

United States Generative AI in Chemical Market Assessment, By Model [Deep Learning, Natural Language Processing, Discriminative Model, Reinforcement Learning, Others], By Application [Complex Structure Predictions, Novel Formulation Optimization, Chemical Process Optimization, Realtime Equipment Monitoring, Production Capacity Optimization, Pricing Optimization, Laboratory Automation, Others], By End-user [Chemical Processing Industry, Research & Development, Others], By Region, Opportunities and Forecast, 2016-2030F

#### https://marketpublishers.com/r/UE1EDA6C559EEN.html

Date: February 2025 Pages: 117 Price: US\$ 3,300.00 (Single User License) ID: UE1EDA6C559EEN

# **Abstracts**

United States Generative AI in Chemical Market size was valued at USD 49.9 million in 2022 and is expected to reach USD 301.3 million in 2030 with a CAGR of 25.2% for the forecast period between 2023 and 2030. The recent advancements in various automation practices have been achieved with the commencement of generative AI models. Generative AI has significant potential that can be implemented in designing products, streamlining operations, analyzing complex scientific literature, and accelerating novel discoveries. In the chemical sector, generative AI delivers important features such as drug development, executing novel chemical reactions, unveiling hidden properties of complex compounds and others.

INS018\_055 a potential novel small molecule inhibitor discovered by Insilico Medicine



using PandaOmics and the generative AI chemistry library Chemistry42. In February 2021, the discovered drug was instigated to treat IPF, a chronic lung disease. In February 2023, the FDA granted INS018\_055 for treating Idiopathic Pulmonary Fibrosis. The collaboration between Insilico Medicine and NVIDIA's DGX systems has resulted in significant achievements in pharma drugs and chemicals discovery. The generative AI and advanced software system are revolutionizing the chemical sector in different aspects and opening opportunities in the United States market.

#### Enhanced Predictive Estimates and Formulations

The conventional trial process to determine the formulation of any compound undergoes several run and testing steps. There are possible chances of error by manually carrying out such a determination process. The implementation of generative AI in these practices has significantly reduced forecast errors and has the potential to predict various essential methods. Generative AI models and advanced analytics can assist in predicting the composition of materials processing in any operation. Mass balance can also predict the real-time quantity of materials required and left simultaneously. Determining complex formulation, which requires different compounds and specific compositions, has become easier as AI models can separately predict the suitable compound along with its design in the formulation.

Advanced forecasting using generative AI has optimized the production process such that the new product can be commenced into the market rapidly, ultimately reducing processing time and increasing the company's revenue. ChemIntelligence is a precise AI tool that incorporates ML-Bayesian algorithms, which assist in developing formulations in a minimum number of performed experiments. Their AI formulation tool can extend its applications to adhesives, coatings, drugs, cleaning solutions, food & drinks, etc. The significance of such generative AI tools can be explored in different chemical sectors, which will open global market opportunities and fascinate chemical companies to invest and make their processes more feasible.

#### Retrosynthesis using Generative AI

Retrosynthesis is a prominent process that assists in creating potential drugs using desired molecules that target specifically and reversibly tracing the chemical reactions for obtaining that specific molecule. The reaction is very challenging and time-consuming which is very difficult to discover such molecules and reaction pathways. Using generative-AI, a tool is developed called G2Retro that automatically generates chemical reactions which can assist in accelerating drug development process. G2Retro



Al model is trained on 40,000 chemical reactions where the model takes input as graphical representation of each molecule and implementing deep neural networks identify novel potential chemical structures to synthesize the molecule.

The generative AI G2Retro tool was tested to predict the reactant configuration of four existing drugs Oteseconazole, Mitapivat, Tapinarof, and Mavacamten. The device successfully generated the patented synthesis routes required for this drug development and provided feasible alternative synthesis routes. The corresponding AI tool can significantly generate hundreds of retrosynthesis predictions within minutes compared to conventional human analysis. This innovative technology will develop infrastructure for lab experiments to increase the accuracy of reaction predictions in drug development. The market-based opportunities can be derived for generative AI models in molecule discovery that ultimately enhance the revenue for AI-driven techniques.

Impact of COVID-19

The COVID-19 outbreak has led to severe disruptions in research practices and the closure of AI laboratories, ultimately lowering experimental research in advanced facilities and significantly hindering data accumulation and acquisition for training generative AI models. The epidemic led to budget cuts on R&D investments for developing AI projects in the chemical sector, as this sector was not very favorable to AI implementation.

Research teams that rely on lab execution of algorithms were affected badly as arrangements for such institutions were shut down because of spreading fear of the COVID-19 virus. However, the pandemic has highlighted the urgency for developing a vaccine to prevent the virus from spreading and protect the world. Generative AI has assisted in developing significant algorithms to manufacture relevant drugs and chemicals in less time.

#### Impact of Russia-Ukraine War

The annexation of Russia on Ukraine has unprecedently led to various sanctions on Russia restricting its trade with other countries. The United States has imposed different legal sanctions on Russia such that it could reduce imports from Russia. Consequently, it has negatively impacted exports of United States AI technologies, including AI-inbuilt chips. Generative AI models in chemicals are significantly troubled in developing more innovations and building proper automation for chemical practices and drug discoveries.



But with the developed smoothness with time, the market for AI technologies can create great potential to expand its innovative models in the chemical industry.

Key Players Landscape and Outlook

The growth in AI and ML industry has encouraged tech companies to invest more in the chemical sector such that innovations and technologies could become faster. Kebotix has emerged as an innovative company that combines cloud technologies with generative AI, physical modeling, and advanced automation. The company's ChemOS product can optimize chemical synthesis and process chemistry using generative AI-powered algorithms. Their advanced formulation and process optimization algorithms have extreme potential to accelerate product development with lesser experimental trials which ultimately reduces process time and costs. Their enhanced AI system can be rolled out to maximize ROI by integrating solutions with their workflow. The generative AI models are advanced type software system that can deliver multiple solutions in a less time which provide prominent opportunities to the United States market to grow.



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\*Companies mentioned above DO NOT hold any order as per market share and can be changed as per information available during research work

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