IQVIA's Drug Discovery & Development Services

Empowering pharmaceutical R&D partners to expedite drug design & development through IQVIA's AI/ML-backed commercial consulting expertise

IQVIA

Deliver faster with greater accuracy

Utilizing AI/ML in clinical R&D creates a paradigm shift around speed, accuracy and cost regarding how pharmaceutical partners bring drugs to market.

Solutions with speed

As an industry, we know it takes 10-15 years and billions of dollars to bring a new drug to market. Adding to that challenge is the knowledge that less than 12% of drugs make it through clinical development. IQVIA's Drug Development & Discovery Services provides solutions aimed at changing that.

IQVIA's highly-skilled machine learning engineers and data scientists, leveraging our unparalleled data, produce solutions for pharmaceutical partners that shorten the development cycle. With advances in high-throughput technologies and data management systems, there are now vast datasets to be applied in the field of biomedicine to provide insights needed to make more informed decisions.

IQVIA extends the results of the analytics with domain expertise to help you make evidence-based decisions. Our offerings help you:

- Produces novel drug designs
- Keep your pipeline healthy
- Find additional uses for new and existing compounds
- Identify the right subpopulations for your trials
- Augment your team with proven expertise
- Maximize the likelihood of clinical trial success

Our Offerings

MOLECULAR DESIGN & OPTIMIZATION	Leveraging computational methods rooted in deep learning to automate the molecular generation process and reduce the search space.
BIOMARKER IDENTIFICATION	Identifying and validating biomarkers from high-throughput gene expression to aid patient stratification and disease progression.
DRUG TARGET INTERACTION FOR DRUG REPURPOSING	Mining existing drugs for new uses and potentially bypassing early drug discovery stages to increase speed to market, lower costs and improve the probability of clinical trial success.
PREDICTING CLINICAL TRIAL SUCCESS	Validating R&D candidates through AI-powered trial simulation and real-world data to forecast clinical trial outcomes to gain better insight into the drug approval process.

Molecular design & optimization

The goal of our molecular design & optimization service is to design molecules or chemical compounds with desired properties by leveraging AI. Refining the molecule at each generative step results in a mechanism that can significantly outperform its previous iteration.

TRADITIONAL METHODS FOR NEW MOLECULES

Traditional processes to identify new molecules often include exhaustive searches through a fixed library or discrete local search methods, such as genetic algorithms. These techniques have led to new molecules in the past; however, they are facing challenges because fixed libraries are costly to utilize and require hand-crafted rules that are difficult and time consuming.

MODELS FOR MOLECULAR DESIGN

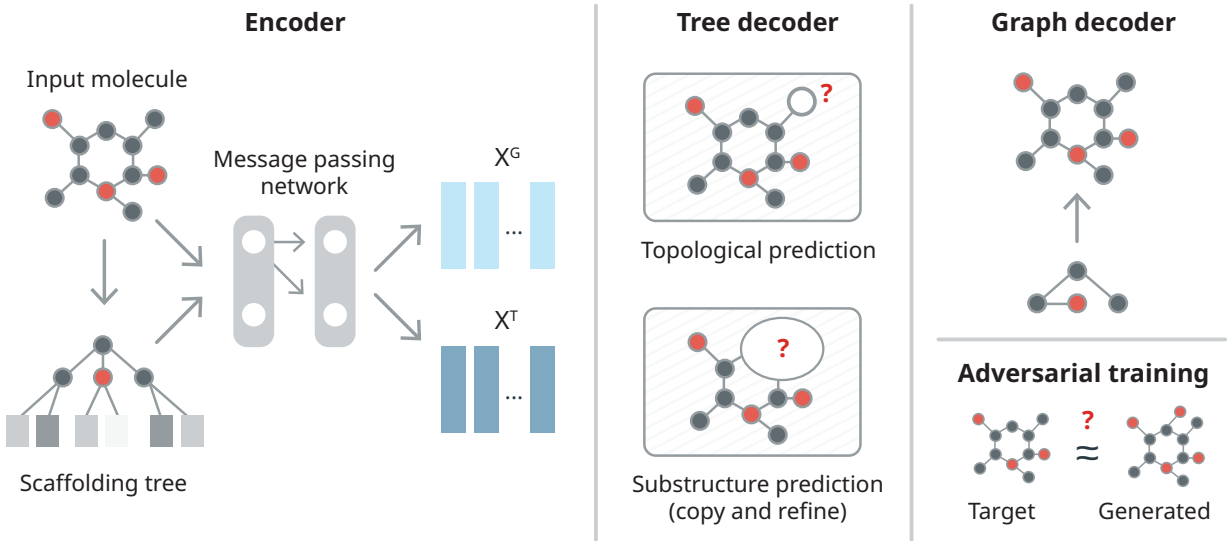
Current models for lead optimization often rely on graph generation methods. These methods can exhibit undesirable behaviors, such as generating inaccurate substructures because the set of all possible substructures is so large.

By using machine learning (ML) with a generative adversarial network (GAN), we are able to automatically generate new compounds. Our models can map molecular representations to desired properties quickly and effectively. These new structures are chemically meaningful molecular compounds that make substantially larger jumps in this innovative space than traditional methods.

OPTIMIZING WITH OUR COPY & REFINE STRATEGY

With IQVIA's Copy & Refine Strategy, our model decides whether to copy a substructure from the input molecule (copy), or to sample a novel substructure from the entire space of substructures (refine) to create novel, but stable, molecules from input molecules. The resulting mechanism enhances accuracy to 90% in substructure prediction. The Copy & Refine Strategy outperforms the latest molecule optimizations baselines, most especially on rare substructures.

Automatic molecule optimization using our Copy & Refine Strategy



Biomarker identification

Identifying patients who would benefit most from specialized treatments is transforming personalized medicine. AI-powered biomarker identification supports R&D in rare diseases by enabling precise patient targeting.

Patient populations in clinical trials are known to be heterogeneous. Biomarkers help characterize and reduce patient heterogeneity, which plays a role in the development of tailored therapies. Biomarker identification improves the likelihood of program success.

TYPES OF BIOMARKERS

Biomarkers include demographic, genetic and clinical data points. **Prognostic markers** are used for identifying subgroups of patients with different outcomes irrespective of the treatment they receive. **Predictive markers** help identify subgroups of patients who are more likely to benefit from a particular treatment, which is key in the development of personalized medicine.

WHY BIOMARKERS ARE IMPORTANT

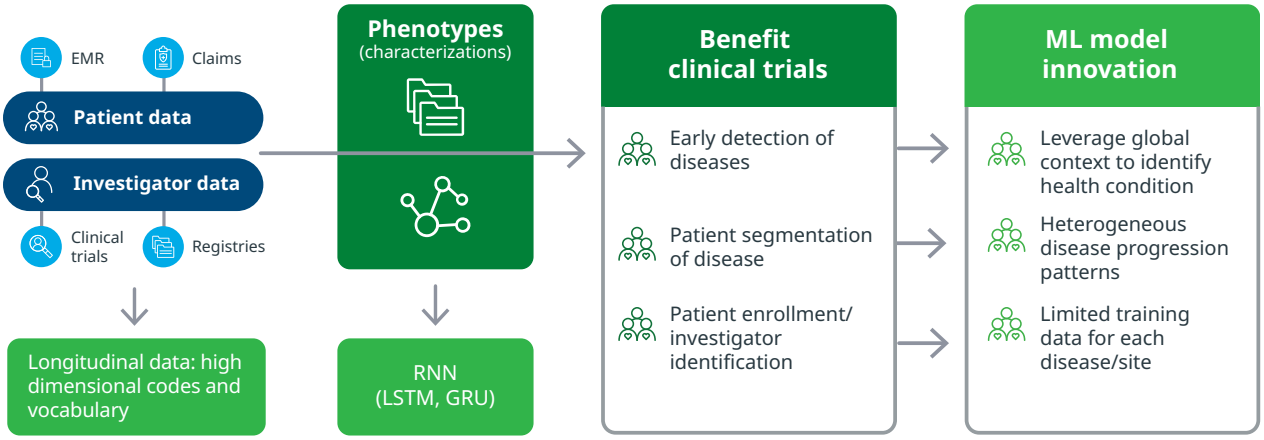
- Drug makers are taking longer to move medicines to approval.
- Novel biomarkers and the ability to draw from pre-screened patient pools provide a productivity boost to the R&D industry.
- Genetic testing leads to a greater understanding of biomarkers linked to disease.
- Improved patient subpopulation selection reduces adverse events and increases overall effectiveness and safety profile of drug candidates.
- The use of biomarkers to recruit patient sub-populations is expected to increase.

Unlocking new possibilities

IQVIA's Drug Discovery & Development team utilizes a combination of data types, including text, omics, phenotypes, assays and molecular structures to create cell-centered learning models. These models are utilized to aid in patient stratification and disease progression through biomarker identification and validation.

IQVIA's machine learning platforms and algorithms identify predictive biomarker(s) in treatment populations with stronger outcomes based on pre-screened patient pools that will drive optimization of trial success and shorter timelines and cost.

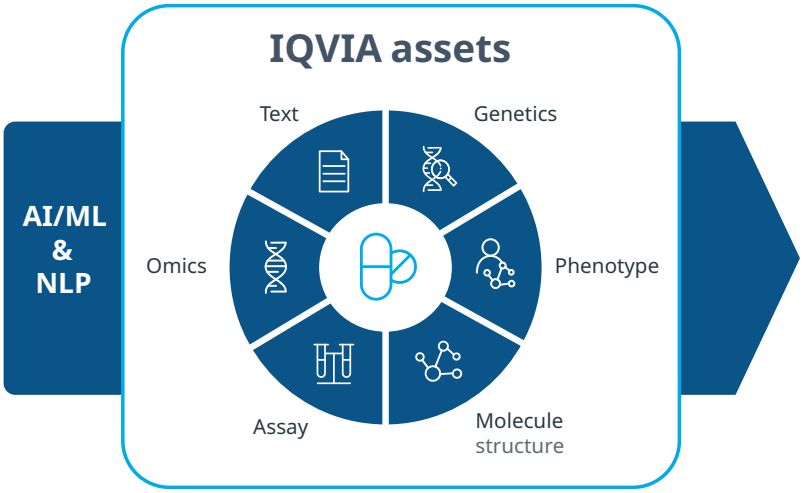
How IQVIA enables your use of Biomarkers



Drug repurposing

Drug repurposing drives increased speed and lower costs by mining existing drugs for new purposes. It allows you to bypass early drug discovery phases and improve the odds that clinical development trials will be successful.

IQVIA's approaches, data assets and expertise enable effective repurposing of existing drugs



Drug centric

- New indications
- Safer drugs
- Less expense

Disease centric

- Specific diseases
- Rare diseases
- Neglected diseases

TRADITIONAL DRUG DEVELOPMENT

Traditional drug development is slow, expensive and high risk. Knowledge of failed assets is often limited and unpublished, which prevents you from having the insights needed to identify successful targets.

AI-POWERED DRUG REPURPOSING

Using AI for drug repurposing gives you confidence in your decision making by providing deeper knowledge and better understanding of potential opportunities.

Streamlined Process

Approved drugs and those that have proven safety in Phase I/II trials save vast amounts of clinical development time and money. By mining existing drugs for new uses, researchers can focus solely on the clinical testing portion of the approval process, shortening development timelines.

Improved drug development success

AI has huge potential to improve the success of drug development, providing new insights into disease drug targets and improving the odds that clinical development trials will be successful.

Earlier patient access

AI provides potential opportunity for patients to access new treatments more quickly due to the potential to bypass early drug discovery stages.

Predicting clinical trial success

Our AI models can predict technical and regulatory success, which not only helps support investment decisions, but also gives you a better understanding of clinical trial features and their impact on the potential success of an asset.

By providing insight into the probability of trial success, IQVIA gives you greater visibility, better protocol design and confidence around where to invest your budget for the biggest value return.

LEVERAGING IQVIA'S PREDICTIVE TECHNOLOGY

IQVIA's solution combs through copious amounts of data and analyzes more than 1,800 variables per pathway to provide prediction that outperform industry-leading models widely used as benchmarks today. This tool, offered with and without expert consulting services can:

- Predict the probability of a compound currently in a trial to achieve FDA approval for the studied indication
- Predict the probability of a trial meeting it's endpoints with statistical significance, gaining insights about key trial, patient and protocol metrics
- Provide insight into the characteristics of existing clinical trials
- Show articles from biomedical literature that describe the effects of a given intervention

Innovate to succeed

The goal of IQVIA's Drug Discovery & Development Services is to drive solutions in pharmaceutical R&D with a focus on expediting drug design and development through to the prediction of clinical trial success. Contact us for more information on how to innovate to succeed.

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