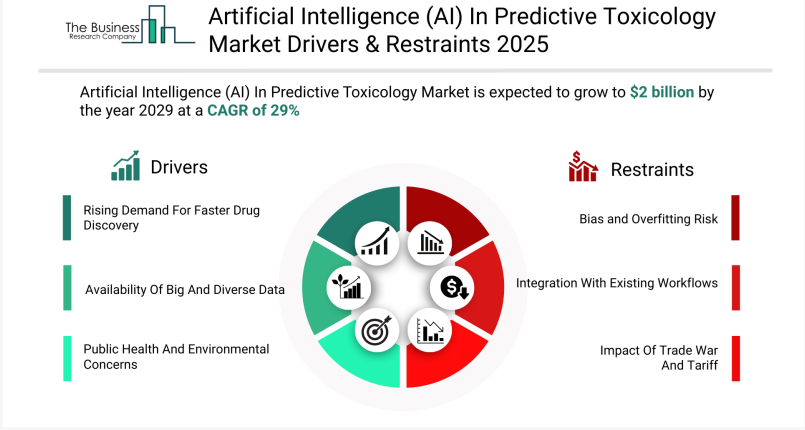
# Artificial Intelligence (AI) In Predictive Toxicology Market Competition Analysis 2025: How Players Are Shaping Growth

*The Business Research Company's Artificial Intelligence (AI) In Predictive Toxicology Global Market Report 2025 – Market Size, Trends, And Forecast 2025-2034*



Artificial Intelligence (AI) In Predictive Toxicology Market Report 2025 – Market Size, Trends, And Forecast 2025-2034

LONDON, GREATER LONDON, UNITED KINGDOM, December 8, 2025 /EINPresswire.com/ -- The Artificial Intelligence (AI) In Predictive Toxicology market is dominated by a mix of established global technology leaders and emerging regional innovators. Companies are focusing on advanced AI-driven toxicology modeling, digital identity solutions for AI agents, and robust governance and compliance frameworks to enhance reliability and regulatory alignment. Understanding the competitive landscape is key for stakeholders seeking growth opportunities and strategic partnerships

Which Market Player Is Leading the Artificial Intelligence (AI) In Predictive Toxicology Market?
According to our research, Simulations Plus Inc led global sales in 2024 with a 3% market share. The total revenue of the company partially involved in the artificial intelligence (AI) in predictive toxicology market provides GastroPlus for simulating drug absorption and pharmacokinetics, ADMET Predictor for chemistry-based molecular property prediction and mechanistic models including DILIsym, NAFLDsym, RENAsym and MITOsym products for quantitative systems toxicology. The company's DILIsym 11 platform incorporates AI-driven predictive capabilities for drug-induced liver injury with advanced pediatric modeling and refined T-cell models, while their NAMVantage package combines PBPK and QSP services with AI/ML integration for predictive toxicology and human-relevant safety assessments.

How Concentrated Is the Artificial Intelligence (AI) In Predictive Toxicology Market?
The market is fairly fragmented, with the top 10 players accounting for 18% of total market revenue in 2024. This level of fragmentation reflects a rapidly evolving and competitive

landscape characterized by numerous innovative companies developing specialized AI-driven toxicology solutions. Leading players such as Simulations Plus Inc., Certara Inc., Schrödinger Inc., and Merative LP (formerly IBM Watson Health) are at the forefront of advancing AI technologies that enhance predictive accuracy, reduce dependency on animal testing, and accelerate drug development timelines. These companies are distinguished by their strong technological capabilities, extensive toxicology data sets, and strategic partnerships that enable them to meet stringent regulatory standards and growing demand for safer, more cost-effective toxicology assessments.

• Leading companies include:
o Simulations Plus Inc. (3%)
o Certara Inc. (3%)
o Schrödinger Inc. (3%)
o Merative LP (formerly IBM Watson Health) (2%)
o BIOVIA (a Dassault Systèmes company) (2%)
o Cyprotex (1%)
o Evalueserve Holding AG (1%)
o Recursion Pharmaceuticals Inc. (1%)
o Eurofins Scientific SE (1%)
o Charles River Laboratories International (1%)

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https://www.thebusinessresearchcompany.com/sample_request?id=14253&type=smp

Which Companies Are Leading Across Different Regions?
• North America: Charles River Laboratories International, Inc., BIOVIA (a Dassault Systèmes company), Recursion Pharmaceuticals, Inc., Insilico Medicine, Inc., Molecular Devices, LLC, Simulations Plus, Inc., Certara, Inc., Instem plc, Schrödinger, Inc., and Valo Health, Inc. are some of the leading companies in this region.
• Asia Pacific: Standigm Inc., Schrödinger Inc., Charles River Laboratories International Inc., Certara Inc., Recursion Pharmaceuticals Inc., Chemaxon Ltd., Insilico Medicine Inc., ArisGlobal LLC, Valo Health Inc., NVIDIA Corporation, PharmCADD Co. Ltd., Syntekabio Inc., AIGEN Sciences Inc., Evalueserve Holding AG, Pharmaron Beijing Co. Ltd., and Syngene International Ltd. are some of the leading companies in this region.
• Western Europe: Cyprotex Limited, SyntheticGestalt Inc., Charles River Laboratories International, Inc., Schrödinger, Inc., Simulations Plus, Inc., Recursion Pharmaceuticals, Inc., Exscientia plc, Lhasa Limited, Chemaxon Ltd., BenevolentAI Limited, and Causaly Ltd. These companies leverage AI-driven modeling, predictive analytics, and molecular simulation tools to advance toxicology research and streamline drug discovery workflows. are some of the leading companies in this region.
• Eastern Europe: Ardigen S.A., Insilico Medicine, Inc., ChemAxon Ltd., and Schrödinger, Inc. are some of the leading companies in this region.
• South America: Instem plc, Lhasa Limited, and Simulations Plus, Inc. are some of the leading

companies in this region.

What Are the Major Competitive Trends in the Market?
• AI-Driven Risk Assessment Platform is transforming development and drug safety predictions.
• Example: GATC Health Derisq (September 2025) designed to streamline the early stages of drug development by providing accurate toxicity predictions.
• These innovations identify safety and off target risks early, thereby reducing the time, cost, and uncertainty associated with traditional preclinical testing.

Which Strategies Are Companies Adopting to Stay Ahead?
• Launching new products development to strengthen market position
• Enhancing strategic funding
• Expanding collaborative partnerships
• Integrating multi-omics and real-world data for more comprehensive toxicological insights and predictive reliability

Access the detailed Artificial Intelligence (AI) In Predictive Toxicology Market report here:
https://www.thebusinessresearchcompany.com/report/artificial-intelligence-ai-in-predictive-toxicology-global-market-report

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