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Generative AI in Chemical Market Assessment, By Model [Deep Learning, Natural Language Processing, Discriminative Model, Reinforcement Learning, Others], By Applications [Complex Structure Predictions, Novel Formulation Optimization, Chemical Process Optimization, Real-time 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

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Abstracts

Generative AI in the Chemical Market size was valued at USD 151.2 million in 2022, which is expected to reach USD 936.4 million in 2030 with a CAGR of 25.6% for the forecast period between 2023 and 2030. AI and ML advancements have impacted various sectors for performing automation and predicting hidden discoveries. The application of generative AI across chemical industries has also benefited enormous practices, making these operations more accessible and practical. Generative AI in the chemical domain has the potential to create momentum in the research and development process by significantly increasing the speed and accuracy compared to previous R&D operations. It can assist in automating data extraction, selecting relevant formulation, enhance quality testing accuracy, supply chain management, etc. With the implementation of Generative AI, chemical reaction monitoring and optimization has been advancing. Proper AI algorithms have boosted the various chemical operations such as computational molecular design, synthesis planning, compound property

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prediction.

Mitsui Chemicals has implemented IBM Watson using a Generative Pre-trained Transformer (GPT) that has already benefited by enhancing the revenue share of Mitsui Chemicals. IBM Watson has significantly transformed around 20 business modules, and over 100 new applications and bugs have been discovered. In 2023, Mitsui extended the application of IBM Watson in various R&D operations using humongous 5 million data points that comprise news, patents, scientific documents, etc. Likewise, chemical companies are putting effort into implementing generative AI in their conventional practices and making their operations more feasible with more accuracy.

Enhanced Predictive Forecasting and Formulation

The conventional trial process to determine the formulation of any compound is very tedious as it must undergo 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 forecasting errors and has the potential to predict various important methods. Generative AI models and advanced analytics can assist in predicting the composition of materials processing in any operations. Mass balance can also predict the real-time quantity of materials required and left simultaneously. The determination of complex formulation which requires different compounds along with specific composition has become easier as AI models can separately predict the suitable compound along with its composition in the formulation.

Advanced forecast methods 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 company’s revenue. ChemIntelligence is a precise AI tool that incorporated ML-Bayesian algorithms which assist in developing formulations in a minimum number of performed experiments. This 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.

Structured Data for Designing Molecules

The deployment of generative AI models requires enlarged high-quality datasets to train the algorithm. Building humongous, structured dataset based on chemical configuration,

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properties, and reaction is very challenging such that the training is difficult on relevant AI models. A proper database comprises of historical information on chemical molecules, their bonding pattern, feasible reactions, and significant characteristics. Designing novel molecular structures along with their properties can be achieved using generative AI algorithms and structured chemical dataset. The steps and time involved in predicting novel molecules are optimized. Generative AI has facilitated the prediction of various molecular properties without any manual intervention and with more effective and accuracy.

Insilico Medicine, an AI company has successfully developed generative adversarial networks (GANs) and reinforcement learning (RL) models to identify novel molecular structures by specifying the suitable parameters. Insilico is extensively using generative AI in different clinical stages and in 2023 it has successfully accomplished the first dose of INS028_055 making it the first anti-fibrotic small molecule inhibitor designed through generative AI algorithms. The automation of molecule discovery has encouraged many AI companies to build selective generative models which is significantly going to transform the potential of global market in generative AI.

Impact of COVID-19

The COVID-19 pandemic peak era was very devastating as due to COVID virus people are succumbs to death. It has created horrific situation which enforced scientists to unveil drug or vaccine to eradicate the virus of COVID-19. Generative AI delivers a prominent role in drug discovery as with manual efforts the scientists would never be able to develop vaccine in limited time. Using chemical molecules and their properties dataset and implementing generative AI models on these datasets consequently led to relevant chemical molecules that could restrict the COVID-19 virus from spreading globally. Indeed, the generative AI has gained interest among the scientists to use it an incredible AI tool for discovering novel drug, chemical molecules in a lesser time.

Impact of Russia-Ukraine War

The annexation of Russia on Ukraine has developed unprecedented impacts globally which turned out to be global economic concern. The disruption in supply chains and novel innovations were some of the negative outcomes of the invasion. The investment in generative AI across chemical sectors got reduced as revenue for new startups in generative AI lowered down due to war. The sanctions imposed by Western countries on Russia enforced these countries to develop their own chemical products and drugs. In 2023 Russian Quantum Center has successfully generated 2331 novel chemical

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structures with medicinal characteristics by implementing generative AI models on ChEMBL dataset. Thus, the war had impacted and halted the development of these startups and companies in both AI generative and chemical market.

Key Players Landscape and Outlook

With AI and ML advancements, big companies and tech startups frequently invest in their research to build generative AI models for specific applications. IBM, one of the giant tech companies, developed the RXN model in 2018 for chemistry-solving problems. Its AI-enabled algorithm effectively predicts possible outcomes of chemical reactions by optimizing synthesis processes. RXN models can be integrated into an autonomous laboratory for executing developed chemical synthesis procedures. Its advanced scientific infrastructure is specialized in training multiple complex AI models for various chemical processes simultaneously and with greater accuracy. The developed platform has an incredibly massive opportunity for the global market to expand in generative AI.

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