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Commentary

Applications of Molecular Interactions in NMR Spectroscopy

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DESCRIPTION

Interest in studying RNA-small molecule interactions has grown significantly as a result of the fascinating findings of biogenic ligand-sensing and disease-related noncoding RNAs. An effective method for describing intermolecular interactions is NMR spectroscopy. The outline techniques and methods for using NMR spectroscopy to examine associations between RNA and small molecules in this review. The RNA sample preparation protocols, techniques for finding RNA-binding small molecules methods for mapping RNA-small molecule interactions, methodologies for figuring out complex structures and specifications for binding kinetics. In order to facilitate both fundamental understandings of RNA activities and biomedical efforts in developing RNA-targeted treatments. This review will serve as a roadmap to expedite NMR applications in researching RNA-small molecule interactions. Understanding of the functions of various non-coding RNAs (ncRNAs) in biology has undergone a revolutionary change as a result of recent findings in addition to directly contributing to protein synthesis these chemically straightforward biomolecules also control a number of other stages of gene expression including transcription translation chromatin remodeling and RNA and ribonucleoprotein (RNP) trafficking. It is now more and more obvious that throughout these processes, RNA molecules, including regulatory ncRNAs and coding mRNAs an take on intricate secondary and tertiary structures.

These RNAs frequently experience significant structural adaptations in response to the detection of certain ligands including as proteins, DNA, metabolites, RNAs and even tiny cations and anions. Numerous RNA species' dysfunctions have also been connected to a number of human diseases, such as cancer, cardiac, and neurological conditions as a result of their crucial roles in gene regulation. Determining how RNA interacts with such a wide range of ligands is therefore of great interest and significance because it can not only offer mechanistic insights into their functions but also open up new opportunities for designing therapies that target disease-specific RNAs. For describing the molecular interactions between RNA and cognate ligands, a wide variety of biochemical and biophysical approaches have been created and put to use. Such techniques as the Electrochemical Cell Shift Assay (EMSA), emission spectra assays, Isothermal Titration Calorimetry (ITC), Surface Plasmon Resonance (SPR), Nuclear Magnetic Resonance (NMR) spectroscopy and others can be used to characterize binding and its related thermodynamic properties. Numerous of these techniques can be improved upon in order to describe RNA-ligand interactions in biological settings. Last but not least high-resolution structures of RNA and their complexes determined using X-ray crystallography, NMR spectroscopy and more recently, cryo-electron microscopy (cryo-EM) outfitted with direct electron detection can be used to determine molecular interactions at the atomic level.

These techniques, which are frequently complementary to one another offer a group of experimental strategies that have significantly advanced understanding of various RNA functions by enabling the clarification of the chemical and physical underpinnings of molecular interactions between RNA and its various types of ligands. Finding tiny compounds that selectively bind to the target RNA is necessary before performing biophysical characterizations of intermolecular interactions. During their molecular characterizations, cognate ligands for metabolite-sensing RNA eukaryotes are frequently found and confirmed and then certain types are annotated.

The nature of a target, whether it is a polypeptide or RNA has no bearing on the experimental setups of these methods because many of them are based on monitoring ligand NMR signals allowing for direct applications in the identification of RNA-binding small molecules. Therefore, the potential conformations that are dynamically sampled by the target RNA cannot be accurately represented by static high-resolution structures from X-ray crystallization or NMR. However, due to the underdeveloped force fields for RNA and the rough energy landscapes of RNA, it can also be difficult to produce strong structural groups from a stationary RNA structure using Molecular Dynamics (MD) simulations.

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