

Artificial Intelligence (Ai) In Predictive Toxicology Market Outlook 2025-2034: Market Share, and Growth Analysis By Component (Solution, Services), By Technology (Machine Learning, Natural Language Processing, Computer Vision, Other Technologies), By Toxicity Endpoints, By End User

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Abstracts

The Artificial Intelligence (Ai) In Predictive Toxicology Market is valued at USD 518 million in 2025 and is projected to grow at a CAGR of 24.5% to reach USD 3733.4 million by 2034. The AI in predictive toxicology market involves the use of AI technologies to predict the toxicity of chemical compounds and drugs. This includes using machine learning for analyzing chemical structures, biological data, and toxicity data to predict potential adverse effects. AI helps to reduce the need for animal testing and accelerate the development of safer chemicals and drugs.

The market is driven by the need for more efficient and ethical toxicity testing, reduced development costs, and improved safety of chemicals and drugs. AI-powered chemical structure analysis can predict potential toxicity based on molecular properties. Biological data analysis can identify potential targets for toxicity. Toxicity data analysis can predict the likelihood of adverse effects based on historical data. The adoption of in silico methods and computational toxicology is further fueling this market.

Challenges include data quality, model validation, and regulatory acceptance of AI-powered predictive toxicology methods. However, the potential benefits, such as reduced animal testing and faster development of safer products, are driving significant investments. The market's future trajectory depends on the successful validation of AI models and the integration of AI into regulatory frameworks.

Key Insights Artificial Intelligence (Ai) In Predictive Toxicology Market

Increased use of AI for chemical structure analysis and toxicity prediction.

Growth of AI-powered biological data analysis for target identification.

Adoption of AI for toxicity data analysis and risk assessment.

Development of AI-driven in silico models for virtual screening.

Use of AI for personalized risk assessment and drug safety monitoring.

Need for more efficient and ethical toxicity testing methods.

Demand for reduced development costs and faster time-to-market.

Growing regulatory pressure to reduce animal testing.

Potential for AI to improve the safety of chemicals and drugs.

Advancements in AI algorithms and computational toxicology.

Data quality and availability for AI model training and validation.

Regulatory acceptance and validation of AI-powered predictive toxicology methods.

Need for robust and reliable AI models for diverse chemical compounds.

Integration of AI into existing toxicity testing workflows and systems.

Ensuring the transparency and explainability of AI-driven toxicity predictions.

Artificial Intelligence (Ai) In Predictive Toxicology Market Segmentation

By Component

Solution

Services

By Technology

Machine Learning

Natural Language Processing

Computer Vision

Other Technologies

By Toxicity Endpoints

Genotoxicity

Hepatotoxicity

Neurotoxicity

Cardiotoxicity

Other Toxicity Endpoints

By End User

Pharmaceutical And Biotechnology Companies

Chemical And Cosmetics

Contract Research Organizations

Other End Users

Key Companies Analysed

Laboratory Corporation of America Holdings (LabCorp)

Eurofins Scientific SE

Wuxi AppTec

Charles River Laboratories International

Medidata Solutions Inc.

Certara Inc.

Schrödinger

Merative L.P.

Molecular Devices LLC

Envigo (Inotiv Inc.)

Instem plc

Simulations Plus

Cyprotex

Recursion Pharmaceuticals

Exscientia PLC

BIOVIA Corporation

Lhasa Limited

Chemaxon Ltd.

Insilico Medicine Inc.

Algorithme Pharma

CiToxLAB

ArisGlobal

Benevolent AI

Berg Health

Cyclica Therapeutics Inc.

Celsius Therapeutics

Biovista Inc.

BioTeam Inc.

Artificial Intelligence (Ai) In Predictive Toxicology Market Analytics

The report employs rigorous tools, including Porter's Five Forces, value chain mapping, and scenario-based modeling, to assess supply–demand dynamics. Cross-sector influences from parent, derived, and substitute markets are evaluated to identify risks and opportunities. Trade and pricing analytics provide an up-to-date view of international flows, including leading exporters, importers, and regional price trends.

Macroeconomic indicators, policy frameworks such as carbon pricing and energy security strategies, and evolving consumer behavior are considered in forecasting scenarios. Recent deal flows, partnerships, and technology innovations are incorporated to assess their impact on future market performance.

Artificial Intelligence (Ai) In Predictive Toxicology Market Competitive Intelligence

The competitive landscape is mapped through OG Analysis' proprietary frameworks, profiling leading companies with details on business models, product portfolios, financial performance, and strategic initiatives. Key developments such as mergers & acquisitions, technology collaborations, investment inflows, and regional expansions are analyzed for their competitive impact. The report also identifies emerging players and innovative startups contributing to market disruption.

Regional insights highlight the most promising investment destinations, regulatory landscapes, and evolving partnerships across energy and industrial corridors.

Countries Covered

North America — Artificial Intelligence (Ai) In Predictive Toxicology market data and outlook to 2034

United States

Canada

Mexico

Europe — Artificial Intelligence (Ai) In Predictive Toxicology market data and outlook to 2034

Germany

United Kingdom

France

Italy

Spain

BeNeLux

Russia

Sweden

Asia-Pacific — Artificial Intelligence (Ai) In Predictive Toxicology market data and outlook to 2034

China

Japan

India

South Korea

Australia

Indonesia

Malaysia

Vietnam

Middle East and Africa — Artificial Intelligence (Ai) In Predictive Toxicology
market data and outlook to 2034

Saudi Arabia

South Africa

Iran

UAE

Egypt

South and Central America — Artificial Intelligence (Ai) In Predictive Toxicology
market data and outlook to 2034

Brazil

Argentina

Chile

Peru

** We can include data and analysis of additional countries on demand.*

Research Methodology

This study combines primary inputs from industry experts across the Artificial Intelligence (Ai) In Predictive Toxicology value chain with secondary data from associations, government publications, trade databases, and company disclosures. Proprietary modeling techniques, including data triangulation, statistical correlation, and scenario planning, are applied to deliver reliable market sizing and forecasting.

Key Questions Addressed

What is the current and forecast market size of the Artificial Intelligence (Ai) In Predictive Toxicology industry at global, regional, and country levels?

Which types, applications, and technologies present the highest growth potential?

How are supply chains adapting to geopolitical and economic shocks?

What role do policy frameworks, trade flows, and sustainability targets play in shaping demand?

Who are the leading players, and how are their strategies evolving in the face of global uncertainty?

Which regional “hotspots” and customer segments will outpace the market, and what go-to-market and partnership models best support entry and expansion?

Where are the most investable opportunities—across technology roadmaps, sustainability-linked innovation, and M&A—and what is the best segment to invest over the next 3–5 years?

Your Key Takeaways from the Artificial Intelligence (Ai) In Predictive Toxicology Market Report

Global Artificial Intelligence (Ai) In Predictive Toxicology market size and growth projections (CAGR), 2024-2034

Impact of Russia-Ukraine, Israel-Palestine, and Hamas conflicts on Artificial Intelligence (Ai) In Predictive Toxicology trade, costs, and supply chains

Artificial Intelligence (Ai) In Predictive Toxicology market size, share, and outlook across 5 regions and 27 countries, 2023-2034

Artificial Intelligence (Ai) In Predictive Toxicology market size, CAGR, and market share of key products, applications, and end-user verticals, 2023-2034

Short- and long-term Artificial Intelligence (Ai) In Predictive Toxicology market trends, drivers, restraints, and opportunities

Porter's Five Forces analysis, technological developments, and Artificial Intelligence (Ai) In Predictive Toxicology supply chain analysis

Artificial Intelligence (Ai) In Predictive Toxicology trade analysis, Artificial Intelligence (Ai) In Predictive Toxicology market price analysis, and Artificial Intelligence (Ai) In Predictive Toxicology supply/demand dynamics

Profiles of 5 leading companies—overview, key strategies, financials, and products

Latest Artificial Intelligence (Ai) In Predictive Toxicology market news and developments

Additional Support

With the purchase of this report, you will receive

An updated PDF report and an MS Excel data workbook containing all market tables and figures for easy analysis.

7-day post-sale analyst support for clarifications and in-scope supplementary data, ensuring the deliverable aligns precisely with your requirements.

Complimentary report update to incorporate the latest available data and the impact of recent market developments.

** The updated report will be delivered within 3 working days*

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