

Global Computational Predictive Toxicology Modeling Service Market Growth (Status and Outlook) 2025-2031

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Abstracts

The global Computational Predictive Toxicology Modeling Service market size is predicted to grow from US\$ 205 million in 2025 to US\$ 276 million in 2031; it is expected to grow at a CAGR of 5.1% from 2025 to 2031.

Computational Predictive Toxicology Modeling based on (Quantitative) Structure-Activity Relationships [(Q)SAR] and metabolic modeling have emerged as fundamental tools in the preliminary safety screening of novel molecules, such as plant extracts, fermentation products, or fungal secondary metabolites that are intended for use in food.

Computational Predictive Toxicology Modeling Service is a professional service that provides the use of computer models and computational methods to predict the toxic effects of chemical substances. Combining chemistry, biology, computer science, and data analysis, this service aims to assess the toxic potential of chemicals to living organisms to support decision-making in areas such as drug discovery, chemical safety assessment, and environmental protection. Collect multiple data sources on chemical substance properties, molecular structure, biological activity, and toxicity test data. Features of chemical substances are extracted from the collected data, which may include molecular descriptors, physicochemical properties, metabolic pathways, etc. Using methods such as machine learning, statistics, and computational chemistry, build predictive models that correlate characteristics of chemical substances with their toxic effects. Validate the model, evaluate its predictive performance using an independent test dataset, and refine the model to improve accuracy. Use the optimized model to predict the toxicity of new chemical substances and explain the prediction results. Based on model predictions, assess the toxicity potential of chemicals and generate

reports that provide decision makers with information on potential toxicity. Computational predictive toxicology modeling services can help speed up the toxicity assessment process, reduce the need for animal experiments, and reduce cost and time investment. It has broad application prospects in drug research and development, new chemical development, food additive safety assessment and other fields.

LPI (LP Information)' newest research report, the "Computational Predictive Toxicology Modeling Service Industry Forecast" looks at past sales and reviews total world Computational Predictive Toxicology Modeling Service sales in 2024, providing a comprehensive analysis by region and market sector of projected Computational Predictive Toxicology Modeling Service sales for 2025 through 2031. With Computational Predictive Toxicology Modeling Service sales broken down by region, market sector and sub-sector, this report provides a detailed analysis in US\$ millions of the world Computational Predictive Toxicology Modeling Service industry.

This Insight Report provides a comprehensive analysis of the global Computational Predictive Toxicology Modeling Service 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 Computational Predictive Toxicology Modeling Service portfolios and capabilities, market entry strategies, market positions, and geographic footprints, to better understand these firms' unique position in an accelerating global Computational Predictive Toxicology Modeling Service market.

This Insight Report evaluates the key market trends, drivers, and affecting factors shaping the global outlook for Computational Predictive Toxicology Modeling Service 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 Computational Predictive Toxicology Modeling Service.

This report presents a comprehensive overview, market shares, and growth opportunities of Computational Predictive Toxicology Modeling Service market by product type, application, key players and key regions and countries.

Segmentation by Type:

On-Premise

Cloud-Based

Segmentation by Application:

Academia

Enterprise

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.

Intertek Group

Harmonic Pharma

Instem (Leadscope)

Inotiv

Simulations Plus Inc

Lhasa Limited

MultiCASE

Schrodinger

Aclaris

Evogene

Deciphex (Patholytix)

Exscientia

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