

Global AI-Designed Small-Molecule Drugs Market 2026 by Manufacturers, Regions, Type and Application, Forecast to 2032

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Abstracts

According to our (Global Info Research) latest study, the global AI-Designed Small-Molecule Drugs market size was valued at US\$ 1321 million in 2025 and is forecast to a readjusted size of US\$ 6010 million by 2032 with a CAGR of 24.2% during review period.

AI-designed small-molecule drugs are synthesizable and developable drug candidates for which machine learning, generative AI, and physics-based modeling make a material contribution to target identification, virtual screening, molecular generation, structure?activity optimization, or ADMET prediction. They are supplied as discovery-stage molecules, preclinical candidates, clinical pipeline assets, or licensed programs and are evaluated by target novelty, potency and selectivity, oral exposure, tissue distribution, safety margin, manufacturability, and intellectual property. Major uses include oncology, immunology and inflammation, neurology, metabolic disease, and infectious disease research. The market scope covers related R&D spending, collaboration revenue, upfront licensing payments, and milestone value rather than end-market prescription drug sales, with an estimated blended gross margin of about 68%.

Demand is driven by pharmaceutical companies seeking to shorten early discovery cycles, expand the range of druggable targets, and improve the quality of candidates entering clinical development. Oncology, immunology and inflammation, neurology, and metabolic diseases are the first areas to build dense AI-enabled pipelines because they combine substantial unmet need with increasingly rich target and molecular data. Demand is particularly strong for oral therapies, brain-penetrant compounds, mutation-selective inhibitors, and programs against historically difficult targets.

Competition is moving beyond stand-alone virtual screening toward closed loops that connect target discovery, generative design, automated synthesis, experimental validation, and clinical translation. Leading suppliers are building proprietary datasets, physics-based simulation, foundation models, and wet-lab infrastructure while validating their systems through internal pipelines and pharmaceutical partnerships. Product development is advancing toward simultaneous multiparameter optimization, more reliable selectivity and toxicity prediction, protein dynamics modeling, active learning, and exploration of new chemical space for protein degradation and nucleic-acid targets.

North America continues to concentrate most AI-native drug developers, capital, and large-pharma partnerships, while the United Kingdom, France, and China are building differentiated capabilities in generative chemistry, structure prediction, laboratory automation, and clinical execution. Customers increasingly evaluate suppliers by delivered candidates, clinical milestones, data feedback loops, and intellectual-property boundaries rather than model benchmarks alone. Key risks include long clinical validation cycles, biased training data, limited synthetic feasibility, and complex ownership of partnered assets. Companies with end-to-end development capability, repeatable delivery records, and cross-regional clinical resources are better positioned to secure licensing and co-development opportunities.

Report Scope

This report is a detailed and comprehensive analysis for global AI-Designed Small-Molecule Drugs market. Both quantitative and qualitative analyses are presented by manufacturers, by region & country, by Type and by Application. As the market is constantly changing, this report explores the competition, supply and demand trends, as well as key factors that contribute to its changing demands across many markets. Company profiles and product examples of selected competitors, along with market share estimates of some of the selected leaders for the year 2025, are provided.

Key Features:

Global AI-Designed Small-Molecule Drugs market size and forecasts, in consumption value (\$ Million), sales quantity (K Dose), and average selling prices (US\$/Dose), 2021-2032

Global AI-Designed Small-Molecule Drugs market size and forecasts by region and country, in consumption value (\$ Million), sales quantity (K Dose), and average selling

prices (US\$/Dose), 2021-2032

Global AI-Designed Small-Molecule Drugs market size and forecasts, by Type and by Application, in consumption value (\$ Million), sales quantity (K Dose), and average selling prices (US\$/Dose), 2021-2032

Global AI-Designed Small-Molecule Drugs market shares of main players, shipments in revenue (\$ Million), sales quantity (K Dose), and ASP (US\$/Dose), 2021-2026

The Primary Objectives in This Report Are:

- To determine the size of the total market opportunity of global and key countries

- To assess the growth potential for AI-Designed Small-Molecule Drugs

- To forecast future growth in each product and end-use market

- To assess competitive factors affecting the marketplace

This report profiles key players in the global AI-Designed Small-Molecule Drugs market based on the following parameters - company overview, sales quantity, revenue, price, gross margin, product portfolio, geographical presence, and key developments. Key companies covered as a part of this study include Recursion Pharmaceuticals, Insilico Medicine, Schrödinger, XtalPi, Isomorphic Labs, Relay Therapeutics, Nimbus Therapeutics, Iambic Therapeutics, BenevolentAI, Accutar Biotechnology, etc.

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

Market Segmentation

AI-Designed Small-Molecule Drugs market is split by Type and by Application. For the period 2021-2032, the growth among segments provides accurate calculations and forecasts for consumption value by Type, and by Application in terms of volume and value. This analysis can help you expand your business by targeting qualified niche markets.

Market segment by Type

Discovery-Stage Candidates

Preclinical Candidates

Clinical-Stage Candidates

Approved Drugs

Market segment by Mechanism of Action

Enzyme Inhibitors

Receptor Agonists

Receptor Antagonists

Targeted Protein Degraders

Molecular Glues

Other Small-Molecule Modulators

Market segment by Route of Administration

Oral Drugs

Injectable Drugs

Inhaled Drugs

Topical Drugs

Other Administration Routes

Market segment by Target Class

Kinases

Other Enzymes

G Protein-Coupled Receptors

Nuclear Receptors

Protein-Protein Interaction Targets

Nucleic Acid Targets

Other Target Classes

Market segment by Application

Oncology

Immunology and Inflammation

Neurology and Psychiatry

Metabolic and Cardiovascular Diseases

Infectious Diseases

Other Therapeutic Areas

Major players covered

Recursion Pharmaceuticals

Insilico Medicine

Schrödinger

XtalPi

Isomorphic Labs

Relay Therapeutics

Nimbus Therapeutics

Iambic Therapeutics

BenevolentAI

Accutar Biotechnology

MindRank AI

Enveda Biosciences

Insitro

Valo Health

Healx

Lantern Pharma

Verge Labs

DeepCure

AQEMIA

Genesis Molecular AI

Terray Therapeutics

CHARM Therapeutics

Anagenex

StoneWise

Market segment by region, regional analysis covers

North America (United States, Canada, and Mexico)

Europe (Germany, France, United Kingdom, Russia, Italy, and Rest of Europe)

Asia-Pacific (China, Japan, Korea, India, Southeast Asia, and Australia)

South America (Brazil, Argentina, Colombia, and Rest of South America)

Middle East & Africa (Saudi Arabia, UAE, Egypt, South Africa, and Rest of Middle East & Africa)

Chapter Outline

Chapter 1, to describe AI-Designed Small-Molecule Drugs product scope, market overview, market estimation caveats and base year.

Chapter 2, to profile the top manufacturers of AI-Designed Small-Molecule Drugs, with price, sales quantity, revenue, and global market share of AI-Designed Small-Molecule Drugs from 2021 to 2026.

Chapter 3, the AI-Designed Small-Molecule Drugs competitive situation, sales quantity, revenue, and global market share of top manufacturers are analyzed emphatically by landscape contrast.

Chapter 4, the AI-Designed Small-Molecule Drugs breakdown data are shown at the regional level, to show the sales quantity, consumption value, and growth by regions, from 2021 to 2032.

Chapter 5 and 6, to segment the sales by Type and by Application, with sales market share and growth rate by Type, by Application, from 2021 to 2032.

Chapter 7, 8, 9, 10 and 11, to break the sales data at the country level, with sales quantity, consumption value, and market share for key countries in the world, from 2021

to 2026. and AI-Designed Small-Molecule Drugs market forecast, by regions, by Type, and by Application, with sales and revenue, from 2027 to 2032.

Chapter 12, market dynamics, drivers, restraints, trends, and Porters Five Forces analysis.

Chapter 13, the key raw materials and key suppliers, and industry chain of AI-Designed Small-Molecule Drugs.

Chapter 14 and 15, to describe AI-Designed Small-Molecule Drugs sales channel, distributors, customers, research findings and conclusion.

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