

Global AI Drug Safety Prediction Software Market Growth (Status and Outlook) 2026-2032

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Abstracts

The global AI Drug Safety Prediction Software market size is predicted to grow from US\$ 401 million in 2025 to US\$ 1766 million in 2032; it is expected to grow at a CAGR of 23.9% from 2026 to 2032.

AI drug safety prediction software uses machine learning, deep learning, QSAR, expert rules, and physics-based models to predict absorption, distribution, metabolism, excretion, toxicity, drug-drug interactions, off-target effects, and safety pharmacology risks from molecular structures, experimental data, and curated knowledge bases. Typical functions include batch screening, applicability-domain and confidence assessment, explainability, custom model training, API or private deployment, and regulatory-ready reporting for drug discovery, preclinical research, and safety decision-making. The average gross margin is approximately 75%.

Demand mainly comes from pharmaceutical companies, biotechnology firms, CROs, and research institutions that are moving safety-risk screening earlier in development. The high cost of terminating candidates at later stages because of toxicity, pharmacokinetic, or drug-interaction liabilities encourages the use of computational prediction during hit screening, lead optimization, and candidate selection. Efforts to reduce animal testing, the expansion of virtual compound libraries, and broader regulatory use of new approach methodologies also support software adoption.

Product development is shifting from isolated QSAR endpoints toward combinations of multitask deep learning, expert knowledge, and physics-based simulation, with greater emphasis on applicability domains, confidence estimates, structural alerts, and analogue evidence. Established vendors retain advantages through curated toxicology databases, validated models, and regulatory workflows, while AI-native platforms are

gaining adoption through faster computation, frequent model updates, and closed design-prediction loops. Purchasing decisions typically focus on endpoint coverage, external validation, proprietary-data model building, deployment security, system integration, and reporting compliance.

North America and Europe remain the leading commercial markets, while China and other Asian markets have strong potential because of expanding innovative-drug investment, local AI drug-discovery companies, and demand for private deployment. Opportunities include localization for regulatory requirements, enterprise-specific model training, multimodal safety assessment, and integration with experimental platforms. Key risks are training-data bias, unreliable predictions outside the applicability domain, limited coverage of biologics, and the continuing need for experimental confirmation and expert review.

Report Scope

LPI (LP Information)' newest research report, the "AI Drug Safety Prediction Software Industry Forecast" looks at past sales and reviews total world AI Drug Safety Prediction Software sales in 2025, providing a comprehensive analysis by region and market sector of projected AI Drug Safety Prediction Software sales for 2026 through 2032. With AI Drug Safety Prediction Software sales broken down by region, market sector and sub-sector, this report provides a detailed analysis in US\$ millions of the world AI Drug Safety Prediction Software industry.

This Insight Report provides a comprehensive analysis of the global AI Drug Safety Prediction Software landscape and highlights key trends related to product segmentation, company formation, revenue, and market share, latest development, and M&A activity. This report also analyses the strategies of leading global companies with a focus on AI Drug Safety Prediction Software portfolios and capabilities, market entry strategies, market positions, and geographic footprints, to better understand these firms' unique position in an accelerating global AI Drug Safety Prediction Software market.

This Insight Report evaluates the key market trends, drivers, and affecting factors shaping the global outlook for AI Drug Safety Prediction Software and breaks down the forecast by Type, by Application, geography, and market size to highlight emerging pockets of opportunity. With a transparent methodology based on hundreds of bottom-up qualitative and quantitative market inputs, this study forecast offers a highly nuanced view of the current state and future trajectory in the global AI Drug Safety Prediction

Software.

This report presents a comprehensive overview, market shares, and growth opportunities of AI Drug Safety Prediction Software market by product type, application, key players and key regions and countries.

Segmentation by Type:

Integrated ADMET Prediction

Toxicity Endpoint Prediction

Drug-Drug Interaction and PK Safety Prediction

Metabolism and Metabolite Prediction

Off-Target and Safety Pharmacology Prediction

Segmentation by Deployment Model:

Cloud-Based

On-Premises

Hybrid Deployment

Segmentation by Modeling Approach:

Machine Learning and Deep Learning

QSAR and Statistical Modeling

Knowledge-Based and Rule-Based

Physics-Based Simulation

Hybrid Modeling

Segmentation by Model Customization:

Fixed Pretrained Models

User-Trained Models

Hybrid Model Platforms

Segmentation by Application:

Hit and Lead Screening

Lead Optimization

Candidate Selection

Preclinical Safety Assessment

Regulatory Safety Assessment

Other Drug Safety Research

This report also splits the market by region:

Americas

United States

Canada

Mexico

Brazil

APAC

China

Japan

Korea

Southeast Asia

India

Australia

Europe

Germany

France

UK

Italy

Russia

Middle East & Africa

Egypt

South Africa

Israel

Turkey

GCC Countries

The below companies that are profiled have been selected based on inputs gathered from primary experts and analyzing the company's coverage, product portfolio, its market penetration.

Simulations Plus

Dassault Syst?mes

Schr?dinger

Certara

Lhasa Limited

Instem

ACD/Labs

Chemical Computing Group

Optibrium

MultiCASE

Insilico Medicine

MindRank

Molecular Discovery

Molecular Networks

OASIS LMC

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