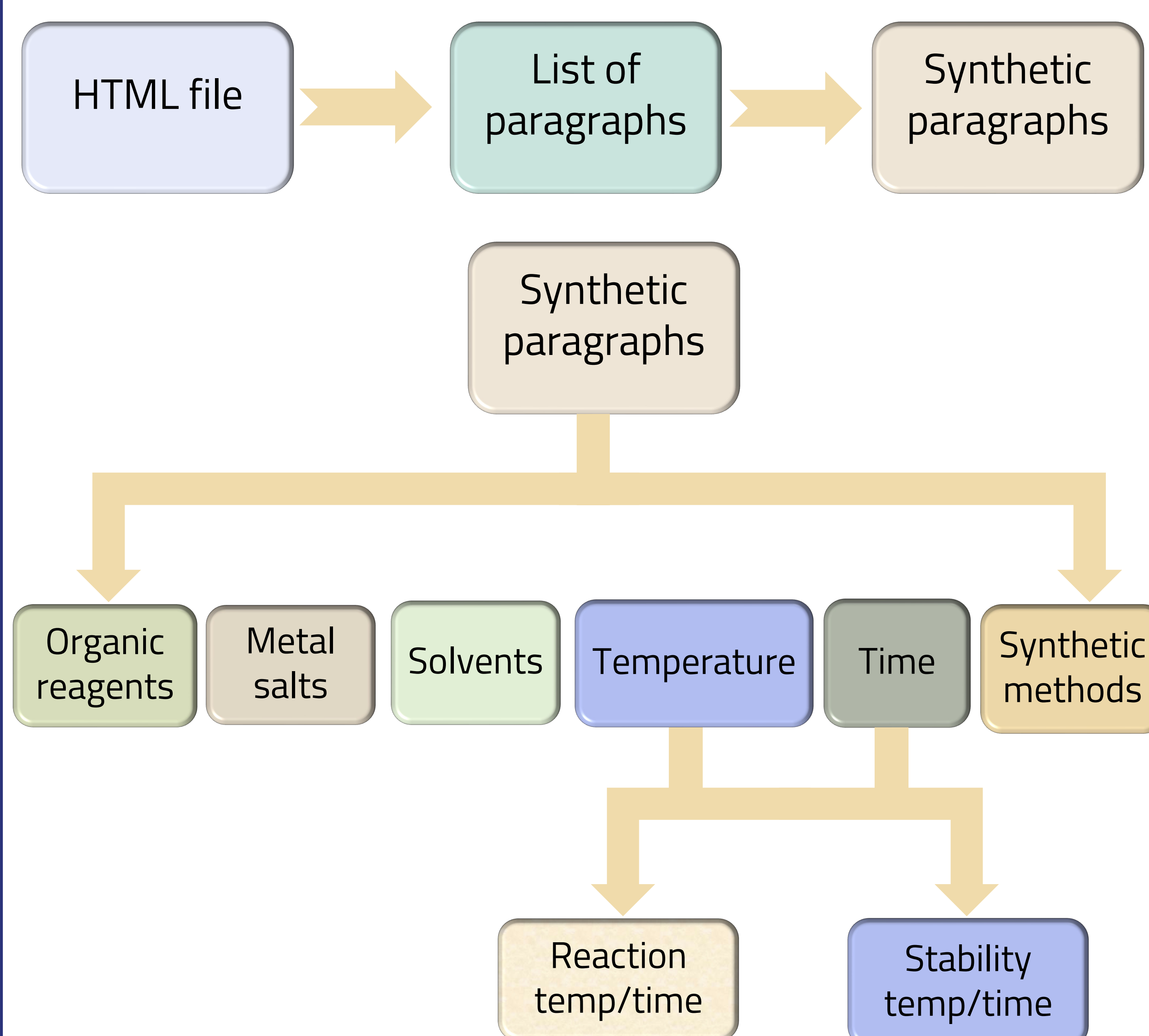


Computed properties

Topology	rCSR code
Porosity	pId, lCd, aSa, av ...
Geometry optimization	GFN-xTB
Thermodynamic stability	ΔH

Synthesis condition extraction

- ❖ Downloaded ~50,000 HTML files using DOIs from the CSD.
- ❖ Text mined the reagents and their quantities using the following procedure



There are several ambiguities in text like:

- Imprecise record of time, e.g. few days, many days, next day
- Abbreviations without definition especially for organic reagents



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