+357 96 030922
info@marketpublishers.com

Global AI Drug Safety Prediction Software Market 2026 by Company, Regions, Type and Application, Forecast to 2032

https://marketpublishers.com/r/GCE2C396DD18EN.html
Date: August 2026
Pages: 115
Price: US$ 3,480.00 (Single User License)
ID: GCE2C396DD18EN

Abstracts

According to our (Global Info Research) latest study, the global AI Drug Safety Prediction Software market size was valued at US$ 422 million in 2025 and is forecast to a readjusted size of US$ 1735 million by 2032 with a CAGR of 22.5% during review period.

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

+357 96 030922
info@marketpublishers.com

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

This report is a detailed and comprehensive analysis for global AI Drug Safety Prediction Software market. Both quantitative and qualitative analyses are presented by company, 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 Drug Safety Prediction Software market size and forecasts, in consumption value ($ Million), 2021-2032

Global AI Drug Safety Prediction Software market size and forecasts by region and country, in consumption value ($ Million), 2021-2032

Global AI Drug Safety Prediction Software market size and forecasts, by Type and by Application, in consumption value ($ Million), 2021-2032

Global AI Drug Safety Prediction Software market shares of main players, in revenue ($ Million), 2021-2026

+357 96 030922
info@marketpublishers.com

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 Drug Safety Prediction Software

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 Drug Safety Prediction Software 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 Simulations Plus, Dassault Syst?mes, Schr?dinger, Certara, Lhasa Limited, Instem, ACD/Labs, Chemical Computing Group, Optibrium, MultiCASE, etc.

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

Market segmentation

AI Drug Safety Prediction Software 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. This analysis can help you expand your business by targeting qualified niche markets.

Market segment by Type

Integrated ADMET Prediction

Toxicity Endpoint Prediction

Drug-Drug Interaction and PK Safety Prediction

Metabolism and Metabolite Prediction

+357 96 030922
info@marketpublishers.com

Off-Target and Safety Pharmacology Prediction

Market segment by Deployment Model

Cloud-Based

On-Premises

Hybrid Deployment

Market segment by Modeling Approach

Machine Learning and Deep Learning

QSAR and Statistical Modeling

Knowledge-Based and Rule-Based

Physics-Based Simulation

Hybrid Modeling

Market segment by Model Customization

Fixed Pretrained Models

User-Trained Models

Hybrid Model Platforms

Market segment by Application

Hit and Lead Screening

Lead Optimization

+357 96 030922
info@marketpublishers.com

Candidate Selection

Preclinical Safety Assessment

Regulatory Safety Assessment

Other Drug Safety Research

Market segment by players, this report covers

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

+357 96 030922
info@marketpublishers.com

OASIS LMC

Market segment by regions, regional analysis covers

North America (United States, Canada and Mexico)

Europe (Germany, France, UK, Russia, Italy and Rest of Europe)

Asia-Pacific (China, Japan, South Korea, India, Southeast Asia and Rest of Asia-Pacific)

South America (Brazil, Rest of South America)

Middle East & Africa (Turkey, Saudi Arabia, UAE, Rest of Middle East & Africa)

Chapter Outline

Chapter 1, to describe AI Drug Safety Prediction Software product scope, market overview, market estimation caveats and base year.

Chapter 2, to profile the top players of AI Drug Safety Prediction Software, with revenue, gross margin, and global market share of AI Drug Safety Prediction Software from 2021 to 2026.

Chapter 3, the AI Drug Safety Prediction Software competitive situation, revenue, and global market share of top players are analyzed emphatically by landscape contrast.

Chapter 4 and 5, to segment the market size by Type and by Application, with consumption value and growth rate by Type, by Application, from 2021 to 2032.

Chapter 6, 7, 8, 9, and 10, to break the market size data at the country level, with revenue and market share for key countries in the world, from 2021 to 2026.and AI Drug Safety Prediction Software market forecast, by regions, by Type and by Application, with consumption value, from 2027 to 2032.

Chapter 11, market dynamics, drivers, restraints, trends, Porters Five Forces analysis.

+357 96 030922
info@marketpublishers.com

Chapter 12, the key raw materials and key suppliers, and industry chain of AI Drug Safety Prediction Software.

Chapter 13, to describe AI Drug Safety Prediction Software research findings and conclusion.

+357 96 030922
info@marketpublishers.com

Contents

+357 96 030922
info@marketpublishers.com

2 COMPANY PROFILES

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

3 MARKET COMPETITION, BY PLAYERS

4 MARKET SIZE SEGMENT BY TYPE

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

14.3 Disclaimer

+357 96 030922
info@marketpublishers.com

List Of Tables

LIST OF TABLES

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

List Of Figures

LIST OF FIGURES

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

+357 96 030922
info@marketpublishers.com

I would like to order

Product name: Global AI Drug Safety Prediction Software Market 2026 by Company, Regions, Type and Application, Forecast to 2032

Product link: https://marketpublishers.com/r/GCE2C396DD18EN.html

Price: US$ 3,480.00 (Single User License / Electronic Delivery)

If you want to order Corporate License or Hard Copy, please, contact our Customer Service:
info@marketpublishers.com

Payment

To pay by Credit Card (Visa, MasterCard, American Express, PayPal), please, click button on product page https://marketpublishers.com/r/GCE2C396DD18EN.html