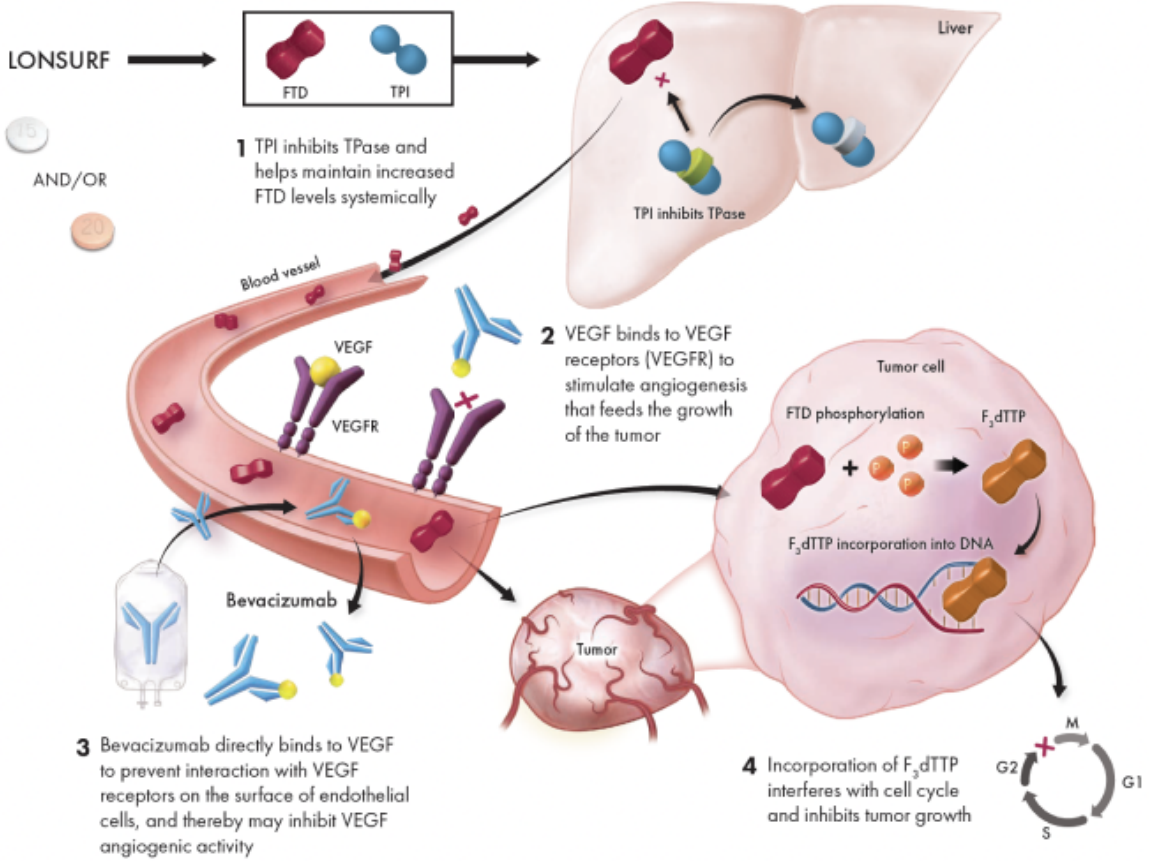
Mechanism of Action (MoA) Analysis

March 13, 2025

What is Mechanism of Action (MoA)?

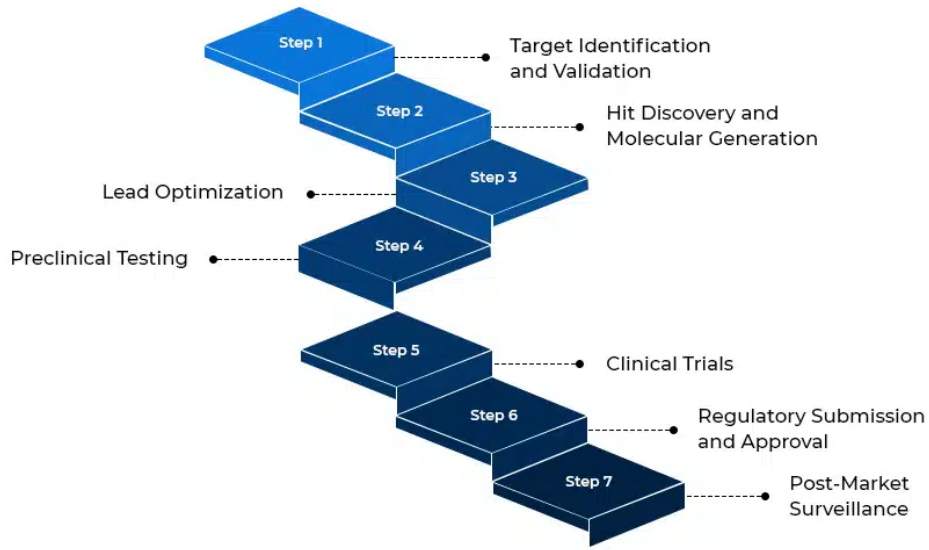
- Defines how a drug interacts with its biological target.
- Can involve receptors, enzymes, signaling pathways, etc.
- Critical for drug discovery and development.



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)



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** deep learning techniques.
- **Identify** key patterns in gene expression & cell viability.
- **Address** multi-label classification challenges.