

FREEDOM SPACE 3.0

Freedom to explore.

5 Billion Molecules

Synthesis on demand, 5-6 weeks. Fixed price

ML-Assisted Space Generation

Reagent statistics from Enamine

ML-assisted classification of reagents

Application of ML models to in-stock reagents (Enamine, AABlocks, Chemscape, etc.)

Enumeration using eight validated procedures

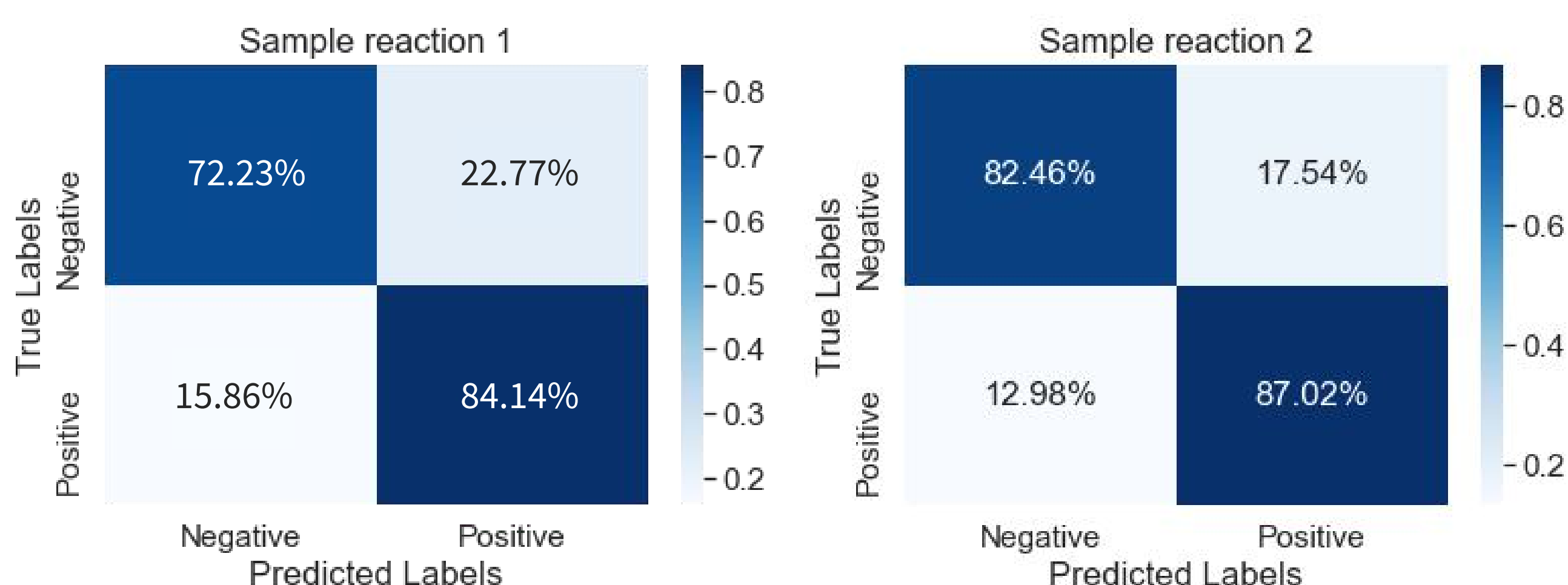
Freedom Space 3.0

Application of ML models to selection of reagents:

Goal is to generate molecules with high synthetic feasibility by filtering out potentially “bad” reagents

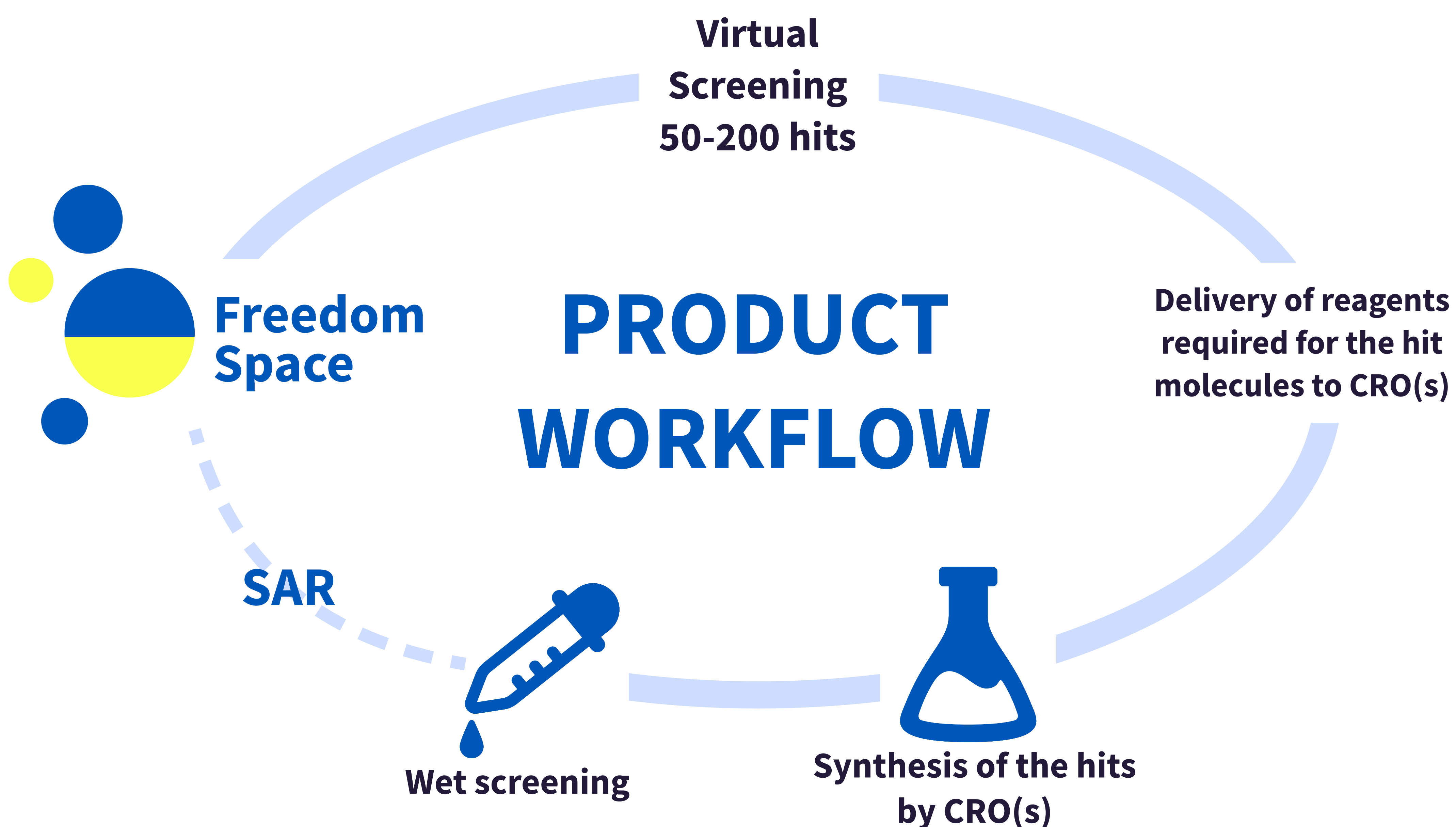
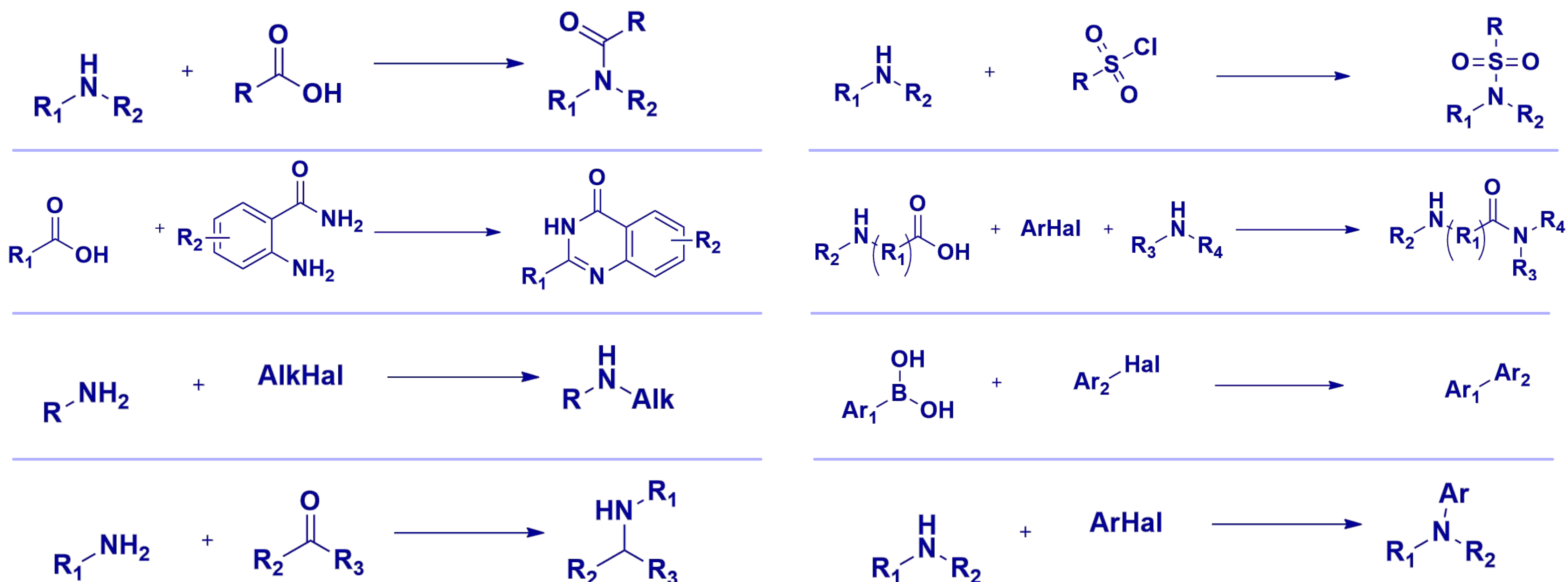
- ML-based classifiers trained on reagent statistics from Enamine
- Neural Network architecture
- Up to **83% recall** of the “bad” reagents
- **90%+ “good” reagents after filtering**

Sample results - performance on the test set (unseen data)



To request the set write an email at cs_sales@chem-space.com

Validated Reactions Space:



Advantages:

- Hit discovery in 10 weeks;
- Well-established workflow with assistance at all stages;
- Unique chemical space, little overlap with other commercial spaces;
- High synthesis success rate, competitive pricing;
- Analogs and custom chemical spaces around hit molecules.

To request the set write an email at cs_sales@chem-space.com