# Applying DNA-encoded library (DEL) screens and machine learning (ML) to drug discovery in animal health

Logan Andrews, Andrew Calabrese, Brett Chevalier Animol Discovery, Inc. ● Boston, MA

### **Introduction**

To address the unmet and emerging needs in animal health, Animol Discovery has engineered a biotechnology platform to identify novel small molecules. Compared to traditional high-throughput methods, the combination of DEL+ML offers a significant reduction in time and cost while increasing the probability of identifying a small molecule development candidate with optimal properties.

## **DNA-Encoded Library (DEL)**

- Chemical building blocks combine to create highly diverse compounds with unique DNA sequence identifiers
- Library of 200 billion+ compounds
- Simultaneously screen target and anti-target(s) activity in multiplexed competitive assays

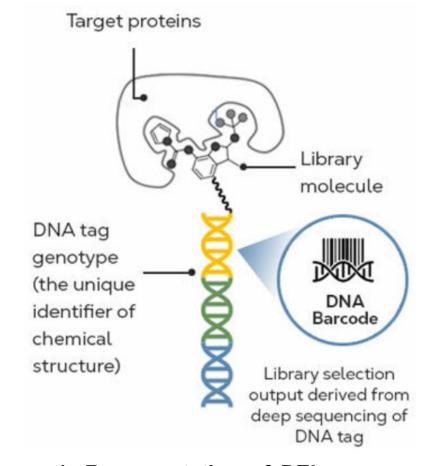


Figure 1: Representation of DEL compound with DNA tag bound to target protein.

## **Machine Learning (ML)**

- Converts DEL binding data to predictive binding models
- Predictive algorithms provide insight to structure-activity relationships following screening
- Expert and automated compound selection to identify lead development candidates

#### **In-Vivo**

- Synthesize and test fewer compounds with improved characteristics
- Primary and secondary in-vitro assays provide gateway to invivo lab and target animal models
- 8-months from concept to in-vivo lead confirmation

#### **Pipeline**

- First project initiated in June 2020
- 10 projects planned for 2021
  - Parasiticide metabolic and non-metabolic pathway targets

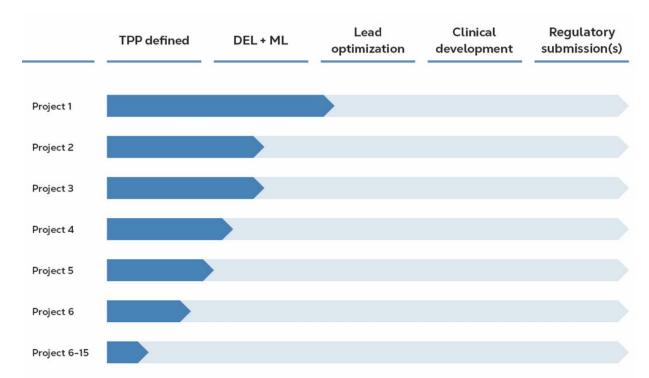


Figure 2: Animol's current project pipeline includes parasiticide and therapeutic targets.

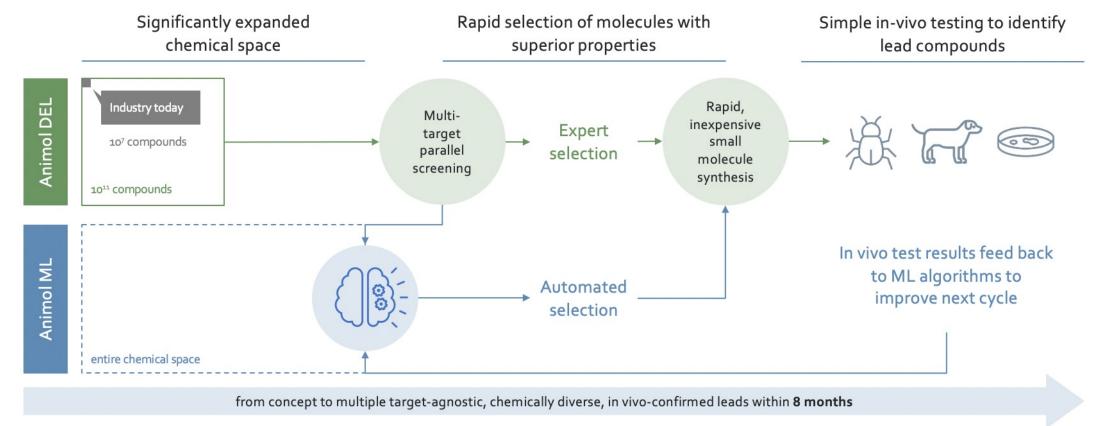


Figure 3: Animol's accelerated screening process to find optimal candidates for a target.