

Title of the workshop: High throughput screening mass spectrometry – current status and future landscape (Pharmaceuticals Interest Group)

Date of the Workshop: June 7th, 2023

Organizers/Presiders list: Kiran Iyer, Senior Scientist, Just Evotec Biologics & Jeremy Manheim, Senior Scientist, Merck and Co. Inc

Description or goals of the workshop: High throughput screening (HTS) systems provide the opportunity to measure several hundred thousand samples a day and is therefore in high demand in the pharmaceutical industry. Coupled to a sensitive and specific technique such as mass spectrometry (MS), HTS-MS systems are employed in several stages of the drug discovery process for applications that include, but not limited to, biomarker discovery, disease monitoring, targeted metabolomics, and the development of new chemical entities. While there are several established MS platforms available for HTS, there are often constraints in trying to balance the throughput and the need for specialized equipment and custom-built software for data analysis. Some common HTS-MS platforms include the RapidFire-MS, multiplexed LC-MS/MS systems, Acoustic systems coupled to MS, MALDI-MS, and the more recently emerging HTS-DESI-MS systems.

This workshop aims to present: 1) The status on the use of HTS-MS systems for pharmaceutical analysis 2) Current developments, instrumentation, limitations and constraints with HTS-MS systems 3) Future outlook. The workshop aims to gather several presenters from instrumentation and pharmaceutical companies. Order of the presentations will be: 1) opening remarks from the presiders covering Topic 1, 2) two presentations from instrument companies (Bruker, Sciex) 3) two presentations from scientists in the pharmaceutical industry, and 4) closing remarks by the presiders. The audience for the workshop will be the industry community, researchers in academia, and analytical contract laboratories. Appropriate time will be designated to encourage participation and idea exchange with the audience. An expected outcome is to trigger the interest in the industry to embrace HTS-MS and for instrument companies to showcase exciting developments within this space.

Titles and summaries of presentations:

Introduction to the topic:

- Introduction to drug discovery and development – Jeremy Manheim
- Purpose of HTS instrumentation in the pharmaceutical industry, analytical techniques employed for HTS – Kiran Iyer
- Ultrahigh-Throughput MALDI MS in Drug Discovery – Sergei Dikler, Bruker Scientific LLC
- Desorption Electrospray Ionization (DESI-MS) and Infrared Matrix-Assisted Laser Desorption ESI Mass Spectrometry (IR-MALDESI-MS) for Ultra-High Throughput MS – James Sawicki (AbbVie)
- Chromatographic and non-chromatographic approaches to HTS-MS – Alternating column regeneration, StreamSelect and RapidFire – Kevin McCann (Agilent Technologies)
- Acoustic Ejection Mass Spectrometry for High-Throughput Screening – Chang Liu, Sciex

The workshop was well attended and engaging with plenty of time for discussion. We had a lot of attendees and the room was rather small with people having to resort to waiting outside after a point since there was standing room only. Additionally, since the adjoining workshops were occurring concurrently, we had a lot of noise pollution from the neighboring workshop.