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Molecular interactions are central to cellular organization and design. Molecular recognition is a key event that dictates the propagation of cellular signals, and it is intra- and intermolecular interactions that facilitate macromolecular folding, stability and elucidation of cellular response. erefore, understanding the interplay of the structural forces that govern recognition and speci city of macromolecular interactions is crucial to decipher the molecular events in a cell. Several spectroscopic techniques such as uorescence, circular dichroism, and Fourier transform infrared spectroscopy, as well as surface plasmon resonance have been successfully used to characterize non-covalent molecular interactions. However, isothermal titration calorimetry (ITC) has been shown to be the most popular and versatile bioanalytical technique that facilitates direct measurement of binding a nity between interacting molecules.

An ITC experiment is a simple titration experiment performed at constant temperature. e secondary ligand, lodged in a syringe, is allowed to titrate its binding partner, the primary ligand, harbored in the heat sensitive sample cell of the calorimeter (Figure 1). e amount

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ITC as a quasi-high throughput technique. For example, quasi-high throughput screening of drugs has been achieved by array calorimetry wherein a series of nanocalorimeters are connected in parallel [8]. Fragment-Based Drug Discovery (FBDD) e orts, in conjunction with ITC, have proved useful in the rapid screening of drugs. e FBDD method involves identi cation, based on enthalpy changes, of smaller fragments of potential drugs that bind to target molecules with high a nity. Subsequently, these high a nity binding fragments are used as building blocks to construct larger drug compounds which bind to their molecular targets with high speci city. ITC-based FBDD methods have provided an avenue for less time-consuming structure-based rational design of drugs, and has found immense favor with the pharmaceutical industry where the consequences of failure could be extremely cost-prohibitive. To this end, Zhou et al. reported an interesting method to identify the target protein(s), present in a mixture of biomolecules, for a drug or lead compound [9]. First, ITC was used as the rst step to verify the binding of a ligand/drug to a protein or protein(s) present in a biomolecular mixture. Next, the mixture was separated by colc11.027d 0esent in a biomolecular 1ne(4ia niihoda endEM

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