

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,
Chemscene, etc.)

Enumeration
using eight
validated
procedures

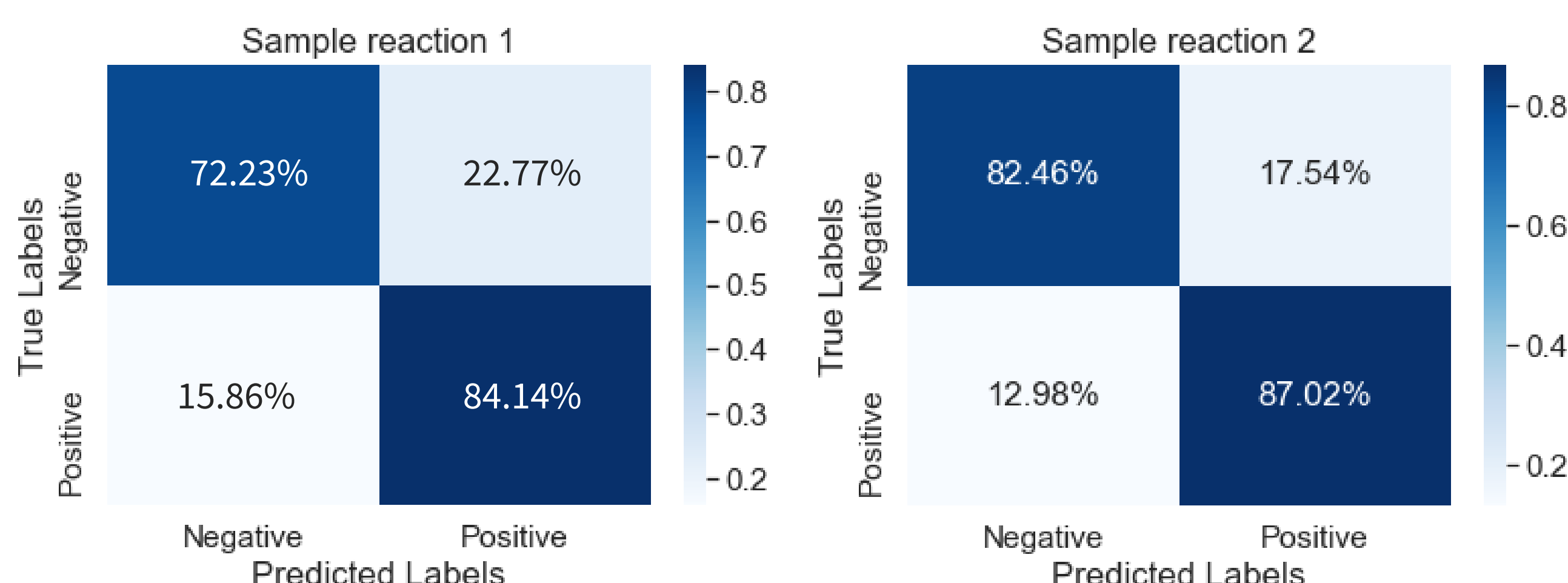
Freedom
Space 3.0

Application of ML models to selection of reagents:

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

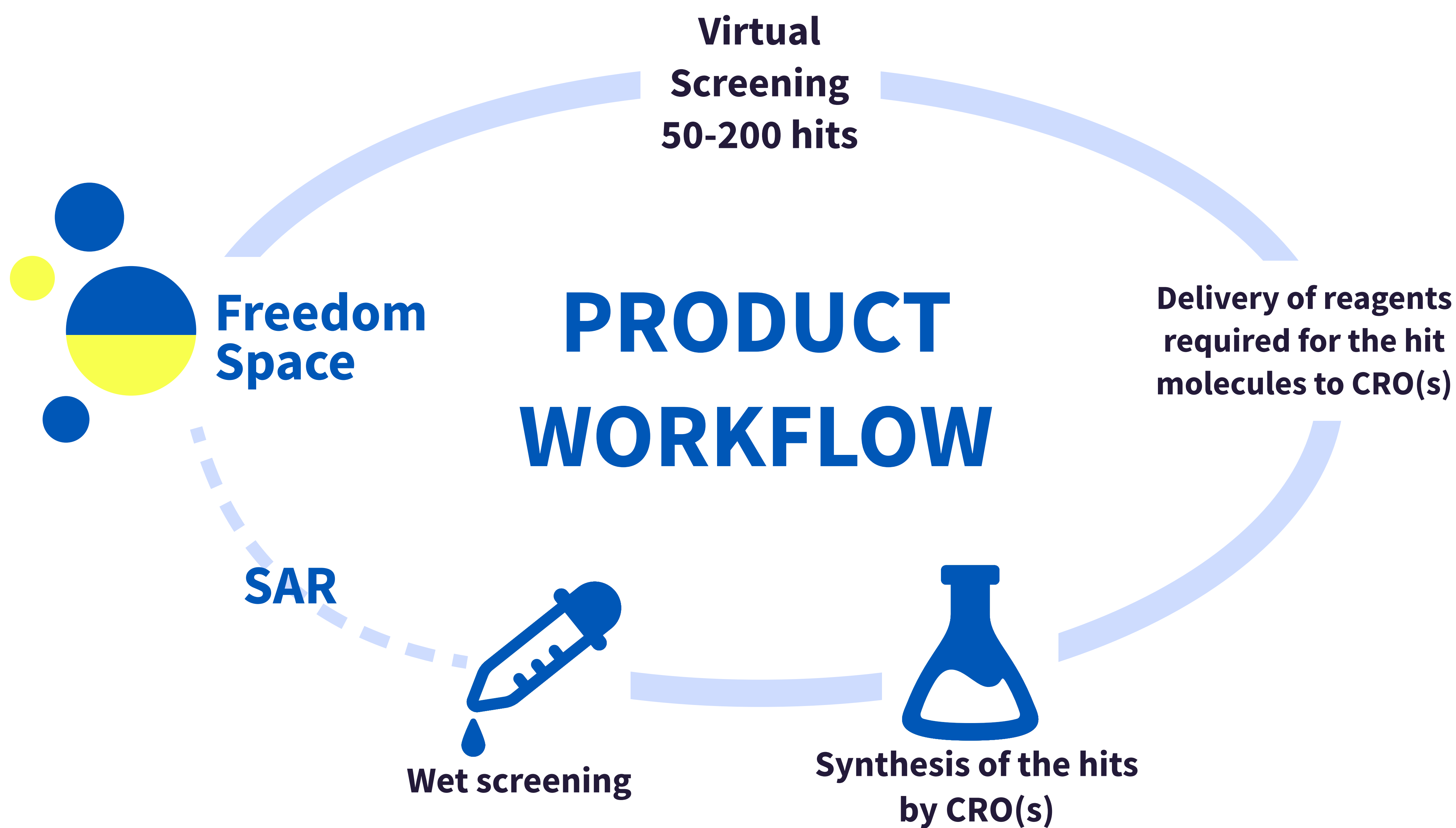
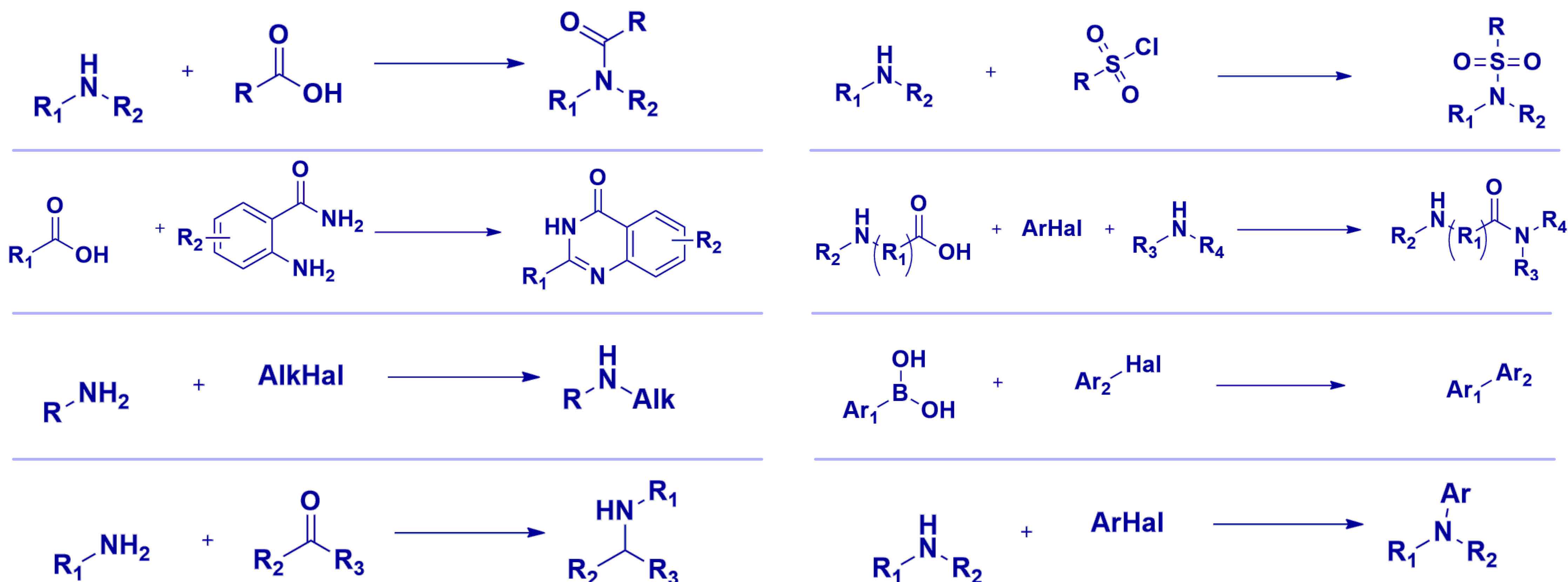
- ML-based classifiers trained on reagent statistics from Enamine
- Neural Network architecture
- Up to **83% recall** of the “bad” reagents
- **90%+ “good” reagents after filtering**

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

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