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Cheminformatics Market - Global Industry Size, Share, Trends, Opportunity, and Forecast, Segmented By Application (Chemical Analysis, Drug Discovery and Validation, Virtual Screening, Others), By End User (Chemical & Pharmaceutical Companies, Academic & Research Institutions, Others), By Region & Competition, 2021-2031F

https://marketpublishers.com/r/C5D4F9D7CAB9EN.html
Date: January 2026
Pages: 180
Price: US$ 4,500.00 (Single User License)
ID: C5D4F9D7CAB9EN

Abstracts

The Global Cheminformatics Market is projected to expand from USD 4.36 Billion in 2025 to USD 8.64 Billion by 2031, achieving a compound annual growth rate of 12.07%. This field utilizes computational strategies to organize and interpret chemical data, supporting the storage, retrieval, and modeling of molecular information. The market's upward trajectory is driven by the growing necessity for streamlined drug discovery processes and the handling of massive datasets generated by high-throughput screening. This momentum is supported by substantial industry funding; for instance, the European Federation of Pharmaceutical Industries and Associations estimated that the research-based pharmaceutical sector invested ?50,000 million in R&D across Europe in 2023. Such spending highlights the essential function of digital solutions in maximizing research productivity and shortening development cycles.

Conversely, market growth faces a significant hurdle due to a shortage of workforce talent holding combined proficiency in chemistry and information technology. This lack of specialized skills hinders the successful deployment of sophisticated informatics infrastructures. Furthermore, the industry struggles with data standardization inconsistencies across various platforms, which impede the seamless integration needed for collaborative scientific efforts. These interoperability challenges threaten to retard the widespread acceptance and application of these advanced technologies

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within the sector.

Market Driver

The rapid incorporation of AI and machine learning into drug discovery acts as a major propellant for the cheminformatics industry. These technologies empower scientists to forecast molecular interactions and refine lead compounds, creating a need for sophisticated software frameworks capable of managing complex data. This technological convergence is particularly crucial for small molecule design, where algorithms analyze extensive chemical libraries. A case in point is Eli Lilly and Company's January 2024 announcement regarding a strategic partnership with Isomorphic Labs, which included a $45 million upfront commitment to advance AI-led drug design. Such alliances underscore the necessity of informatics platforms to connect computational forecasts with experimental validation in the lab.

Additionally, escalating R&D expenditures by pharmaceutical corporations serve as a primary catalyst for the market. Firms are directing significant funds toward digital transformation tools that optimize the research lifecycle to sustain competitive development pipelines. This financial backing enables the acquisition of essential screening and modeling software. As reported by Merck & Co., Inc. in February 2024, the company?s full-year R&D expenses for 2023 surged to $30.5 billion. This trend is further strengthened by regulatory requirements for strict data integrity; the U.S. Food and Drug Administration approved 55 new molecular entities in 2023, a volume that necessitates powerful informatics systems to handle the rigorous data management associated with regulatory submissions.

Market Challenge

A critical obstacle facing the Global Cheminformatics Market is the shortage of professionals who possess dual competency in both chemistry and information technology. As biotechnology and pharmaceutical firms increasingly depend on computational techniques to model compound data, the requirement for staff capable of understanding scientific fundamentals alongside complex data structures has exceeded availability. This talent deficit creates barriers to the seamless implementation of informatics systems, compelling organizations to postpone the rollout of vital digital solutions. Without a workforce equipped to bridge these distinct fields, companies face difficulties in optimizing large-scale chemical data management, effectively halting key research and development endeavors.

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Recent industry statistics confirm that this skills gap is widening, creating an operational bottleneck. According to the Pistoia Alliance, 34 percent of life science laboratories identified the lack of skilled personnel as a major impediment to adopting advanced digital technologies in 2025, a rise from 23 percent the prior year. This growing shortage of technical proficiency directly limits the market's capacity to maintain its expansion. If organizations fail to acquire the necessary human capital to manage these platforms, the anticipated efficiency improvements from cheminformatics remain out of reach, leading to prolonged development schedules and constrained market growth.

Market Trends

The shift toward Cloud-Native and SaaS deployment models is transforming the Global Cheminformatics Market by supplanting rigid on-premise hardware with scalable digital platforms. This migration enables pharmaceutical companies to decentralize their research activities, promoting fluid collaboration among dispersed teams. By utilizing cloud infrastructures, organizations can effectively handle the rapid expansion of chemical data without incurring the heavy capital costs linked to traditional hardware. This strategic pivot is highlighted by leading industry players moving their digital operations to cloud frameworks; for instance, Veeva Systems announced in June 2025 an extension of its collaboration with AWS to support over 50 life sciences applications, emphasizing the sector's dependence on cloud-native environments for operational flexibility.

Simultaneously, the rise of specialized tools designed for biologics and large molecules is becoming increasingly significant as the industry shifts focus from small-molecule drugs to complex therapeutic proteins. This trend drives the creation of innovative informatics solutions tailored to manage the intricate structural data of biologics, which older systems cannot sufficiently process. As R&D pipelines place greater emphasis on large-molecule therapies, there is a surging need for specific software to model and simulate these entities. This market progression is bolstered by strong financial forecasts for biologics-dominated sectors; the IQVIA Institute for Human Data Science reported in June 2025 that global spending on oncology is expected to reach $441 billion by 2029, underlining the urgent requirement for advanced informatics to sustain this growing field.

Key Market Players

Agilent Technologies Inc.

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Bio-Rad Laboratories Inc.

PerkinElmer NC.

Accelrys Software Inc.

Chemical Computing Group, Inc.

Certara, L.P.

Advanced Chemistry Development, Inc.

BioSolveIT GmbH

Dassault Systemes

ChemAxon Inc.

Eurofins Panlabs Inc.

Jubilant Biosys Inc.

Molecular Discovery Ltd.

OpenEye Scientific Software Inc.

SchrOdinger Inc.

Report Scope

In this report, the Global Cheminformatics Market has been segmented into the following categories, in addition to the industry trends which have also been detailed below:

Cheminformatics Market, By Application

Chemical Analysis

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India

Japan

Australia

South Korea

South America

Brazil

Argentina

Colombia

Middle East & Africa

South Africa

Saudi Arabia

UAE

Competitive Landscape

Company Profiles: Detailed analysis of the major companies present in the Global Cheminformatics Market.

Available Customizations:

Global Cheminformatics Market report with the given market data, TechSci Research offers customizations according to a company's specific needs. The following customization options are available for the report:

Company Information

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Detailed analysis and profiling of additional market players (up to five).

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