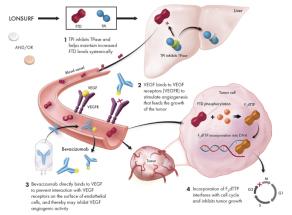
Mechanism of Action (MoA) Analysis

March 13, 2025

What is Mechanism of Action (MoA)?

- Defines how a drug interacts with its biological target.
- Can involve receptors, enzymes, signaling pathways, etc.
- Critical for drug discovery and development.



Why is MoA Important?

How to Determine It?

Why is MoA Important?

- ► Identifies drug targets (Step 1)
- ► Guides hit discovery optimization (Steps 2-3)
- Supports preclinical clinical evaluations (Steps 4-5)
- ► Ensures safety regulatory approval (Steps 6-7)

Target Identification and Validation And Validation Lead Optimization Preclinical Testing Step 3 Clinical Trials Regulatory Submission and Approval Approval Step 7 Step 7 Regulatory Submission and Approval Step 7 Step 7 Step 7 Step 7 Step 8 Clinical Trials Regulatory Submission and Approval Step 7 Step 7 Step 7 Step 7 Step 8 Step 8 Step 8 Step 8 Step 8 Step 8 Step 9 Step

How to Determine MoA?

- **Expose** human cells to drugs.
- ▶ Measure responses (e.g., gene expression, cell viability).

Dataset Overview & Project Objective

Dataset Overview

- Contains gene expression and cell viability data.
- **Covers** responses from 100 human cell types.
- ► Annotated with MoA labels for 5000+ drugs.
- ► **Enables** multi-label classification of drug effects.

Project Objective

- ▶ Develop a model to predict MoA based on drug response data.
- Utilize machine learning techniques.
- ▶ **Identify** key patterns in gene expression & cell viability.
- ▶ Address multi-label classification challenges.