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Abstract:

One strategy to transform early Drug Discovery into a more competitive process is to reduce the Design-Make-Test-Analyze (DMTA) cycle time and its associated costs.[1] Through a postdoc project at AstraZeneca, we developed a novel miniaturized[2] and automated high throughput (HT) hit identification method to produce and screen large arrays of compounds in less than a week using acoustic technologies. Reaction mixtures were prepared at nanoscale using the Echo® 655 acoustic liquid handler (reaction volume: 0.5 -1 µL in 1536-well microtiter plates). Then, acoustic mist ionization mass spectrometry (AMI-MS) was employed for both analysis and bioassays screening against MTH1 protein target. Finally, we also investigated the compatibility of various HT mass spectrometry technologies (beyond AMI-MS) with picomolar compound libraries and compared sensitivity, speed, and sustainability.

1.Paul, S. M. et al. *Nat. Rev. Drug Discovery*, **2010**, *9*, 203.

2.Lin, S. et al. Science 10.1126/science.aar6236 (**2018**)

3.Kettle, J. G. et al *J. Med. Chem*. **2016**, *59*, 2346.