Measuring Intermolecular Interactions in Solution

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Most pharmaceutical, biomanufacturing, and specialty chemical companies spend more than 40% of new chemical plant costs on separations. These industries default to resource-intensive distillation and crystallization because the monetary risk of implementing a new chemical separation process frequently outweighs the potential savings of improving the yield. Improving a separation's yield without resorting to distillation and crystallization often requires controlling intermolecular interactions between solutes, solvents, and ions. Unfortunately, current state-of-the-art analytical techniques are insensitive to many of these critical competing intermolecular interactions, forcing manufacturers to optimize their processes by costly iteration alone. Here, we present an overview of several projects aimed at closing the measurement gap for intermolecular interactions. The three aims are to: (1) pioneer an electric-acoustic spectrometer that selectively drives and detects intermolecular interactions; (2) develop new electric spectral simulations to map measurements to intermolecular interactions; and (3) develop state-of-the-art nuclear magnetic resonance (NMR) for intermolecular interactions. Solving this measurement problem enables scientists to tailor intermolecular interactions to increase separation yield and reduce design iterations.