

Overview

Here we present advances in automated multi-ionization mass spectrometry (MS). The Ionique platform offers ESI, matrixassisted ionization (MAI) and solvent-assisted ionization (SAI).

Introduction

MAI, SAI and vMAI are new ionization technologies capable of high sensitivity and different selectivity relative to ESI and MALDI and operate without use of high voltages or a laser^{1,2,3,5}. MSTM built the first automated multi-ionization platform capable of analyses with ESI, MAI, and SAI and later two different vMAI automated ionization sources⁴. The Ionique platform typically delivers between 0.1 and 1 µL of sample solution from a variety of formats (e.g., 96-well plates) for analysis on API mass spectrometers. The most extensive use of the multi-ionization platform was analysis of ca. 5000 bacterial extract sample by ESI and MAI and fewer with SAI to demonstrate the ability to differentiate various bacteria even on the strain level. Here we demonstrate a variety of platform upgrades, methodology improvements, and applications where multiple ionization delivers superior results.

Methods

The MS[™] lonique upgraded platform was interfaced to Thermo Exactive, Q-Exactive Focus, and Waters SYNAPT G2S mass spectrometers. The platform delivers sample solution using a stainless steel capillary tubing to the ionization region of the API mass spectrometer. For ESI, *ca.* 1 µL of solution is expelled from the capillary about 1 cm from the MS inlet tube of the mass spectrometer while voltage is applied to the capillary (for the SYNAPT G2S an inlet tube is retrofitted). With SAI, the capillary is inserted into the heated inlet tube before ca. 1 µL of solution is expelled. With MAI, 0.1-0.2 µL of matrix: analyte solution is expelled from the tube and allowed to air dry before insertion into the inlet.

Ionique Multifunctional Automated Platform





Figure 1. MSTM Ionique platform on mass spectrometers (A) the Thermo Orbitrap Exactive, (B) the Waters Synapt G2S.





Figure 2. MSTM Ionique platform: (1) flange for attachment, (2) instrument override, (3) camera, (4) robotic arm, (5) delivery probe, (6) matrix container, (7) wash container, (8) sample well plate

Figure 8. Mass spectra of DH5 alpha bacteria extract acquired by (A) MA and (**B**) ESI using the MSTM Ionique automated platform.

Advances in Automated Multi-Ionization Mass Spectrometry: ESI, SAI, MAI and vMAI

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