

Global AI Drug Discovery Supply, Demand and Key Producers, 2026-2032

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Abstracts

The global AI Drug Discovery market size is expected to reach \$ 47759 million by 2032, rising at a market growth of 29.2% CAGR during the forecast period (2026-2032).

AI Drug Discovery refers to the use of artificial intelligence (AI) technologies, machine learning (ML) algorithms, and big data analysis to accelerate drug discovery, design, screening, and optimization. The core advantage of AI drug discovery lies in its high data processing and pattern recognition capabilities, which can help identify potential drug candidates, predict biological activities, optimize preclinical drug effects, and shorten the drug development cycle. Common applications in AI drug discovery include target discovery, virtual screening, drug repurposing, molecular design, and clinical data analysis.

The upstream of the industry chain involves data resources and algorithm technologies, such as genomic data, protein structure databases, chemical libraries, and AI platforms. Downstream applications are concentrated in pharmaceutical companies, new drug R&D institutions, and contract research organizations (CROs), supporting drug discovery, target validation, drug repositioning, and personalized medicine design. Pharmaceutical companies leverage AI to shorten development cycles, reduce costs, and improve drug success rates. CROs utilize AI for compound screening, toxicity prediction, and clinical trial design, enhancing overall R&D efficiency.

Development trends include multimodal data integration, generative AI for drug design, AI-assisted clinical trial optimization, and precision medicine integration. Driving factors include high costs of traditional drug development, long R&D timelines, high clinical failure rates, and enhanced AI computational capabilities. Constraints include difficulty in acquiring high-quality data, limited algorithm interpretability, regulatory uncertainties,

and shortage of specialized talent. Overall industry gross margins are relatively high, typically ranging from 40% to 60%, driven by the added value of software and AI services to pharmaceutical companies and technological barriers.

This report studies the global AI Drug Discovery demand, key companies, and key regions.

This report is a detailed and comprehensive analysis of the world market for AI Drug Discovery, and provides market size (US\$ million) and Year-over-Year (YoY) growth, considering 2025 as the base year. This report explores demand trends and competition, as well as details the characteristics of AI Drug Discovery that contribute to its increasing demand across many markets.

Highlights and key features of the study

Global AI Drug Discovery total market, 2021-2032, (USD Million)

Global AI Drug Discovery total market by region & country, CAGR, 2021-2032, (USD Million)

U.S. VS China: AI Drug Discovery total market, key domestic companies, and share, (USD Million)

Global AI Drug Discovery revenue by player, revenue and market share 2021-2026, (USD Million)

Global AI Drug Discovery total market by Type, CAGR, 2021-2032, (USD Million)

Global AI Drug Discovery total market by Application, CAGR, 2021-2032, (USD Million)

This report profiles major players in the global AI Drug Discovery market based on the following parameters - company overview, revenue, gross margin, product portfolio, geographical presence, and key developments. Key companies covered as a part of this study include Recursion, Insilico Medicine, Schrödinger, DeepMind, Insitro, Generate Biomedicines, XtalPi, Relay Therapeutics, BenevolentAI, Roivant Sciences, etc.

This report also provides key insights about market drivers, restraints, opportunities, new product launches or approvals.

Stakeholders would have ease in decision-making through various strategy matrices used in analyzing the world AI Drug Discovery market

Detailed Segmentation:

Each section contains quantitative market data including market by value (US\$ Millions), by player, by regions, by Type, and by Application. Data is given for the years 2021-2032 by year with 2025 as the base year, 2026 as the estimate year, and 2027-2032 as the forecast year.

Global AI Drug Discovery Market, By Region:

United States

China

Europe

Japan

South Korea

ASEAN

India

Rest of World

Global AI Drug Discovery Market, Segmentation by Type:

Machine Learning Type

Deep Learning Type

Natural Language Processing Type

Data Mining Type

Global AI Drug Discovery Market, Segmentation by Drug Type:

Small Molecule Drugs

Biomacromolecules

Novel Therapies

Global AI Drug Discovery Market, Segmentation by Computational Power:

High-Performance Computing Type

Cloud Computing Type

Edge Computing Type

Global AI Drug Discovery Market, Segmentation by Application:

Target Discovery and Validation

Virtual Screening and Molecular Docking

Drug Repurposing and Precision Medicine

Clinical Data Analysis and Optimization

Companies Profiled:

Recursion

Insilico Medicine

Schrödinger

DeepMind

Insitro

Generate Biomedicines

XtalPi

Relay Therapeutics

BenevolentAI

Roivant Sciences

Ginkgo Bioworks

Exscientia

Merck KGaA

Novartis

Biotus

Huazhi Bio

MindRank AI

Ubigene

WuXi AppTec

Key Questions Answered

1. How big is the global AI Drug Discovery market?
2. What is the demand of the global AI Drug Discovery market?
3. What is the year over year growth of the global AI Drug Discovery market?
4. What is the total value of the global AI Drug Discovery market?
5. Who are the Major Players in the global AI Drug Discovery market?
6. What are the growth factors driving the market demand?

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