Nuclear Magnetic Resonance and Artificial Intelligence

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This review explores the current applications of artificial intelligence (AI) in nuclear magnetic resonance (NMR) spectroscopy, with a particular emphasis on small molecule chemistry. Applications of AI techniques, especially machine learning (ML) and deep learning (DL) in the areas of shift prediction, spectral simulations, spectral processing, structure elucidation, mixture analysis, and metabolomics, are demonstrated. The review also shows where progress is limited.

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NMR spectroscopy is indispensable for the identification and structural elucidation of small compounds (e.g., metabolites). The resonance frequencies of each spin (mainly ^{13}C and ^{1}H), also known as chemical shifts, together with their multiplicities, provide a unique fingerprint for different chemical environments within a molecule. By analyzing these shifts and peak profiles, analysts can deduce the connectivity, arrangement, and electronic environments of atoms in a molecule, making NMR an essential tool for determining the precise structure of organic and inorganic compounds. NMR spectroscopy also plays a crucial role in studying molecular dynamics and interactions. The technique can probe how molecules behave in different environments, offering insights into conformational changes, reaction mechanisms, and molecular interactions. This makes NMR invaluable not only for structural chemistry but also for understanding complex biological systems and metabolic pathways. In metabolomics, NMR is used to identify and quantify metabolites in biological samples, providing a comprehensive overview of metabolic processes [1]. By analyzing the NMR spectra of biofluids, tissues, or cells, researchers can gain insights into the metabolic state of an organism, detect biomarkers for diseases, and study the effects of drugs and other interventions [2].

Integrating artificial intelligence (AI) into NMR spectroscopy has been revolutionizing the field, enhancing the accuracy, efficiency, and scope of analyses. This review outlines this progress. Most techniques mentioned here can be classified as machine learning (ML), so we mostly use the terms AI and ML interchangeably. Deep learning (DL) is a subset of newer ML techniques. We do not delve into details of the definition of artificial intelligence, but comprise everything here which is helping to replace human expertise and input. The aim of this is to transform data handling and interpretation, enabling more complex and large-scale studies automatically. This review focuses on advancements in small molecule chemistry and the potential for future developments. Apart from the references given in the text, we point the reader to two recent special issues on the topic [3][4] and the reviews [5][6][7][8] for more

materials and references. As part of this overview paper, we do not claim to cover the extensive literature exhaustively.

References

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