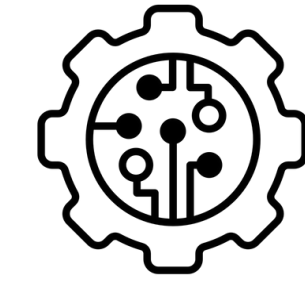


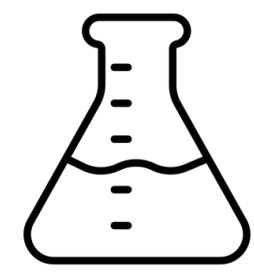
What we do & why it matters

Bringing new small molecules to market is a complex and lengthy process. Poor ADME properties are a leading cause of drug attrition, often identified late in the development cascade, leading to wasted resources and delayed breakthroughs.



AI-ready ADME

>10,000 compounds
 ML-guided analysis of large datasets drives **shorter cycle times** and **fewer cycles** required to lead optimization

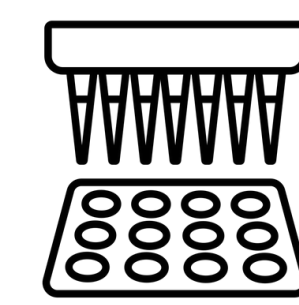


Traditional ADME

10 - 100 compounds
 Historically, generating ADME data on lead compounds has been the standard. This approach limits testing of library compounds, resulting in longer hit-to-lead cycles.

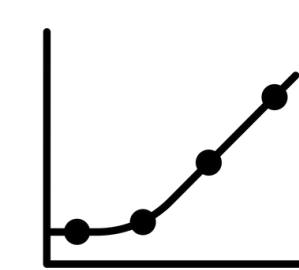
In a traditional drug discovery workflow, ADME (absorption, distribution, metabolism, and excretion) properties are evaluated during the lead optimization phase, typically on a small number of compounds. This often necessitates additional hit-to-lead cycles to improve compound ADME profiles. Current ADME workflows are prohibitively costly and time-consuming to implement at high throughput, preventing researchers from obtaining this crucial data earlier in the process.

To address this need, we developed a high-throughput ADME service capable of generating large, high-quality, reproducible datasets across key Tier 1 ADME assays. Our platform is **highly automated and purpose-built for scale to generate the large-scale datasets** required to train robust machine learning (ML) models. Ginkgo Datapoints brings its extensive small molecule screening expertise, automated labs built for scale, and streamlined fee-for-service business model to generate more data per dollar and ultimately to reduce hit-to-lead cycle times



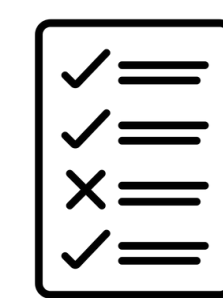
First-in-class screening capabilities

Our team of scientists has expertise in high throughput small molecule profiling, with decades of combined experience in everything from assessing metabolites in unique and hard to work with matrices to natural product discovery and development.



Extensive miniaturization and scaling expertise

Automation touches upon every part of our platform. Our labs are equipped with top of the line integrated workcells and automated data pipelines, which together enable scale and ease of execution of ADME assays.



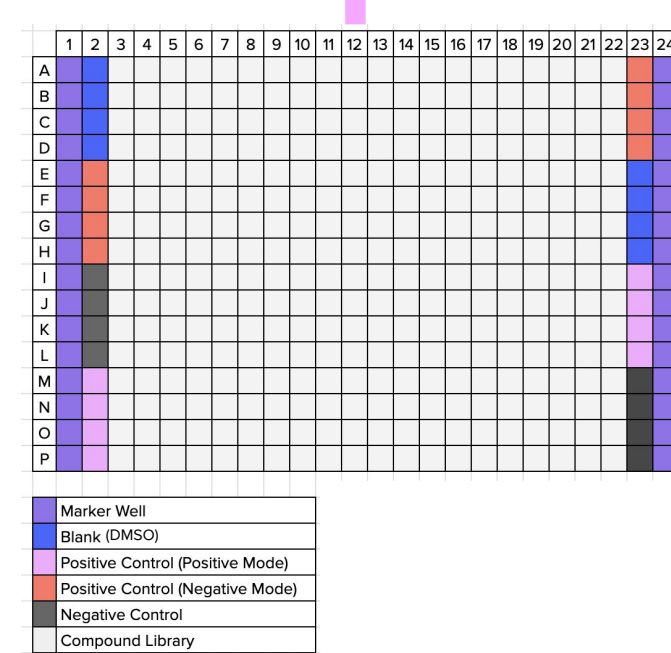
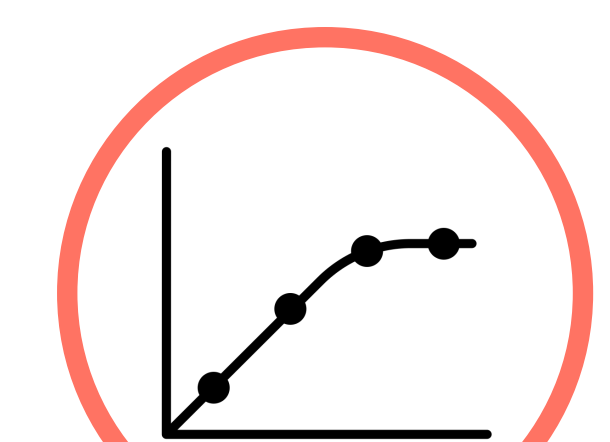
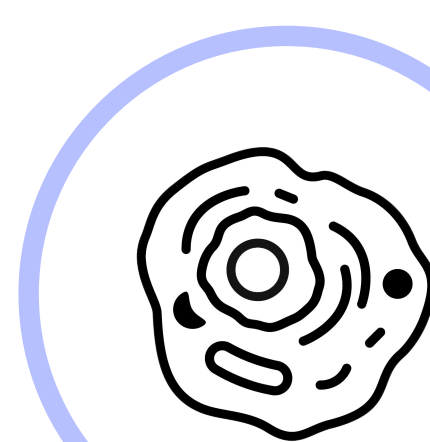
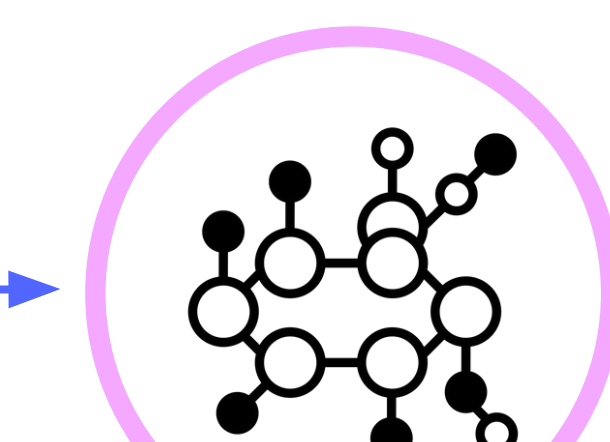
Rigorous QC

We are committed to delivering the high quality, reproducible ADME results that are critical to your workflows. Our assays are rigorously validated, and we share QC metrics for all controls to ensure adherence to industry best practices.

Our product

We profiled a 320-compound subset of the Library of Pharmacologically Active Compounds (LOPAC 1280) across key Tier 1 ADME assays.

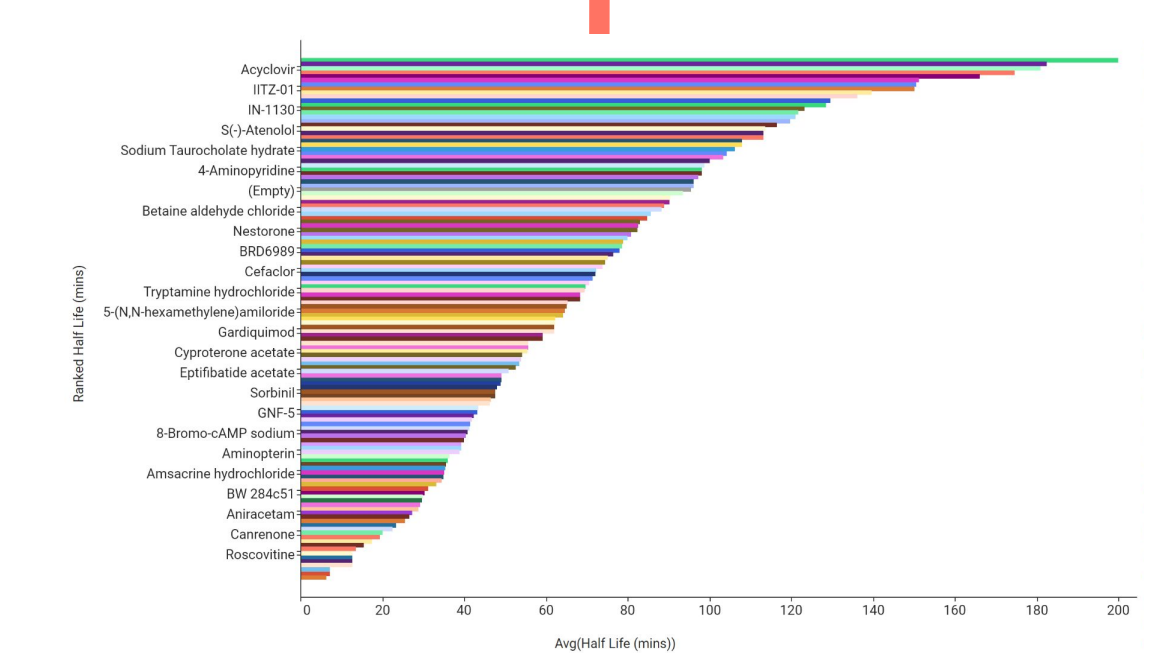
The assays were executed in 384-well format and analyzed by acoustic ejection mass spectrometry (AE-MS) on the SciEx EchoMS system coupled with a QQQ 6500 mass spectrometer in positive ionization mode. All assays were run with technical replicates and robust QC to ensure data quality and adherence to industry standards.



Microsomal Stability
 Assess the rate at which a compound is metabolized by liver microsomes
 • 5 time points
 • 3 different microsomes [human, mouse, rat]

Kinetic Solubility
 Assess the solubility of a compound in a biologically relevant medium
 • 1 pH [7.4]
 • 1 medium [phosphate buffer]

P450 Inhibition
 Assess a compound's ability to cause drug-drug interactions using P450 inhibition
 • 1 or 8 concentrations
 • 5 CYP isoforms [3A4, 2D6, 2C9, 1A2, 2C19]



Speak to our team about your ADME needs!

Partner provides compound library

You provide your test compounds at 10 mM for screening

We used standardized plate formats to increase precision and accuracy, allowing Robust Z' calculations per plate and %CV per compound, per control, and per reference material while maximizing plate space for compound testing

We've partnered with **Tangible Scientific** to provide compound management, assay-ready plate preparation, and access to a streamlined data management platform to enable rapid data turnaround.

Selected assays executed

Choose from our *in vitro* ADME menu

We tested our 320 compounds across all three assays with a single microsome species (human) and CYP (2D6)

All controls passed QC, with verapamil showing the expected degradation up to 45 minutes for microsomal stability. A robust Spearman's correlation between replicates ($p < 0.001$ $r^2 = 0.98$) for kinetic solubility and and IC50 dose response for quinidine against CYP2D6

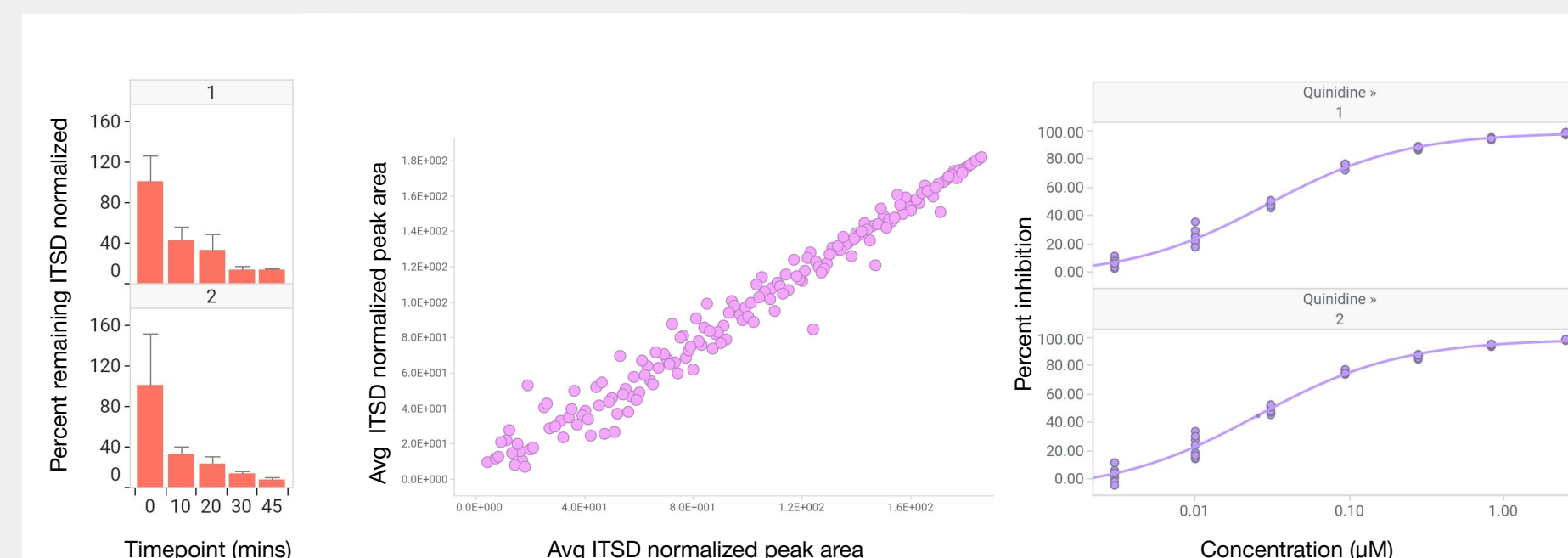


Figure 1: Microsomal stability percent remaining and standard deviation for verapamil

Figure 2: Spearman's rank correlation for LOPAC compounds run as n=2

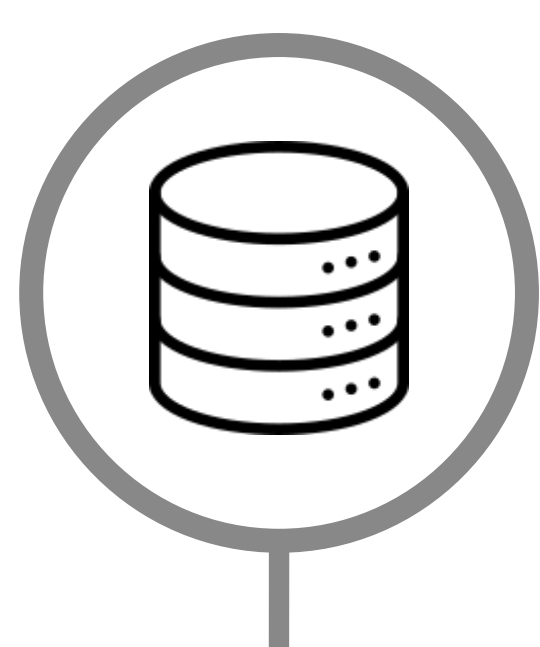
Figure 3: Dose response curve for quinidine, positive control for CYP2D6 inhibition

Download our ADME dataset



320-compound ADME dataset analyzed from a subset of the LOPAC 1280 chemical library

Our findings



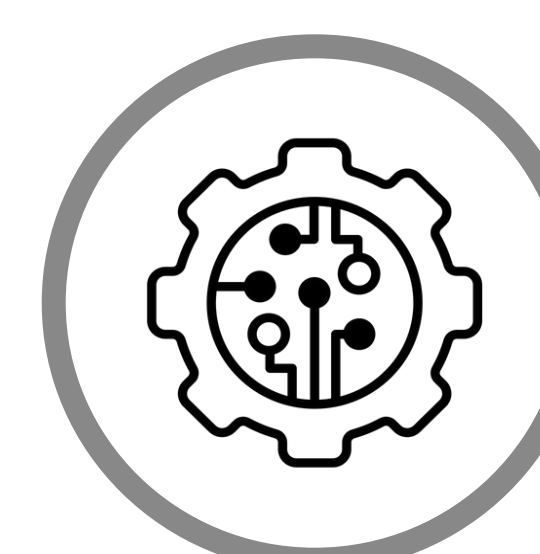
We understand the importance of delivering precise, reliable data on a large scale, specifically formatted for seamless integration into AI/ML models. By providing a high volume of high-quality data, we empower your machine learning algorithms to predict and optimize drug candidates more accurately, dramatically shortening lead optimization cycles.

Table 1: Structure activity relationship (SAR) table for a subset of the 320 compounds tested

	Microsomal Stability		Kinetic solubility	P450 Inhibition
	Intrinsic Clearance (μL/min/mg)	Half Life (mins)	Solubility (μg/mL)	IC50
Roscovitine	104.43	13.27	4.67	1.33
Torin2	16.60	83.47	0.9	0.19
BAY 60-7550	45.75	30.30	6.20	0.1
KT203	75.59	18.33	2.01	

4 of 17254 rows 4 of 45 columns

Expanding our platform



Available now

- Microsomal stability
- Kinetic solubility
- P450 inhibition

Coming soon

- MDCK permeability
- Plasma protein binding

We are growing our *in vitro* ADME platform with a focus on AI/ML ready data for SAR modelling to accelerate your drug discovery pipeline.

We streamline and expedite medicinal chemistry workflows

- Get more data per dollar
- Reduce hit-to-lead cycle times and time to identifying development candidates
- Leverage our lab-in-the-loop infrastructure to make more informed decisions, faster

We provide ADME at every stage of your discovery journey

- Early hit screening
- Lead optimization
- AI-driven discovery workflows

For technical inquiries, please contact:

Hilary Ranson

Ginkgo Bioworks, Inc.

Email: hranson@ginkgobioworks.com