# **Agentic AI:** Your Truly Intelligent Assistant (Or Your Virtual Team)

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# Objectives for Today

- **Introduce Agentic AI**

  - Unveil the frontier concept of agentic AI

- **Demonstrate an Agentic AI Drug-Discovery Platform – Medicine.AI**

  - Real-time demo of selected use cases

- **Q&A and Learn from Everyone**

  - Hear your feedback on the agentic AI platform, and how I may help you solve your problems

# Agenda

1. Introduction
    a) About Me and Medicine.AI
    b) Agentic AI
2. Demo
    a) Disease of interest for demo
    b) Platform’s interactive mode
    c) Platform’s auto-pilot mode
    d) Platform’s full-self driving (FSD) mode

# About Me

- **Interdisciplinary Academic Foundation**
  - College: Chemistry and Finance
  - Graduate studies in Chemistry, Computer Science, and Business (MBA)
  - Chartered Financial Analyst (CFA), awarded in 2006

- **Diverse Industry Experience**
  - 20+ years across finance and technology sectors
  - Roles spanning financial engineering, quantitative research, data science, machine learning, and AI

- **Progressive Leadership & Entrepreneurship**
  - Corporate progression: Analyst → Manager → Director → VP → Division Head
  - Founder of Human & AI Harmony Consulting (Machine Learning & AI)
  - Founder of Medicine.AI – an agentic-AI-powered drug discovery platform

*Kevin Hou's LinkedIn*

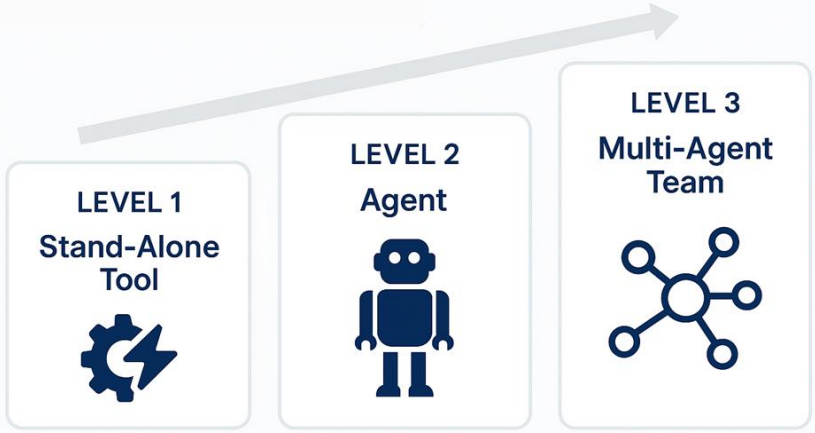
# About Medicine.AI

**Medicine.AI** is pioneering a new era of pharmaceutical innovation with its **agentic AI-driven drug discovery platform**. Our open-architecture approach integrates the best computational and AI models, fine-tuned with public and proprietary data towards targeted therapeutic objectives.

We focus on **empowering frontier researchers** and **small-to-medium-sized biotech** and **pharmaceutical companies**.

Our platform is now a **fully functional MVP**, validated through collaborations with multiple leading research and industry partners.

# Evolving AI: From Stand-Alone Tool to Multidisciplinary Partner




- **LEVEL 1 – Stand-Alone Tool/Bot**
  - **Fully human-driven**: you supply prompts, run the model, and interpret every result
- **LEVEL 2 – Autonomous Agent**
  - **Delegate defined tasks**: the AI analyzes inputs, invokes specialized functions, reviews its own output, and self-corrects.
- **LEVEL 3 – Collaborative Multi-Agent Team**
  - **High-level orchestration**: you state the objective; the platform decomposes it into subtasks and coordinates a suite of specialized agents (e.g., target ID, docking, lead optimization).

Team/Organization

# Agent and Agentic AI

- **“Agent” – Defined**
  - A person or entity authorized to act on behalf of another
  - Someone empowered to take action or make decisions
  - An individual working for or managing an agency
  - A representative acting in an official capacity (e.g., for a government)
  - A person responsible for carrying out a specific task.
- **In Practice**
  - Scientists, engineers, analysts, and executives — all are agents driving progress through specialized actions and decisions
- **Agentic AI**
  - An AI paradigm where autonomous systems function as agents, making informed decisions and executing tasks based on defined goals and context

# What is Agentic AI?

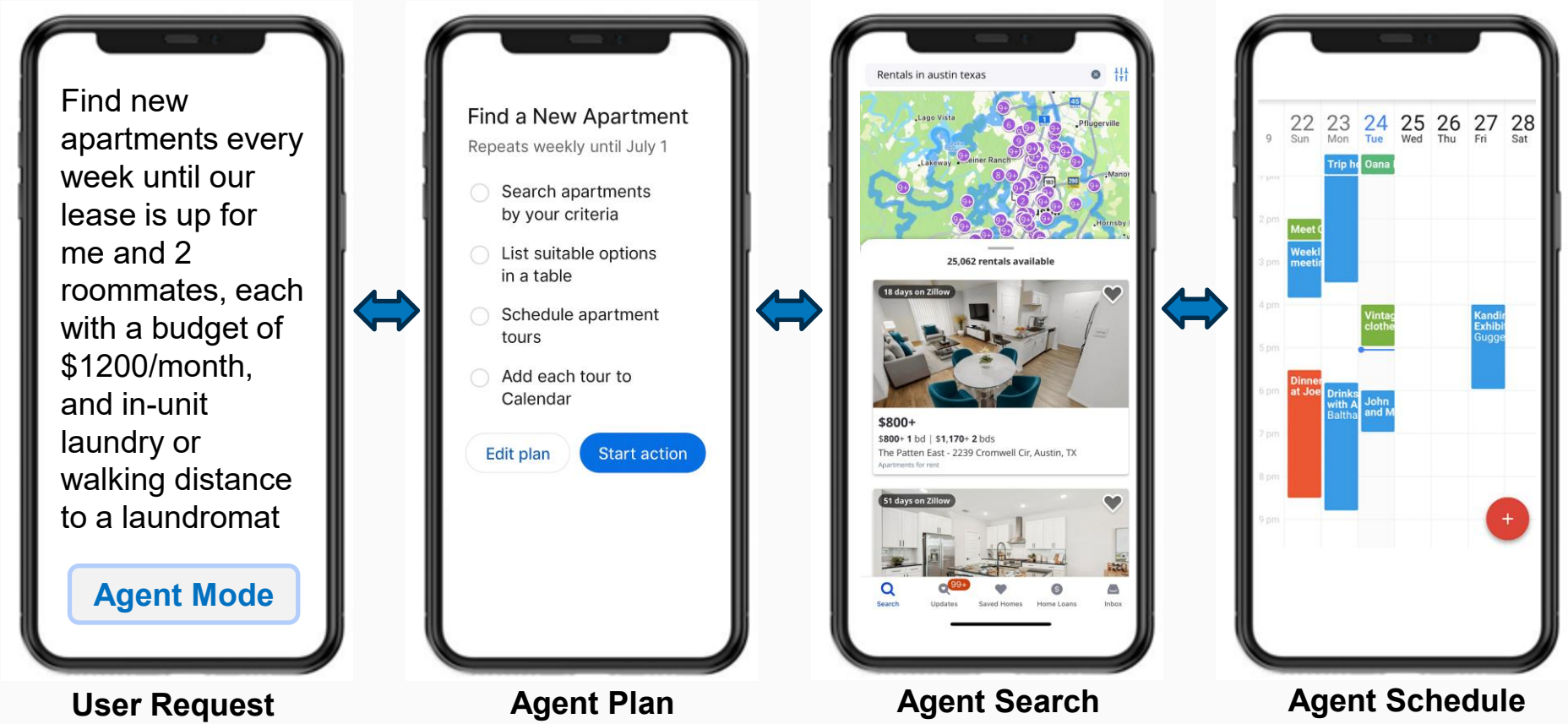
- **Definition:** An AI framework where systems operate autonomously as agents, making decisions and taking actions based on goals and environmental interactions.

- **Components:**
  - **Perception:** Understanding inputs or environmental data.
  - **Reasoning and Planning:** Deciding on actions to achieve goals.
  - **Action Execution:** Carrying out planned actions.
  - **Feedback Loop:** Learning from outcomes to refine future behavior.

- **Characteristics:**
  - **Autonomous Operation:** Minimal human intervention.
  - **Goal-Oriented:** Focused on achieving specific objectives.
  - **Adaptive Learning:** Continuously improves through experience.

# An Example of Agentic AI: Smart Apartment Search to Save Time & Hassle

** Reference a soon-to-be-launched use case presented at Google I/O 2025.*




**User Request** | **Agent Plan** | **Agent Search** | **Agent Schedule**

# Agentic AI: From Daily Life to Breakthrough Science

- **Powerful:** Agentic AI is designed for complex, information-intensive, and goal-driven tasks — far surpassing the capabilities of stand-alone AI bots. These tasks are often neither well-suited for nor engaging to humans.

- **Daily Lives:**
  - Whether finding homes, booking trips, shopping, or learning, AI agents are there to assist at every step.
  - Leading technology, service, and product companies will compete to deliver these intelligent assistants to billions of people worldwide.

- **Industries & Science:**
  - By integrating domain expertise with Agentic AI, we can drive transformative impact across industries and accelerate scientific discovery.

# Medicine.AI's Agentic-AI Drug Discovery Platform

**Planning Agent**

- Literature Analysis Agent
- Target Identification Agent
- Ligand Screening Agent
- Molecule Design Agent
- Pathway Analysis Agent
- ADMET Prediction Agent
- Experiment Design Agent
- Report Generation Agent

- Data Tools
- Prediction & Analysis Tools
- Docking & Simulation Tools
- Visualization & Reporting Tools
- Molecules Generation Tools

# Agentic AI and Human Roles – Our Multi-Agent AI Platform forms a virtual team

| AI Agent | Human Role | Skills & Responsibilities |
|---|---|---|
| 👤 **Planning Agent** | Drug Discovery Program Manager / Project Manager | Oversees and coordinates project strategies, sets milestones, and refines overall research plans. Manages strategic planning, resource allocation, and cross-functional coordination. |
| 🎯 **Target Identification Agent** | Target Identification Scientist / Bioinformatics Scientist | Utilizes bioinformatics, genomics, and molecular biology to identify and prioritize potential drug targets. Requires expertise in data mining, omics technologies, and computational modeling. |
| 🔬 **Ligand Screening Agent** | HTS Scientist / Assay Development Scientist | Designs and executes assays to screen compound libraries against targets. Manages large datasets from screening campaigns and optimizes assay conditions. |
| 🧩 **Molecule Design Agent** | Medicinal Chemist / Computational Chemist | Designs, synthesizes, and optimizes molecular structures with desired biological activity. Relies on structure–activity relationships, in silico modeling, and iterative chemical optimization. |
| ⚖️ **ADMET Prediction Agent** | ADMET Scientist / Pharmacokinetic–Toxicologist | Predicts absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiles using computational tools. Requires expertise in pharmacokinetics, toxicology, and metabolism. |
| 📈 **Pathway Analysis Agent** | Systems Biologist / Pathway Analyst | Investigates and interprets biological pathways and networks to understand drug action mechanisms. Integrates high-dimensional data using systems-level analytical methods. |
| 🔍 **Literature Analysis Agent** | Scientific Research Analyst / Information Specialist | Performs comprehensive reviews of scientific literature to extract insights, trends, and data. Skilled in literature mining, data curation, and staying current with emerging research. |
| ⚗️ **Experiment Design Agent** | Experimental Design Scientist / Research Scientist | Develops robust experimental protocols to validate hypotheses and test drug candidates. Proficient in design of experiments (DOE), statistical analysis, and hands-on laboratory techniques. |
| 📑 **Report Generation Agent** | Scientific Writer / Technical Documentation Specialist | Synthesizes complex scientific data and analysis into clear, comprehensive reports. Expert in technical writing, data visualization, and regulatory documentation. |

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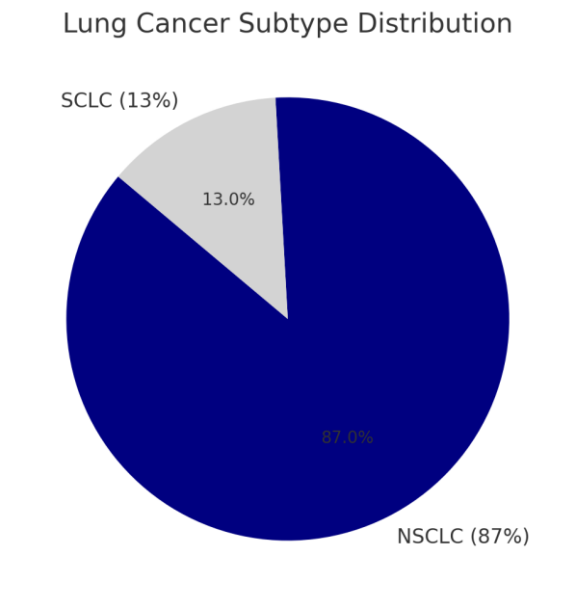
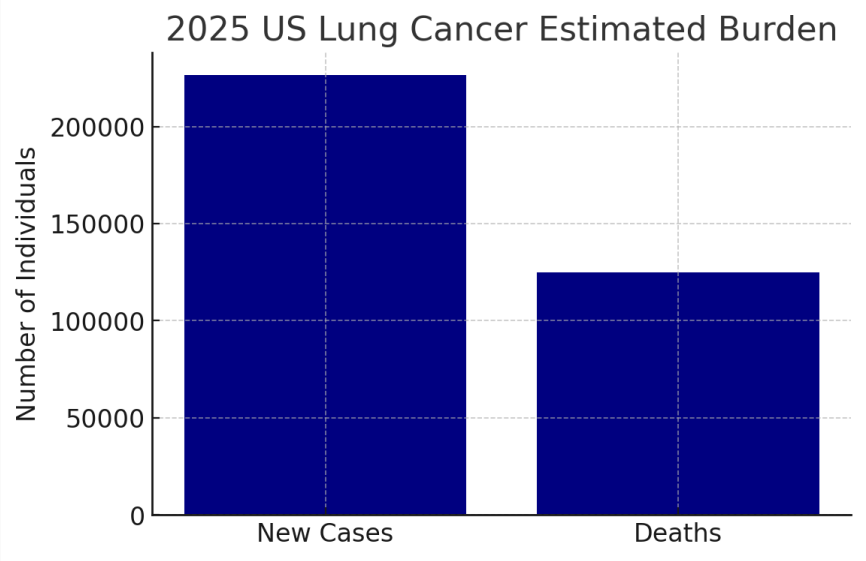
# Disease of Interest for Demo: Non–Small Cell Lung Cancer

- **Lung cancer is the 2nd most common cancer in US adults (behind prostate in men, breast in women)**



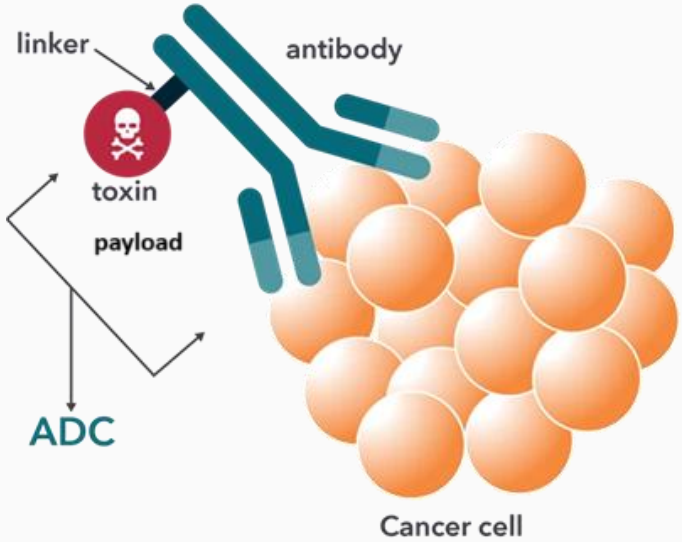




*Source: https://www.cancer.org/cancer/types/lung-cancer/about/key-statistics.html*

# Disease of Interest for Demo: ADCs in Breast Cancer

## Antibody-Drug Conjugates (ADCs)

ADCs - Precision medicines that deliver powerful anti-cancer drugs directly to tumor cells




### How?

- Antibody targets tumor-specific antigen
- Linker joins antibody to cytotoxic drug (i.e. payload)
- Payload released inside cancer cell

### Advantages:

- Highly specific targeting
- Fewer side effects vs. standard chemotherapy
- "Bystander effect" kills nearby tumor cells

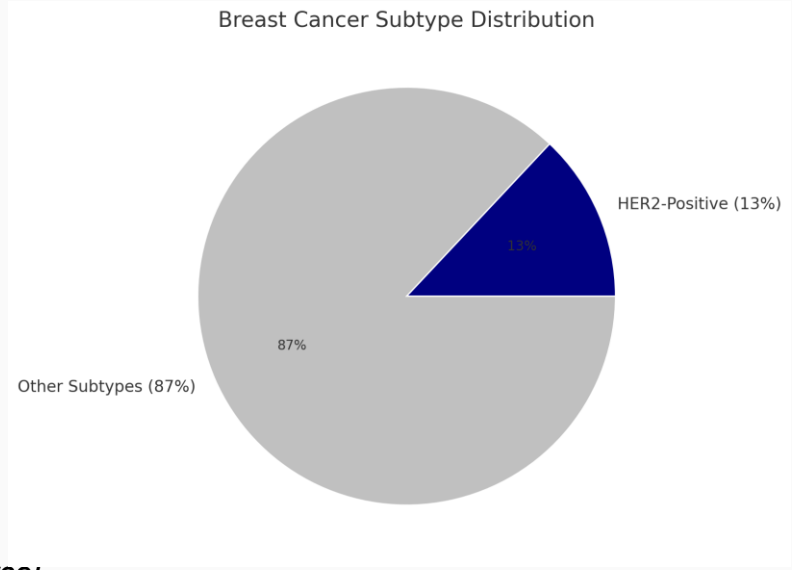
### Challenges:

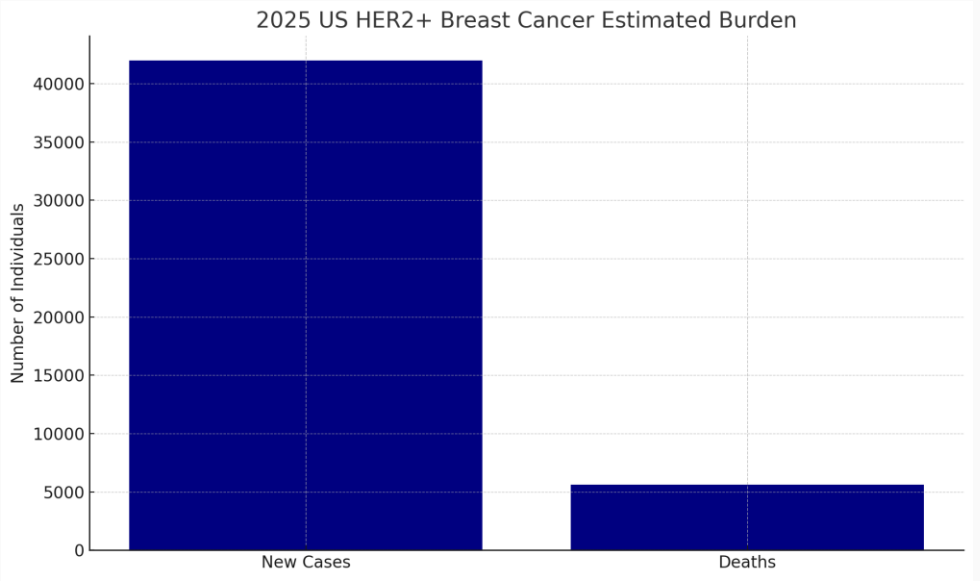
- Need for tumor-specific antigens
- Linker and payload stability
- Managing off-target toxicity

ADCs like *T-DM1* and *T-DXd* have improved outcomes in HER2+ breast cancer.

# Disease of Interest for Demo: ADCs in Breast Cancer

- **Breast cancer is the most common cancer in US women and the second leading cause of cancer death**
- **HER2+ (positive) is defined by overexpression of the HER2 receptor, which drives more aggressive tumor growth**




*Source:*
*https://seer.cancer.gov/statfacts/html/breast-subtypes.html*
*https://www.cancer.org/content/dam/cancer-org/research/cancer-facts-and-statistics/annual-cancer-facts-and-figures/2025/2025-cancer-facts-and-figures-acs.pdf*

# Demo Modes: Interactive → Auto-Pilot → Full-Self Driving

**Full-Self Driving Mode**

**Level 3 Multi-Agent Team**

End-to-end orchestration of specialized AI agents

**Auto-pilot Mode**

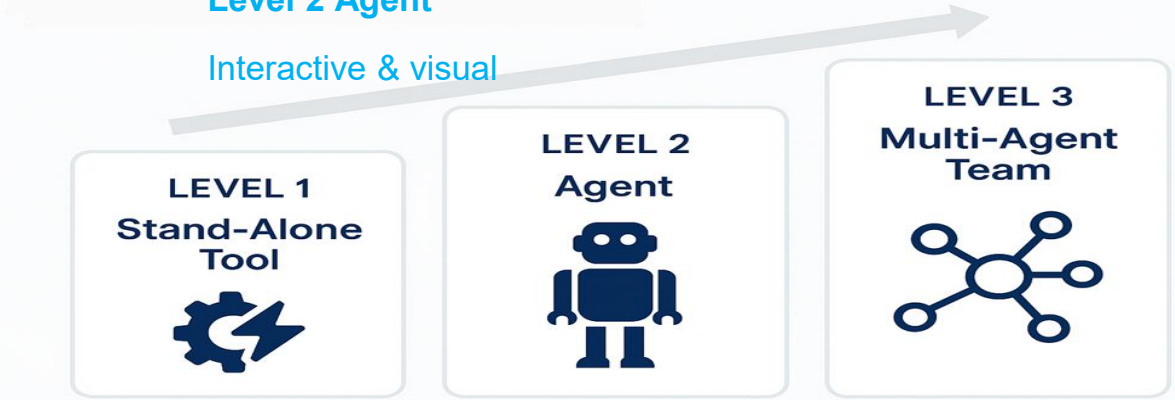
**Advance Level 2**

Pre-configured workflows that self-review and adjust

**Interactive Mode**

**Level 2 Agent**

Interactive & visual



# Demo Mode: Interactive Mode

## Drug Discovery Platform

Diseases => Drugs/Compounds for Cure | Targets => Drugs/Compounds for Analysis | Drugs/Compounds => Analysis and Generation

**Disease Names:**

non-small cell lung carcinoma ×

Type to search diseases...

Search

### Results

**Disease-Target Associations**

| Associated Disease | Symbol | UniProt | Target Name | Target Type | Target TDL | Target Fam |
|---|---|---|---|---|---|---|
| non-small cell lung carcinoma (Learn More) | EGFR | P00533 | Epidermal growth factor receptor | Single Protein | Tclin | Kinase |
| | CD274 | Q9NZQ7 | Programmed cell death 1 ligand 1 | Single Protein | Tclin | |
| | TP53 | P04637 | Cellular tumor antigen p53 | Single Protein | Tchem | TF |
| | ALK | Q9UM73 | ALK tyrosine kinase receptor | Single Protein | Tclin | Kinase |
| | KRAS | P01116 | GTPase KRas | Single Protein | Tclin | Enzyme |
| | VEGFA | P15692 | Vascular endothelial growth factor A | Single Protein | Tclin | |

Our system identifies 3,213 associated targets at different target development levels

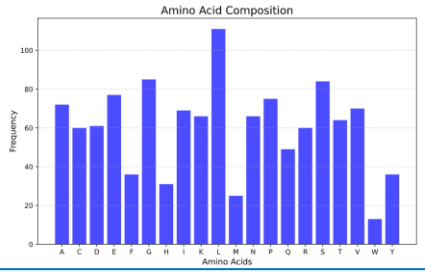
## Protein Sequence Analysis

**UniProt ID: P00533**

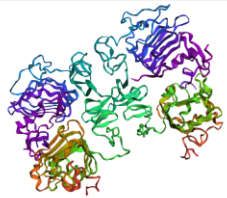
**Sequence**

```
MRPSGTAGAALLALLAALCPASRALEEKKVCQGTSNKLTQLGTFEDHFLSLQRMFNNCEVVLGNLEITYVQRNYDLSFLKTIQEVAGYVLIALNTVERIPLENLQIIRGNMYYENSYALAVLSNYDANKTGLKELPMRNLQEILHGAVRFSNNPALCNVESIQWRDIVSSDFLSNMSMDFQNHLGSCQKCDPSCPNGSCWGAGEENCQ
KLTKIICAQQCSGRCRGKSPSDCCHNQCAAGCTGPRESDCLVCRKFRDEATCKDTCPPLMLYNPTTYQMDVNPEGKYSFGATCVKKCPRNYVVTDHGSCVRACGADSYEMEEDGVRKCKKCEGPCRKVCNGIGIGEFKDSLSINATNIKHFKNCTSISGDLHILPVAFRGDSFTHTPPLDPQELDILKTVKEITGFLLIQAWPENRTD
LHAFENLEIIRGRTKQHGQFSLAVVSLNITSLGLRSLKEISDGDVIISGNKNLCYANTINWKKLFGTSGQKTKIISNRGENSCKATGQVCHALCSPEGCWGPEPRDCVSCRNVSRGRECVDKCNLLEGEPREFVENSECIQCHPECLPQAMNITCTGRGPDNCIQCAHYIDGPHCVKTCPAGVMGENNTLVWKYADAGHVCHLCHPNC
TYGCTGPGLEGCPTNGPKIPSIATGMVGALLLLVVALGIGLFMRRRHIVRKRTLRRLLQERELVEPLTPSGEAPNQALLRILKETEFKKIKVLGSGAFGTVYKGLWIPEGEKVKIPVAIKELREATSPKANKEILDEAYVMASVDNPHVCRLLGICLTSTVQLITQLMPFGCLLDYVREHKDNIGSQYLLNWCVQIAKGMNYLEDRR
LVHRDLAARNVLVKTPQHVKITDFGLAKLLGAEEKEYHAEGGKVPIKWMALESILHRIYTHQSDVWSYGVTVWELMTFGSKPYDGIPASEISSILEKGERLPQPPICTIDVYMIMVKCWMIDADSRPKFRELIIEFSKMARDPQRYLVIQGDERMHLPSPTDSNFYRALMDEEDMDDVVDADEYLIPQQGFFSSPSTSRTPLLSSLSA
TSNNSTVACIDRNGLQSCPIKEDSFLQRYSSDPTGALTEDSIDDTFLPVPEYINQSVPKRPAGSVQNPVYHNQPLNPAPSRDPHYQDPHSTAVGNPEYLNTVQPTCVNSTFDSPAHWAQKGSHQISLDNPDYQQDFFPKEAKPNGIFKGSTAENAEYLRVAPQSSEFIGA
```

**Composition Graph**




**3D Structure Visualization**



Zoom in EGRF

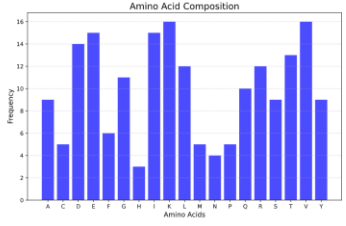
## Protein Sequence Analysis

**UniProt ID: P01116**

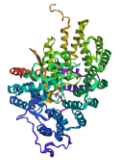
**Sequence**

```
MTEYKLVVVGAGGVGKSALTIQLIQNHFVDEYDPTIEDSYRKQVVIDGETCLLDILDTAGQEEYSAMRDQYMRTGEGFLCVFAINNTKSFEDIHHYREQIKRVKDSEDVPMVLVGNKCDLPSRTVDTKQAQDLARSYGIPFIETSAKTRQRVEDAFYTLVREIRQYRLKKISKEEKTPGCVKIKKCIIM
```

**Composition Graph**




**3D Structure Visualization**



Zoom in KRAS

# Demo Mode: Interactive Mode (cont.)

**Ligands that hit Targets that Impact Disease of Interest**

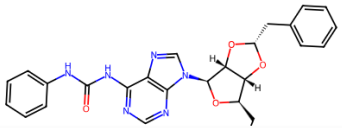
Showing the first 5000 rows from the result that contains 146560 rows!

| Count | Ligand Name | Ligand Is Drug | Ligand Activity Type | Ligand Action | Ligand References |
|---|---|---|---|---|---|
| 1 | (((2R,3S,4R,5R)-5-(6-(cyclopentylamino)-2-(methoxymethyl)-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methoxy)methylphosphonic acid | No | • IC50 | | • J Med Chem, (2021) |
| 2 | ((3aS,4R,6R,6aS)-2-benzyl-6-(6-(3-phenylureido)-9H-purin-9-yl)tetrahydrofuro[3,4-d][1,3]dioxol-4-yl)methyl-trihydrogen Diphosphate | | | | • J. Med. Chem., (200 |
| 3 | ((3S,4S)-4-(2-fluoro-6-methylphenoxy)-3,4-dihydro-1H-isochromen-3-yl)-N-methylmethanamine | | | | • Bioorg. Med. Chem. 18:16:4491 |
| 4 | ((cis)-3-(5-(3-(7-oxabicyclo[2.2.1]heptan-1-ylmethoxy)phenyl)-4-amino-7H-pyrrolo[2,3-d]pyrimidin-7-yl)cyclobutyl)methanol | | | | • Bioorg. Med. Chem. 26:8:2057 |

**SMILES:**

O=C(Nc1ccccc1)Nc1ncnc2c1ncn2[C@@H]1O[C@H](COP(=O)(O)OP(=O)(O)O)[C@H]2O[C@@H](Cc3ccccc3)O[C@H]21

**Molecule:**



Our system retrieves 146,560 ligand records—approved and experimental—with their associated targets and activity profiles.

# Demo Mode: Interactive Mode (cont.)

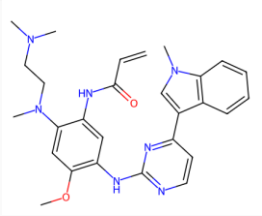
**Scoring Results**

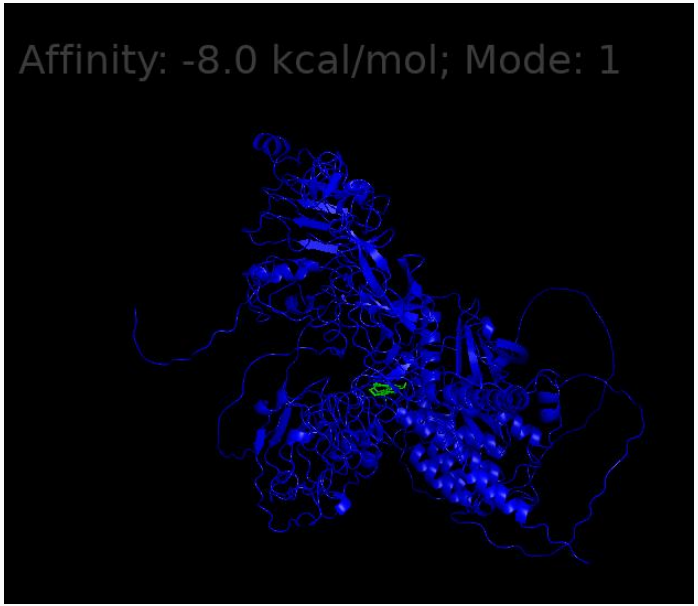
| Rank | Ligand Name | Ligand Is Drug | AI-1 Score | AI-2 Score | AI-3 Score | Final Ligand Score | Binding Affinity (kcal/mol) |
|---|---|---|---|---|---|---|---|
| 1 | osimertinib | Yes | 7.95 | 8.10 | 8.10 | 8.06 | P00533: -8.00 |
| 2 | gefitinib | Yes | 8.05 | 8.30 | 7.10 | 7.94 | P00533: -8.10 |
| 3 | erlotinib | Yes | 7.20 | 8.75 | 7.05 | 7.94 | P00533: -7.20 |
| 4 | brigatinib | Yes | 7.95 | 7.85 | 7.40 | 7.76 | P00533: -8.80 |
| 5 | dacomitinib | Yes | 7.95 | 8.00 | 7.05 | 7.75 | P00533: -8.90 |
| 6 | afatinib | Yes | 7.95 | 7.90 | 7.10 | 7.71 | P00533: -8.50 |
| 7 | ceritinib | Yes | 7.20 | 8.05 | 7.10 | 7.60 | P00533: -8.80 |
| 8 | mobocertinib | Yes | 7.00 | 7.75 | 7.10 | 7.40 | P00533: -7.90 |
| 9 | amivantamab | Yes | 7.05 | 7.30 | 7.00 | 7.16 | P00533: 0.00 |
| 10 | icotinib | Yes | 6.95 | 7.25 | 6.80 | 7.06 | P00533: -9.00 |

3rd-generation EGFR TKI

For example, our system ranks approved EGFR-targeting drugs by a composite, AI-derived weighted score.

# Demo Mode: Interactive Mode (cont.)






Example: binding affinity of osimertinib

**AI Model 2 Evaluation**

**Safety Profile**

**Score:** 7.00

**Rationale:** Osimertinib has an established safety profile as an FDA-approved drug for NSCLC. While side effects such as diarrhea, rash, and more serious risks like QT prolongation and interstitial lung disease exist, these are manageable with monitoring and dose adjustments. Regulatory approval by FDA, EMA, and PMDA indicates acceptable safety for clinical use.

**Efficacy Indicators**

**Score:** 9.00

**Rationale:** Osimertinib effectively targets mutant forms of EGFR prevalent in NSCLC, showing high binding affinity (-8.0 kcal/mol) and irreversible inhibition. Clinical trials have demonstrated significant improvements in progression-free and overall survival in patients, supporting strong efficacy.

**Pharmacokinetics**

**Score:** 8.00

**Rationale:** Osimertinib has favorable pharmacokinetic properties, including good oral bioavailability (~70%), adequate absorption, long half-life (48 hours), and extensive volume of distribution, allowing for effective dosing regimens.

**Treatment Potential**

**Score:** 9.00

**Rationale:** As an irreversible inhibitor of mutant EGFR, osimertinib overcomes resistance mechanisms in NSCLC and impacts key pathways such as EGFR signaling and PI3K/AKT, leading to cell cycle arrest and apoptosis in tumor cells, indicating high treatment potential.

**Drug Likeness**

**Score:** 8.00

**Rationale:** Osimertinib possesses favorable chemical properties consistent with drug-like molecules, is an approved drug, and has been successfully used clinically, indicating good drug-likeness.

Example: one AI's explanation of its scoring of osimertinib

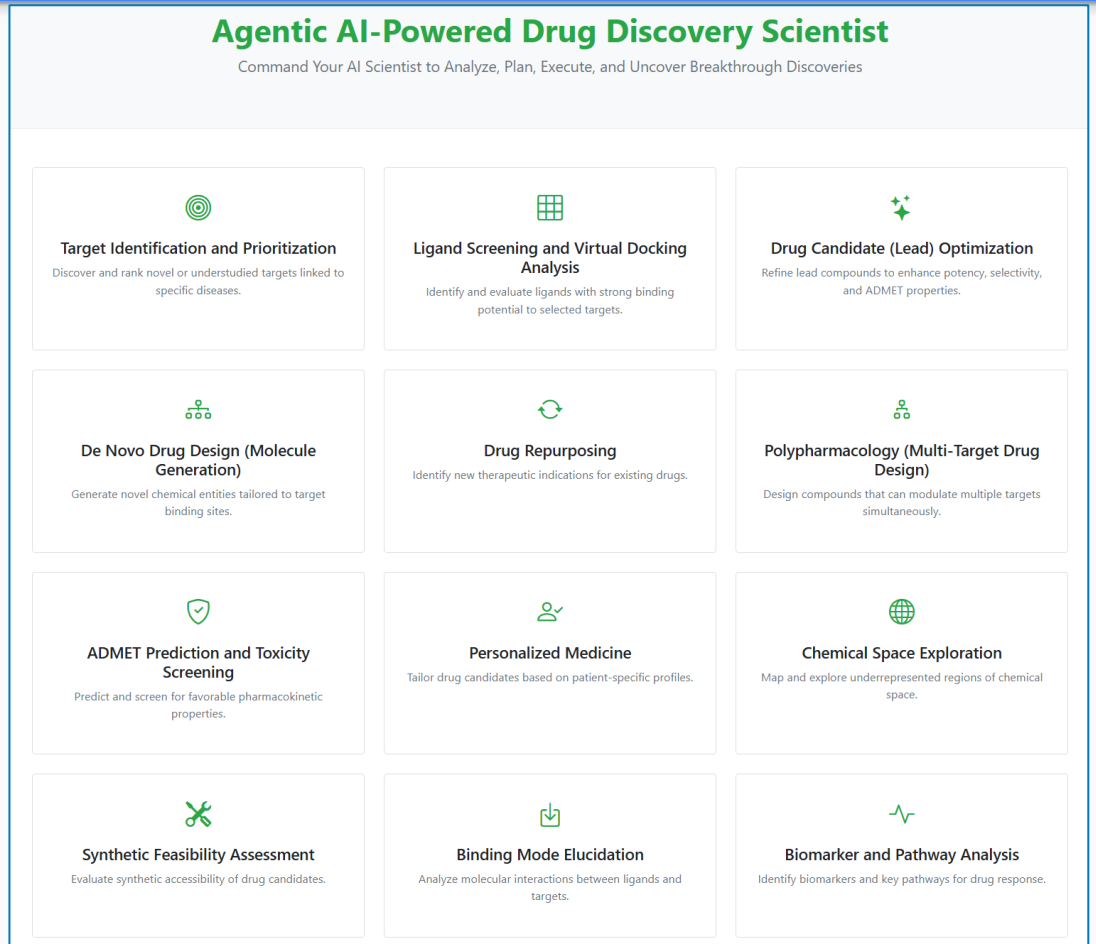
# Pause for Reflection

**Non–Small Cell Lung Cancer: The Opportunity**

- **~100 approved drugs**—but all act on just **a dozen targets**
- **Over 3,200 potential targets** have been associated with NSCLC
- **Hundreds of thousands to millions of compounds** may interact with those targets

Question: Should we deploy Agentic-AI to comprehensively discover new drugs and unlock untapped targets for Non–Small Cell Lung Cancer?

# Demo Mode: Auto-pilot Mode

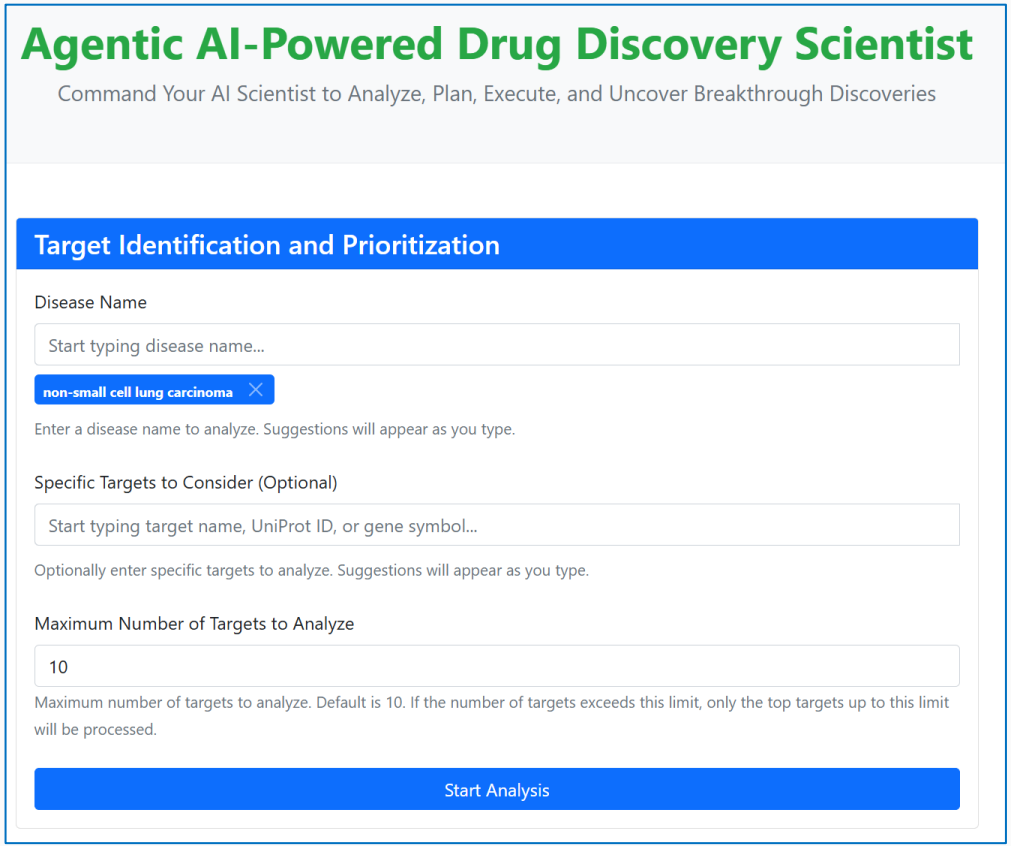



## Autonomous workflow

- Each box is the entry point to an AI agent, such as
  - Target Identification and Prioritization
  - Drug Repurposing
  - Molecule Generation
- Each AI agent self-reviews & adapts for certain highly complex drug-discovery tasks

# Demo Mode: Auto-pilot Mode (cont.)

**Non–Small Cell Lung Cancer on Target Identification and Prioritization as Example**




## Input Interface

### Step1 ) Type & Auto-Complete

Enter a few characters—our system will auto-fill the rest

### Step 2) Review & Adjust

Adjust optional inputs or take no action

### Step 3) Launch & Relax

Click “Start Analysis” and let the AI handle the rest

# Demo Mode: Auto-pilot Mode (cont.)

**Non–Small Cell Lung Cancer on Target Identification and Prioritization as Example**

## Analysis Results

### Target Prioritization

- EGFR (P00533): Score 9.00
- ALK (Q9UM73): Score 8.25
- KRAS (P01116): Score 7.61
- TP53 (P04637): Score 7.23
- VEGFA (P15692): Score 7.11
- CD274 (Q9NZQ7): Score 7.09
- ROS1 (P08922): Score 6.99
- CDH1 (P12830): Score 6.24
- PDCD1 (Q15116): Score 6.23
- CEACAM5 (P06731): Score 5.57

EGFR (P00533)

**Target Information**

**Target Name:** Epidermal growth factor receptor
**Protein Name:** EGFR_HUMAN
**Type:** Single Protein
**Family:** Belongs to the protein kinase superfamily. Tyr protein kinase family. EGF receptor subfamily.
**Description:** Epidermal growth factor receptor

2

Disease Association Factors

Disease Evidence Factors

Expression, Pathway, Network, Regulation Factors

Structure, Sequence Factors

Docking Prediction

Unboxed: Clinical Relevance

**Analysis Results:**

- Weighted Score: 9.00
  - Model 1 (AI): 9.50 (weight: 0.40)
  - Model 2 (AI): 9.20 (weight: 0.40)
  - Model 3 (Rule-Based): 7.59 (weight: 0.20)
- Key Factors:
  - High expression in 9 tissues with good confidence
  - High DisGeNET Score: 0.7
  - High expression and pathway involvement
  - High network connectivity (degree: 52, avg confidence: 0.80)
  - Has disease evidence: 16 PubMed IDs; 27 SNPs; ECO:0000033: traceable author statement; marker/mechanism
  - Structure available: AF-P00533-F1-model_v4.pdb
  - Has 149210 publications
  - Well-characterized structure and binding properties
  - Good secondary structure (helix: 0.29, sheet: 0.31)
  - Very high druggability score (7.59)
  - High Tinx Importance Score: 147.44
  - High disease association scores
  - Regulated by 11 factors
  - Co-expressed with 8389 proteins
  - 26 known drugs and 1556 clinical trials
  - Involved in 238 expression-related pathways
  - Extensive literature support (149,210 publications)
  - High TPM values in 31 tissues
  - Has 26 known drugs
  - Large surface area: 88003.4
  - Has 1556 clinical trials
  - Involved in 489 enriched pathways
  - Low docking confidence (score: -1.95)

# Example: EGFR scoring

3 models 1

- Strengths: 3
  - Multiple approved drugs
  - High tissue specificity
  - Robust expression data across tissues
  - Established clinical efficacy
  - Multiple known drugs targeting EGFR
  - Extensive literature and clinical trial evidence
  - Well-understood mechanism
- Limitations: 4
  - Low docking confidence (-1.95)
  - Low docking confidence (-1.95), indicating potential challenges in drug binding
  - Resistance development
- Recommendations:
  - Continue to explore EGFR inhibitors and combinations
  - Explore combination strategies
  - Focus on resistance mechanisms 5
  - Develop next-generation inhibitors
  - Leverage structural data for novel inhibitor design
  - Investigate resistance mechanisms and alternative pathways

**Clinical Evidence:** 149210 publications, 1556 clinical trials, 26 known drugs

Known Ligands (2541) 6

| Name | Type | Activity | Source |
|---|---|---|---|
| dasatinib | IC50 | 7.70 | - |
| docetaxel | Kd | 9.09 | - |
| erlotinib | IC50 | 7.55; 7.64; 7.69; 7.70; 7.71; 7.72; 7.80; 7.82; 7.96; 8.00; 8.19; 8.20; 8.30; 8.41; 8.44; 8.51; 8.52; 8.59; 8.66; 8.70; | - |

# Demo Mode: Auto-pilot Mode (cont.)

## Non–Small Cell Lung Cancer on Target Identification and Prioritization as Example

### Recommendations

- Prioritize EGFR for drug development (druggability score: 7.59)
- Consider CD274 for further validation studies
- Consider TP53 for further validation studies
- Prioritize ALK for drug development (druggability score: 7.24)
- Prioritize KRAS for drug development (druggability score: 7.07)
- Consider VEGFA for further validation studies
- Consider CEACAM5 for further validation studies
- Consider PDCD1 for further validation studies
- Consider ROS1 for further validation studies
- Consider CDH1 for further validation studies

### Therapeutic Strategies

- Leverage known ligands for EGFR as starting points for drug design
- Consider pathway-based approaches for EGFR to modulate disease network
- Leverage known ligands for CD274 as starting points for drug design
- Consider pathway-based approaches for CD274 to modulate disease network
- Leverage known ligands for TP53 as starting points for drug design
- Consider pathway-based approaches for TP53 to modulate disease network
- Leverage known ligands for ALK as starting points for drug design
- Consider pathway-based approaches for ALK to modulate disease network
- Leverage known ligands for KRAS as starting points for drug design
- Consider pathway-based approaches for KRAS to modulate disease network
- Leverage known ligands for VEGFA as starting points for drug design
- Consider pathway-based approaches for VEGFA to modulate disease network
- Consider fragment-based screening for CEACAM5 to identify initial hits
- Consider pathway-based approaches for CEACAM5 to modulate disease network
- Leverage known ligands for PDCD1 as starting points for drug design
- Consider pathway-based approaches for PDCD1 to modulate disease network
- Leverage known ligands for ROS1 as starting points for drug design
- Consider pathway-based approaches for ROS1 to modulate disease network
- Consider fragment-based screening for CDH1 to identify initial hits
- Consider pathway-based approaches for CDH1 to modulate disease network

# Pause for Reflection

- Traditionally, prioritizing drug targets demands the coordinated effort of a diverse, highly-trained team—each bringing deep domain knowledge.

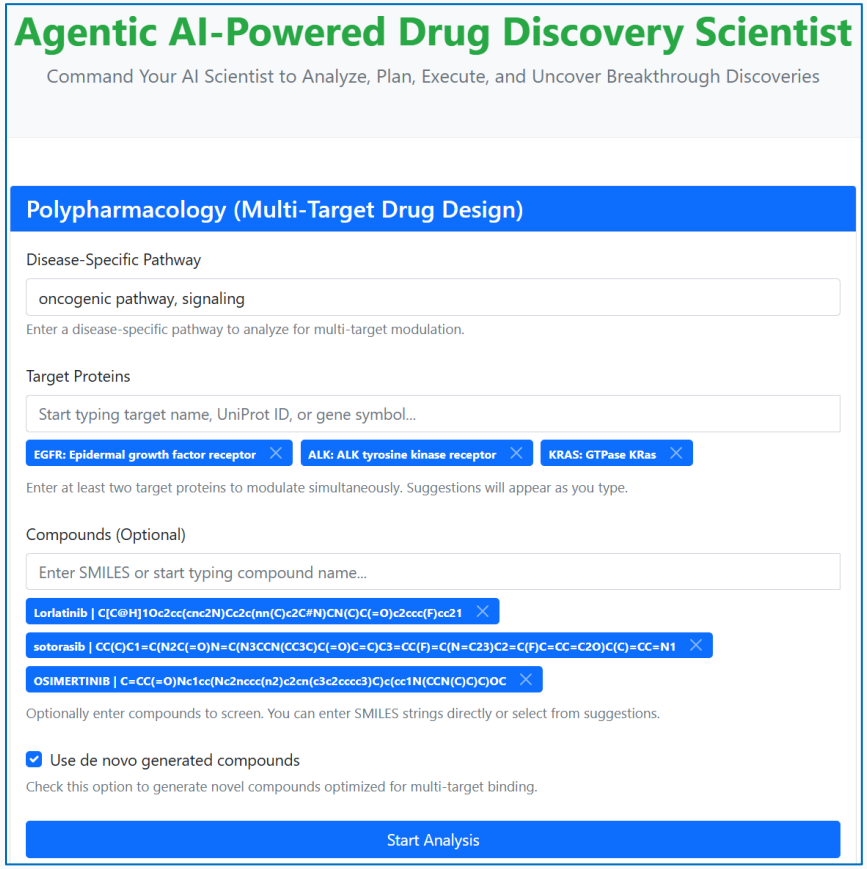
| Target Prioritization Area | Typical Human Roles |
|---|---|
| Disease Association | Geneticist, Bioinformatician, Epidemiologist |
| Disease Evidence | Clinical Researcher, Medical Writer |
| Expression, Pathway, Network, Regulation | Systems Biologist, Pathway Analyst, Molecular Biologist |
| Structure, Sequence | Structural Biologist, Computational Chemist, Protein Scientist |
| Docking Prediction | Medicinal Chemist, Computational Modeler |
| Clinical Relevance | Clinical Scientist, Pharmacologist, Data Analyst |

- Today, Agentic-AI is able to orchestrate, automate, and even scale many of these complex workflows—acting as a virtual multidisciplinary team.

**Should we reimagine how discoveries happen?**

# Demo Mode: Auto-pilot Mode (cont.)

## Non–Small Cell Lung Cancer on Polypharmacology (Multi-Target Drug Design) as Example




## Input Interface

**Step1 ) Select Targets:** EGFR, ALK, KRAS

**Step 2) Add Ligands**

- osimertinib – EGFR
- lorlatinib – ALK
- sotorasib – KRAS

**Step 3) Toggle on “De Novo Generated Compounds”**

Toggle on “De Novo Generated Compounds”

**Step 4) Launch & Relax**

Click “Start Analysis” and let the system run automatically

# Demo Mode: Auto-pilot Mode (cont.)

## Analysis Results

### Target Set

- ALK (Q9UM73)
- EGFR (P00533)
- KRAS (P01116)

### Pathway Interactions

**Interaction Strength:** 0.99

**Network Density:** 1.00

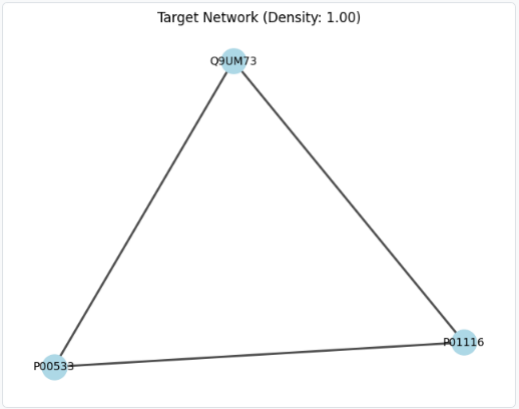
Network density range: 0 (no connections) to 1 (fully connected)

**Common Pathways:**

- Non-small cell lung cancer (3 targets, 100.0%)
- PD-L1 expression and PD-1 checkpoint pathway in cancer (3 targets, 100.0%)
- Signaling by FGFR4 in disease (3 targets, 100.0%)
- Constitutive Signaling by EGFRvIII (3 targets, 100.0%)
- Signaling by ERBB2 ECD mutants (3 targets, 100.0%)
- MET in type 1 papillary renal cell carcinoma (3 targets, 100.0%)
- Constitutive Signaling by Ligand-Responsive EGFR Cancer Variants (3 targets, 100.0%)
- Signaling by FGFR3 in disease (3 targets, 100.0%)
- Signaling by ERBB2 KD Mutants (3 targets, 100.0%)
- Diseases of signal transduction by growth factor receptors and second messengers (3 targets, 100.0%)
- Signaling by FGFR1 in disease (3 targets, 100.0%)
- Signaling by FGFR2 in disease (3 targets, 100.0%)
- Signaling by Receptor Tyrosine Kinases (3 targets, 100.0%)
- Signaling by EGFR (3 targets, 100.0%)
- Lung cancer (3 targets, 100.0%)
- Glioma (3 targets, 100.0%)
- EGFR tyrosine kinase inhibitor resistance (3 targets, 100.0%)
- ErbB signaling pathway (3 targets, 100.0%)
- Glioblastoma signaling pathways (3 targets, 100.0%)
- Choline metabolism in cancer (3 targets, 100.0%)

## Non–Small Cell Lung Cancer on Polypharmacology (Multi-Target Drug Design) as Example

Target Network Visualization



# Demo Mode: Auto-pilot Mode (cont.)

The system designs de novo multi-target compounds for EGFR, ALK, and KRAS—ranking Compound 4 as the top candidate.

| Rank | Compound | Structure | Balance Score | Potency Score | Combined Score |
|---|---|---|---|---|---|
| 1 | Compound_4 | | 0.13 | 5.33 | 4.87 |
| 2 | Compound_6 | | 0.65 | 6.22 | 3.39 |
| 3 | Compound_7 | | 0.52 | 5.13 | 3.26 |
| 4 | Compound_8 | | 0.44 | 4.35 | 3.00 |

Balance Score: Lower is better, 0 is perfect; Potency and Combined Scores: Higher is better; 10 is perfect.

### Target Docking Profiles

Docking Profile for Top Candidate: Compound_4

| Target | Confidence Score |
|---|---|
| ALK | -1.18 |
| EGFR | -1.10 |
| KRAS | -1.22 |

Note: Score >0, high confidence; btw 0 and -1.5, moderate; below -1.5, weak.

### ADMET Profiles

ADMET Profile for Top Candidate: Compound_4

Absorption

- **oral bioavailability: high** (confidence: 0.55)
- **caco2 permeability: high** (confidence: 0.60)
- **pgp substrate: low** (confidence: 0.60)

Distribution

- **plasma protein binding: low** (confidence: 0.50)
- **blood brain barrier: low** (confidence: 0.50)
- **volume of distribution: low** (confidence: 0.50)

Metabolism

- **cyp inhibition:**
  - **3A4: low** (confidence: 0.50)
  - **2D6: low** (confidence: 0.50)
  - **2C9: low** (confidence: 0.50)
- **half life: short** (confidence: 0.55)

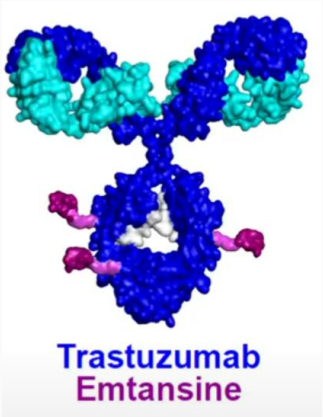
Toxicity

- **herg inhibition: low** (confidence: 0.56)
- **hepatotoxicity: low** (confidence: 0.50)
- **carcinogenicity: low** (confidence: 0.50)
- **mutagenicity: low** (confidence: 0.50)

Confidence scores near 0.5 indicate predictions close to threshold values. Higher confidence (>0.7) indicates stronger predictions.

# Switching to the demo of ADCs for Breast Cancer

**Two Generations of ADCs, T-DM1 and T-DXd, that treat HER2+ breast cancer**




Approved 2013

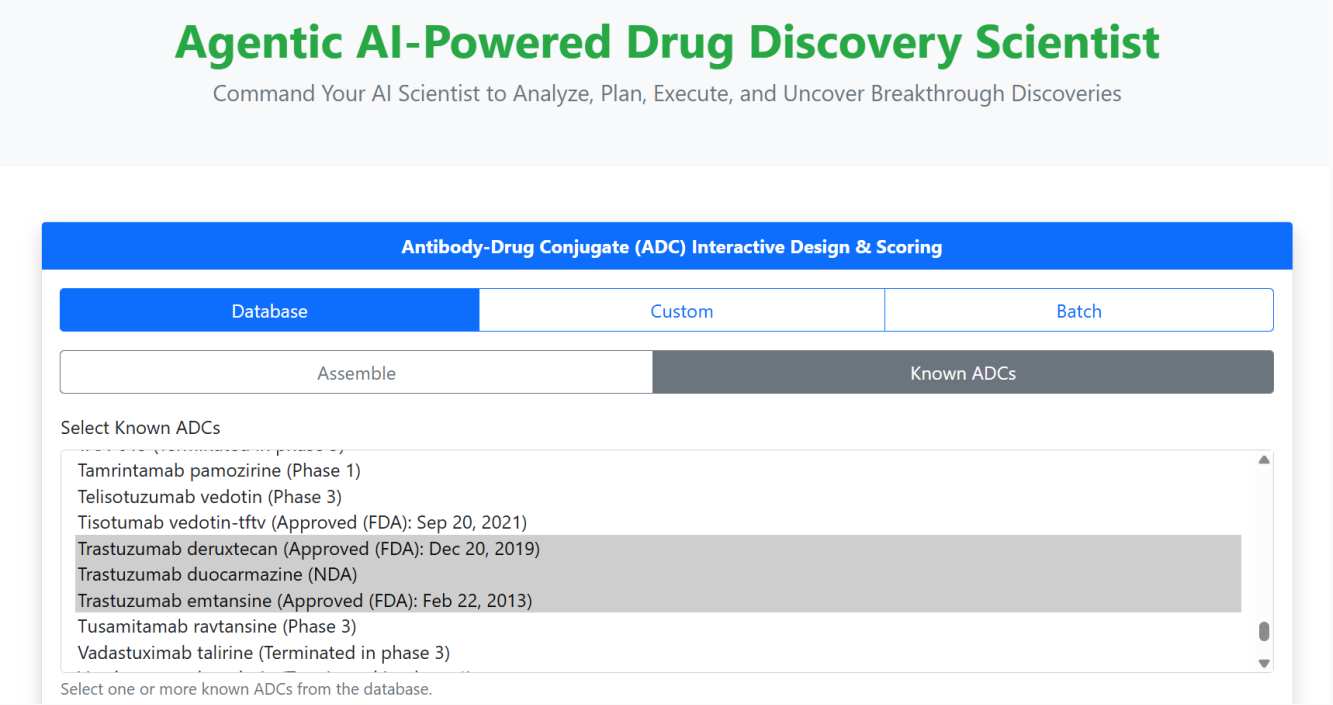
| T-DM1 | ADC Attributes | T-DXd |
|---|---|---|
| Trastuzumab | Antibody | Trastuzumab |
| Emtansine | Payload | Deruxtecan |
| Anti-microtubule | Payload MoA | Topoisomerase I inhibitor |
| ~3.5:1 | Drug-to-antibody ratio | ~8:1 |
| No | Tumor-selective cleavable linker? | Yes |
| No | Evidence of bystander anti-tumor effect? | Yes |

Approved 2019

# Demo Mode: Auto-pilot Mode (cont.)

## ADC Scoring with the antibody of Trastuzumab as Example

### Input Interface: Step 1) Select Three ADCs



# Demo Mode: Auto-pilot Mode (cont.)

| ADC Name | Drug Status | Indications | Target Name | Antigen Name | Antibody Name | Payload Name | Linker Name | DAR |
|---|---|---|---|---|---|---|---|---|
| Trastuzumab emtansine | Approved (FDA): Feb 22, 2013 | ['Breast cancer [ICD11:2C60-2C65] (Approved)', 'HER2(+) breast cancer [ICD11:2C60-2C65] (Approved)', 'Metastatic breast cancer [ICD11:2C6Y] (Approved)', 'Solid tumors [ICD11:2A00-2A0Z\|2B50-2F9Z] (Phase 2)', 'Gastric cancer [ICD11:2B72] (Terminated in phase 3)', 'Bladder cancer [ICD11:2C94] (Terminated in phase 2)', 'Intrahepatic bile ducts cancer [ICD11:2C12] (Terminated in phase 2)', 'Non-small cell lung cancer [ICD11:2C25] (Terminated in phase 2)', 'Pancreatic cancer [ICD11:2C10] (Terminated in phase 2)'] | Microtubule (MT) | Receptor tyrosine-protein kinase erbB-2 (ERBB2) | Trastuzumab | Mertansine DM1 | Succinimidyl-4-(N-maleimidomethyl)cyclohexane-1-carboxylate (SMCC) | 3.5 |

Score All

**Input Interface:**

**Step 2) Receive Detailed ADC Information**

**&**

**Click on “Score All”**

# Demo Mode: Auto-pilot Mode (cont.)

## User Interface: Step 3) Potency Probabilities Returned

Results Dashboard

Export CSV

| ADC ID | Antigen Name | Antibody Name | Payload Name | Linker Name | DAR | Probability of Potency |
|---|---|---|---|---|---|---|
| Trastuzumab deruxtecan | Receptor tyrosine-protein kinase erbB-2 (ERBB2) | Trastuzumab | DX-8951 derivative (DXd) | Mc-Gly-Gly-Phe-Gly | 8 | 93.94% |
| Trastuzumab duocarmazine | Receptor tyrosine-protein kinase erbB-2 (ERBB2) | Trastuzumab | seco-DUBA | Mal-PEG2-Val-Cit-PABA-Cyclization Spacer | 2.8 | 59.61% |
| Trastuzumab emtansine | Receptor tyrosine-protein kinase erbB-2 (ERBB2) | Trastuzumab | Mertansine DM1 | Succinimidyl-4-(N-maleimidomethyl)cyclohexane-1-carboxylate (SMCC) | 3.5 | 91.07% |

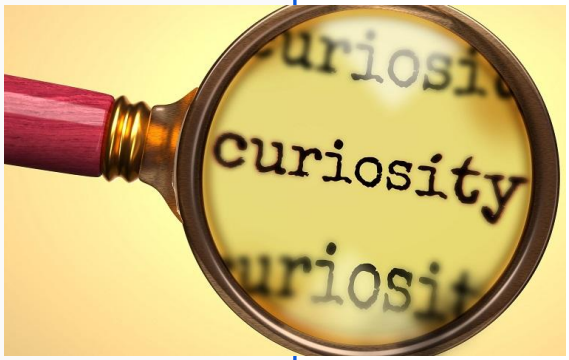
**T-DXd: Approved 2019**

**New Drug Application**

**T-DM1: Approved 2013**

# Demo Mode: Auto-pilot Mode (cont.)

Out of curiosity, on June 12, 2025, I asked Gemini Deep Research for its opinion on the **trastuzumab duocarmazine** New Drug Application.




Gemini

2.5 Pro (preview)

Regarding your questions about trastuzumab duocarmazine (SYD985):

**1. How likely is this ADC to be approved in the US by the FDA?**

The likelihood of trastuzumab duocarmazine (SYD985) receiving FDA approval in the US for HER2-positive metastatic breast cancer, based on the data from the TULIP trial, currently appears to be low.

- In May 2023, the FDA issued a Complete Response Letter (CRL) for the Biologics License Application (BLA) of trastuzumab duocarmazine. A CRL indicates that the FDA cannot approve the application in its present form and has requested additional information. The developer, Byondis, stated that addressing this request would require additional time and resources beyond the review period. The specific details of the information requested by the FDA were not publicly disclosed.
- Further compounding the challenges, the European Medicines Agency (EMA) marketing authorisation application for the drug (under the name Jivadco) was withdrawn by the applicant in September 2023. This withdrawal followed significant concerns raised by the EMA's Committee for Medicinal Products for Human Use (CHMP) regarding the analysis of progression-free survival (PFS) data, the handling of patients who discontinued treatment, adequacy of patient follow-up, and findings from clinical trial site inspections. The CHMP's provisional opinion was that the benefits of the drug did not outweigh its risks.

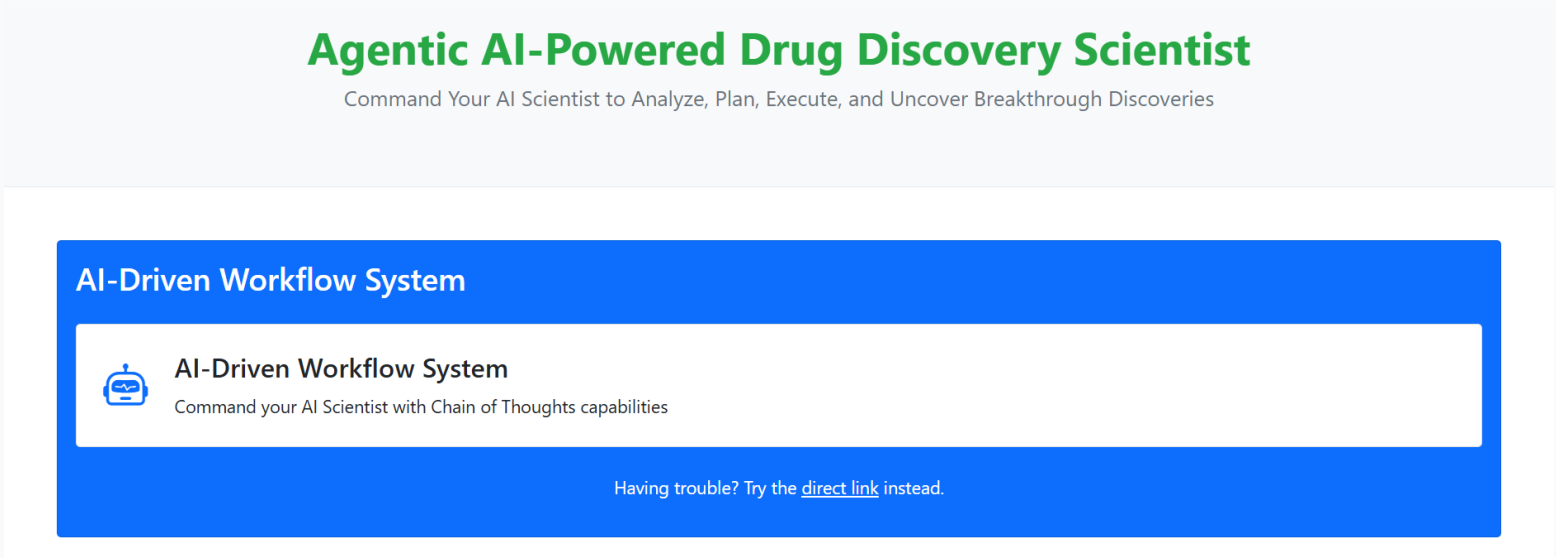
# Pause for Reflection

- The preclinical development of an ADC candidate, from initial concept through to Investigational New Drug (IND) submission, typically spans 15 to 30 months.
- With Agentic-AI's ability to assemble or generate vast libraries of novel antibodies, payloads, and linkers—and instantly evaluate the potency of every new ADC combination—we're witnessing a true game-changer in ADC discovery.

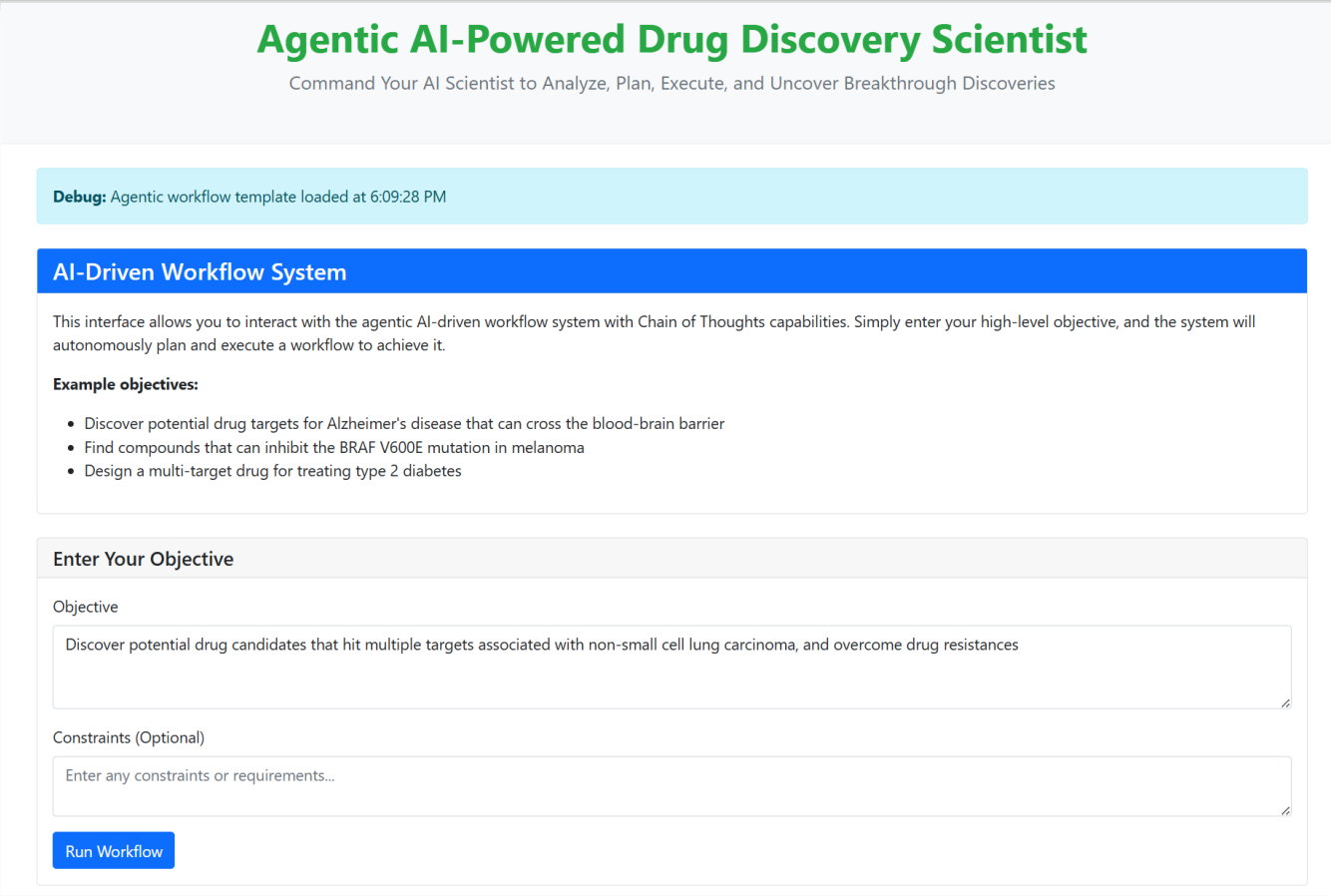
Agentic-AI enables rapid generation and evaluation of countless novel ADCs—transforming the pace and scale of discovery.

# Demo Mode: Full-Self Driving Mode

## Step 1: Enter the robotic interface



# Demo Mode: Full-Self Driving Mode

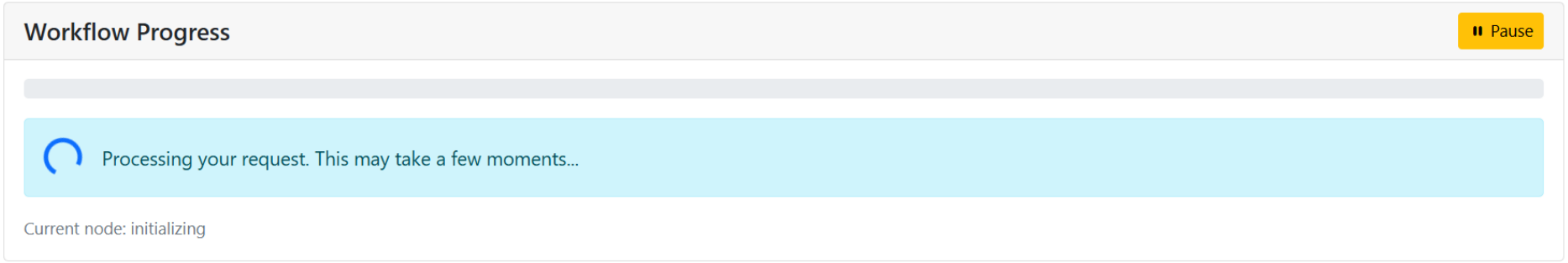



**Step 2: Define Objective (with or without additional requirements)**

**Step 3: Hit "Run Workflow" and relax**

# Demo Mode: Full-Self Driving Mode

**Then, you will see ….**



# Demo Mode: Full-Self Driving Mode

## Review and Approve Plan

The workflow has reached a checkpoint. Please review the plan and decide how to proceed.

**Initial Inputs**

**Objective:** Identify drug candidates that can target multiple proteins associated with non-small cell lung carcinoma and address drug resistance issues.

**Objective Analysis:**

The objective is to discover drug candidates that can interact with multiple targets related to non-small cell lung carcinoma, with a focus on overcoming drug resistance. No specific ligands or targets are mentioned, so the default mode for both ligands and targets is 'addition', meaning any relevant ligands or targets identified by the workflow should be considered. The absence of constraints allows for a broad exploration of potential candidates and targets.

**Disease:** non-small cell lung carcinoma (close match of 'non-small cell lung carcinoma')

**Sorted Targets (Showing Top 20 Targets Out of 3213)**

- EGFR (P00533)
- CD274 (Q9NZQ7)
- TP53 (P04637)
- ALK (Q9UM73)
- KRAS (P01116)
- VEGFA (P15692)
- CEACAM5 (P06731)
- PDCD1 (Q15116)
- ROS1 (P08922)
- CDH1 (P12830)
- GAPDH (P04406)
- EML4 (Q9HC35)
- ERCC1 (P07992)
- PTEN (P60484)
- CTNNB1 (P35222)
- MYC (P01106)

**The system returns a detailed analysis of your objective and a proposed plan for you to review, refine, or execute.**

# Demo Mode: Full-Self Driving Mode

**Execution Plan**

**Main Path**

- Analyzing target structures
- Analyzing target druggability
- Screening ligands against targets
- Analyzing binding modes
- Predicting ADMET properties
- Screening for toxicity
- Generating novel molecules
- Optimizing molecules

**Drug Repurposing Path**

- Analyzing target druggability
- Identifying repurposing candidates
- Analyzing repurposing mechanisms

**Polypharmacology Path**

- Analyzing target druggability
- Identifying target combinations
- Designing multi-target ligands

**Next Steps**

1. Analyze target structures
2. Assess target druggability
3. Screen ligands against targets
4. Analyze binding modes
5. Predict ADMET properties
6. Screen for toxicity
7. Generate novel molecules
8. Optimize molecules
9. Identify repurposing candidates
10. Analyze repurposing mechanisms
11. Identify target combinations
12. Design multi-target ligands

**The system returns a detailed analysis of your objective and a proposed plan for you to review, refine, or execute.**

Edit Plan

Approve and Continue

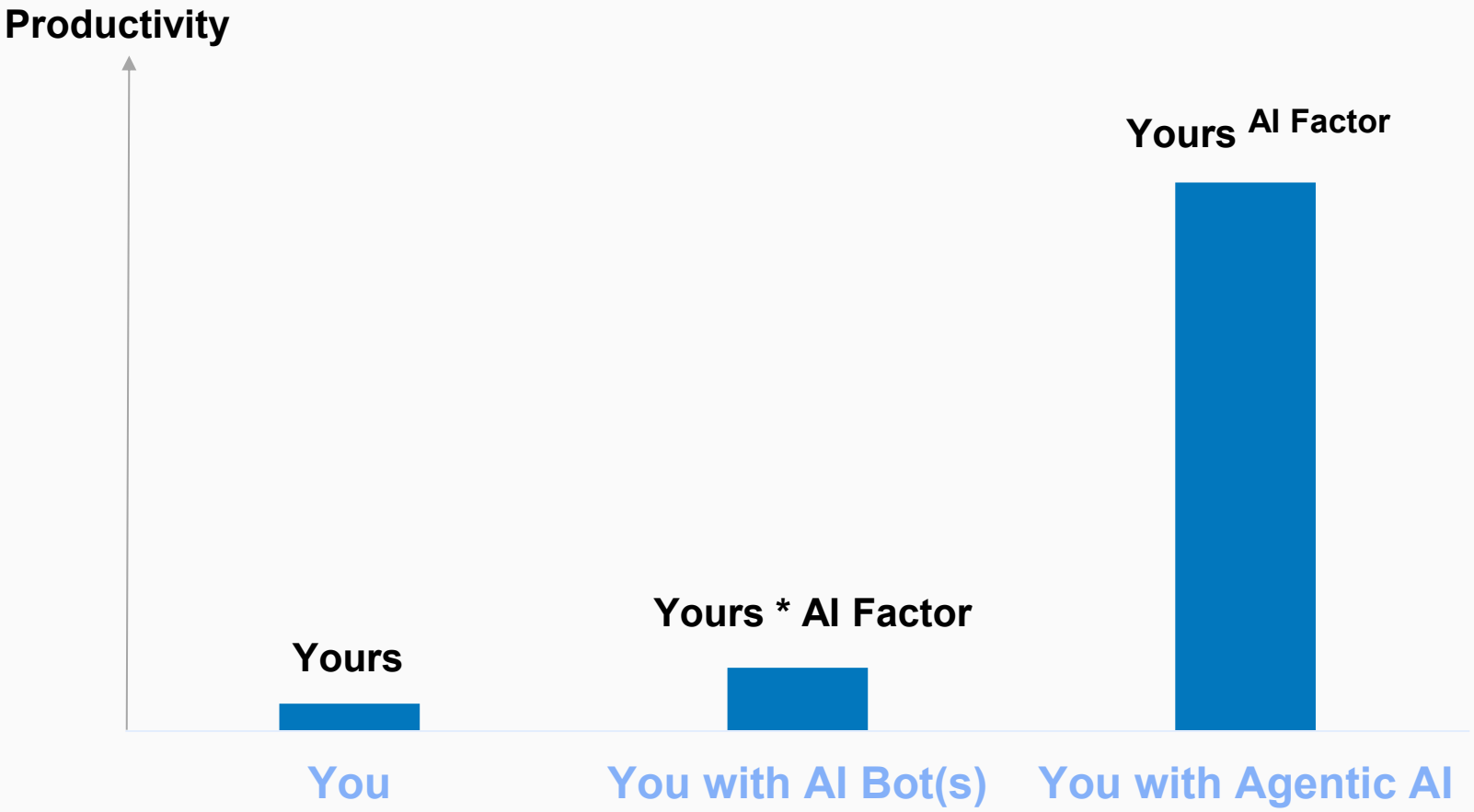
# Where To Next?

**Shift over 90% of routine tasks (R&D or whatever your business) to agentic AI, delivering:**

- **10× Your Team** with only modest incremental cost
- **A Tireless Workforce** operating at unmatched speed and scale
- **Diverse Expertise On-Demand** across every relevant domain
- **Minimized operational errors** and **miscommunication inefficiencies**

## Outcome: Exponential Productivity Growth

# How productivity could be different?



# The Future is in Our Hands