High throughput fragment screening at the nano-scale: laboratory miniaturization and beam-line integration

Alexei Soares Brookhaven National Laboratory

Fragment based drug discovery has emerged as a mainstream tool for identifying small molecules which interact with biological targets. As the method matures the scope expands to include projects that would previously have been considered unsuitable due to complications such as poor expression and instability of the protein target. Here we describe a collection of acoustic based sample handling techniques that improve the likelihood of successful fragment screening in sub-optimal circumstances (and which greatly increase speed and throughput for well behaved systems). These techniques have grown in popularity for rapidly screening a large chemical space using a limited quantity of purified protein and a limited size of compound library.