

# DNA-ENCODED LIBRARIES WITH ML-SUPERVISED DATA PROCESSING

DNA encoded library technology (DELt) is a cutting-edge technology for early-stage drug discovery. It gives access to screening billions of compounds in a single tube! We offer end-to-end solution leveraging the full potential of this approach, enabling efficient screening of diverse compounds, and hit identification.

## DNA-encoded libraries

- Commercially available
- Custom DEL design/production

### Experiment planning

Possibility to address selectivity and include information about off-targets

## Affinity Selection

- Protein production & acquisition
- Target investigation
- Preselection test
- Affinity selection

## Sequencing

- gPCR quantification
- PCR amplification
- Sample purification
- NGS by partner company

## DEL-ML-CS Workflow



DEL data



ML



CS

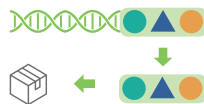
Using ML on DEL data to explore chemical spaces of choice

- ✓ Subset of 1B molecules from Enamine REAL Space
- ✓ Prediction using Tompson sampling (Enamine REAL Space 70B, Freedom Space 4.0 142B)

## Data Analysis

- NGS raw data recording
- 3D plots preparation
- Features identification
- Report preparation

## Off-DNA Synthesis

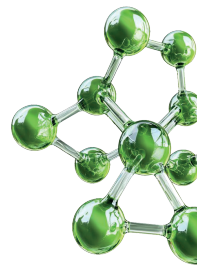


✓ Chemical diversity

## Hit Validation

Assay development:

- ✓ Cell-based assay
- ✓ Biochemical
- ✓ Biophysical



## Deliverables:

- ✓ Full moderation of the project
- ✓ Detailed reports for each stage of the project
- ✓ Two groups of hits resulting from DEL screen and ML prediction
- ✓ Easy follow up using synthon modularity of Enamine REAL Space and Freedom Space

