

The development and applications of artificial intelligence in chemistry

Davit Abramishvili

E-mail: daviti.abramishvili626@ens.tsu.edu.ge

Department of Chemistry, Faculty of Exact and Natural Sciences

Ivane Javakhishvili Tbilisi State University, I. Chavchavadze Ave 1, 0179 Tbilisi, Georgia

Artificial intelligence has significantly transformed the landscape of chemical research. Its impact has become particularly pronounced in recent years with the emergence of new and powerful computational tools. This paper discusses the evolution of artificial intelligence in chemistry, from the period when it was limited to rule-based systems and simulations intended for simple data analysis, to the present stage in which advanced machine learning methods are employed. The latest achievements in artificial intelligence, especially deep learning, possess great potential for revolutionizing chemistry. The application of these advanced computational approaches enables scientists to save time in extracting diverse information from large datasets. This capability to identify patterns within big data leads to accurate prediction of molecular properties. Furthermore, since its implementation, the technology has brought substantial progress in drug discovery, materials science research, chemical synthesis, and many other areas of chemistry, which is reflected in ecological benefits as well as the saving of time resources and financial costs.