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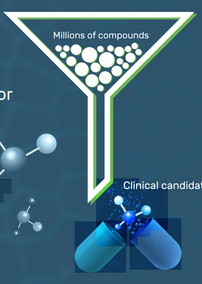
Drug discovery in the ultra-high throughput and acoustic ejection mass spectrometry age

Today's drug discovery involves the evaluation of massive compound libraries of thousands or even millions of potential drug candidates. Thus, **high-throughput screening (HTS)** to assess the pharmacokinetic (PK) properties of molecules is essential for **lead candidate selection** in a practical timeframe.

Industry need: to speed up high-throughput drug discovery.



Analyses are typically performed using **plate reading technology** due to speed but have inherent development costs and specificity issues, whereas liquid chromatography (LC) or high-performance LC (HPLC) for separation and mass spectrometry (MS) for detection has the specificity and information rich data but currently lacks the speed for wider applicability.

Technology pro's & con's

For **plate reading technology**, the output is typically based on a reaction of the compound that generates an absorption or emission. This is a simple endpoint but lacks specificity and can become complicated to develop and troubleshoot. Often, secondary screens are needed to evaluate false positives.

LC–MS/MS methodologies currently have high specificity but low throughput due to sample preparation and separation workflows, which are rate limiting bottlenecks for HTS.

There is a need for simple ultra-high throughput sampling that directly measures product and substrate, enables HTS screening with complex biology and delivers an unequivocal endpoint(s) to reduce ambiguity and enable better decision-making on progression of therapeutic along the development pipeline.

The best of both worlds: acoustic ejection mass spectrometry

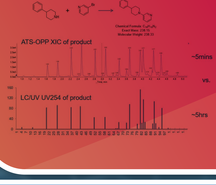
True high-throughput LC–MS/MS screening of candidate compounds during drug discovery has been hindered by the limitations of traditional LC. **Acoustic Ejection Mass Spectrometry (AEMS)** leveraging Acoustic Droplet Ejection (ADE) technology combined with an Open Port Interface (OPI) allows sample analyses at speeds up to 50 times faster than conventional LC–MS.

# Samples (sampling volume ~2.5 nL)	Analysis Time Per Compound	Number Mass Spec Days Required for Screen
500K	0.5 sec	~2.9 days
1000K		~5.75 days
3000K		~17.4 days

- ☑ Speed – ultra high-throughput enabled
- ☑ High specificity, separating true active compounds from false positives
- ☑ High sensitivity (ng/ml)
- ☑ Universality of mass spectrometry detection
- ☑ Limited sample preparation
- ☑ Cost savings in consumables and solvents

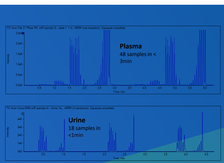
Impact examples

Industry insight: SYNTHESIS
Syncing high-speed plate-based chemistry with high-throughput mass spectrometry analysis.



- Rapid read on reaction success saving cycle times
- Content-rich information including by-products
- Minimal sample needed saving precious templates
- Minimal purification saving cycle time and FTE

Industry insight: BIOANALYSIS



- Rapid analysis with real-time experiment
- Minimal sampling reducing animal use
- Minimal cleanup enabling speed and cost savings

This infographic has been created as part of a Bioanalysis Zone feature in association with SCIEX.

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