

TuneLab-at-Revvity Federated Learning Program

By Revvity Signals

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Overview

This document outlines:

- The functioning of the federated learning consortium initiated by Eli Lilly and co-funded with Revvity Signals
- How your data contribute while preserving your IP
- How to join the program

Program Overview

Lilly TuneLab™ is a first-of-its-kind, collaborative AI/ML drug discovery platform with a unique Access/Contribute value proposition:

- **Access:** Lilly provides participating biotech companies access to powerful models trained on decades of proprietary data (representing over \$1B investment) to accelerate their therapeutic programs
- **Contribute:** Participants contribute training data to improve the models via privacy-preserving federated learning

Revvity Signals operationalizes the TuneLab program by providing

- Necessary software to host, invoke and manage TuneLab models (complimentary for the first year)
- A pool of modelling credits
- Signals secure scientific data platform

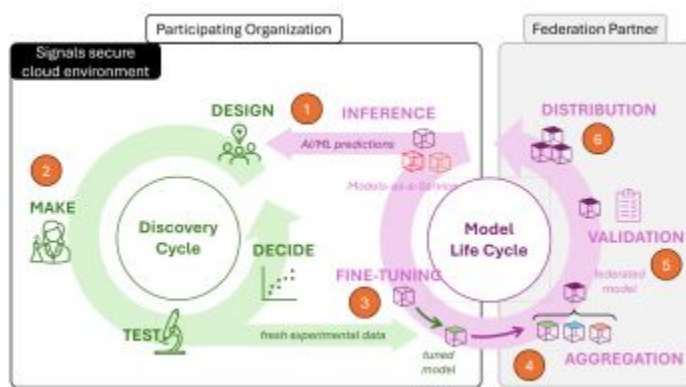
Roles & Responsibilities of Partners

- **Eli Lilly:** Program initiator who provides the original AI/ML models, funds and leads the program
- **Revvity Signals:** Provides the software and secure cloud environment necessary for operationalization of the TuneLab program
- **Participating Organizations:** Access TuneLab model predictions in exchange for retraining models with proprietary data within the Signals platform, and share updated

models Lilly federation partners.

- **Lilly Federation Partners:** Third-party companies with AI expertise whose role is to aggregate models updated by all participating organizations, monitor model performances, and, once validated, distribute back the new global models in your Signals cloud environment, ready to be used.

Workflow Process



1. Biologists and medicinal chemists invoke TuneLab models to prioritize and select molecules for synthesis in the laboratory. Depending on the computational cost of the invoked models, a certain number of modeling credits will be consumed.
2. Selected molecules are experimentally profiled, including assays with endpoints to TuneLab models.
3. Molecular structures and experimental endpoints are used to retrain corresponding models within your Signals secure environment.
4. Updated models are securely shared with the federation partner selected by Lilly
5. Federation partners aggregate updated models into a new global model that is verified and distributed back to your Signals secure cloud environment.
6. The cycle then repeats with models that are better aligned with your research

Benefits for Participating Organizations

- **Access to premium AI/ML models generated by TuneLab** directly from the software they use daily. Model performance will further improve as they are retrained with participants' data.
- **Complimentary licenses** for a 1-year period specifically for use with the TuneLab program:
 - Up to 5 licenses of [Signals One](#) (multi-tenant)
 - Up to 5 licenses of [Signals Synergy](#) (multi-tenant)
 - Up to 5 licenses of [Signals ChemDraw](#)
- **Early access to [Signals Xynthetic](#)** to host and manage TuneLab models in their own environment.
- **A pool of modeling credits.** Additional modeling credits may be purchased.

TuneLab Models

Small Molecule Models

Models for small molecules cover **several tens of ADMET models** (classification and regression models) such as thermodynamic and kinetic solubility, MDCK apparent permeability, fraction unbound in plasma of various species, microsomal stability in various species, CYP inhibition of several isoforms, hERG binding.

[See Addendum #1 for more information](#)

Antibody Models

Models for **antibodies** provide insight into their **developability** with properties such as thermal stability, hydrophobicity and viscosity.

[See Addendum #2 for more information](#)

Information About your Proprietary Data

Experimental protocol sharing

For AI models to perform, standardized quality data are essential. Consequently, Lilly will ask participating organizations to share their experimental protocols, compare with their own, and decide on the data compatibility.

Data Contribution (volume)

Federated learning programs allow access to larger and more diverse datasets which increases the accuracy and predictability domain of a given model. Diversity is a direct consequence of the number of organizations who participate to the TuneLab program, while quality and quantity are provided by each organization.

All organizations are requested to provide a **minimum of 1,000 experimental endpoint each year**. For example, 200 molecules profiled on 5 endpoints suffice.

[See Addendum #3 for more information](#)

Historical data are accepted, although we recommend using fresh data from current research projects to get the most of the program.

Data Protection

Protection of participating organizations' proprietary data and IP is essential for the success of the program. The TuneLab-at-Revvity programs ensures security by design. In this regard, the following key security measures should be mentioned:

- Proprietary data of participating organizations (molecules – existing and virtual-, predictions, experimental results) remain within your Signals cloud environment which is safeguarded by a “defense in depth” security strategy [[learn more](#)]
- TuneLab models are hosted within your Signals cloud environment, so your small molecules or antibodies will never leave this secure infrastructure.
- Updated model sharing with Lilly’s federation partner will be encrypted
- Federation partners will only send back updated models, making it impossible for other organizations -including Lilly- to know about the training data.

How to join the Program?

Eligibility Criteria

- **Revvity Signals customers** currently licensing Signals software: Signals One or Signals Notebook.
- Drug discovery organizations, primarily biotech companies and startups investigating **small molecules and/or antibodies**. Other organizations, pharmaceutical companies, and research institute are invited to apply as well.
- Organizations that can contribute **1,000 experimental data points per year** relevant to retraining TuneLab models within the federated learning framework implemented by Lilly (see list of endpoints in Addendum #3)

Organizations applying to the TuneLab program will be reviewed and approved by Lilly before joining.

Legal Agreement

A legal agreement between Eli Lilly and each selected organization will be required.

Experimental protocols followed by selected organizations will be shared as part of the agreement package.

Onboarding Process

Newly approved participating organizations will be provided access to relevant software, TuneLab models, and a pool of modeling credits by the Revvity Signals service department directly within your Signals cloud environment.

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Unleash that big, beautiful science.