Atmospheric pressure ionization (API) sources

The Agilent 6545 Q-TOF mass spectrometer at the Western Illinois Mass Spec Center is equipped with the following interchangeable API sources: Dual Agilent Jet Stream Electrospray Ionization (Dual AJS ESI), Atmospheric Pressure Chemical Ionization (APCI), and GC-APCI. A common atmospheric sampling interface introduces ions from these various sources into the mass spectrometer vacuum system.

Dual AJS ESI.

ESI relies in part on chemistry to generate analyte ions in solution before the analyte reaches the mass spectrometer. As shown in the following **Figure 1**, the LC eluate is sprayed into a spray chamber at atmospheric pressure in the presence of a strong electrostatic field and heated drying gas. The electrostatic field occurs between the nebulizer, which is at ground in the Agilent design, and the capillary, which is at high voltage. The spray occurs at right angles to the capillary. This design reduces background noise from droplets, increases sensitivity, and keeps the capillary cleaner for a longer period of time.

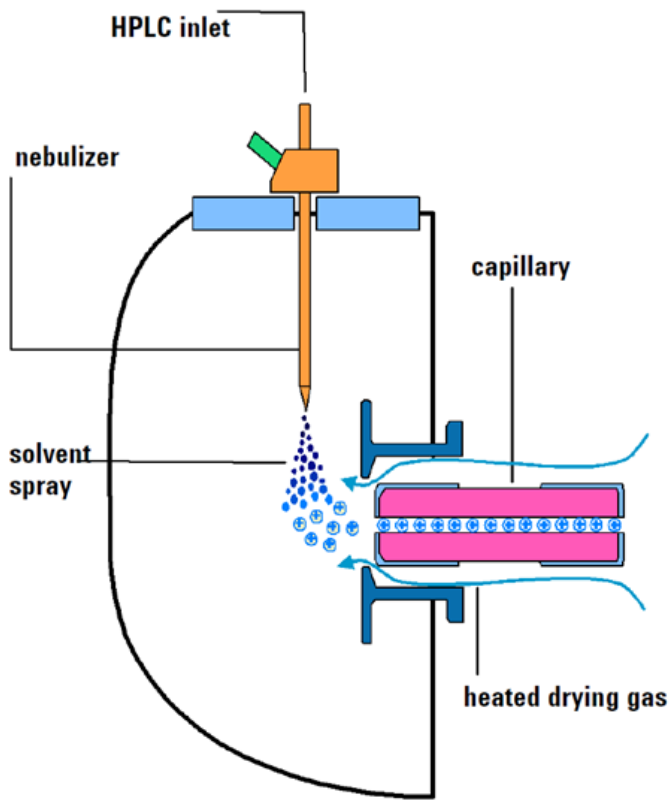

Figure 1. The Agilent ESI

AJS thermal gradient focusing consists of a superheated nitrogen sheath gas that is introduced collinear with and concentric to the pneumatically assisted electrospray. Thermal energy from the superheated nitrogen sheath gas is focused to the nebulizer spray producing the most efficient desolvation and ion generation possible. The enhanced desolvation results in more

ions entering the sampling capillary as shown in **Figure 2** and concomitant improved signal to noise.

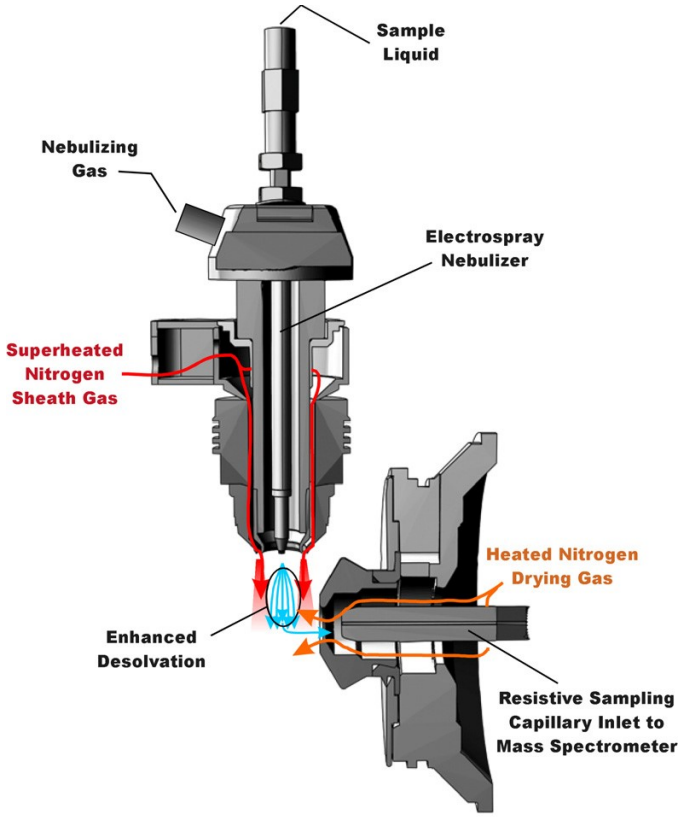

Figure 2. The AJS ESI

The Dual AJS ESI source consists two nebulizers: a standard nebulizer and a capillary nebulizer. The internal diameter (ID) of the internal needle for the standard and the capillary nebulizer is 120 and 50 µm, respectively. The recommended flow range for the standard and the capillary nebulizer is 50 to 250 µL/minute and 1 to 50 µL/minute, respectively. While the standard nebulizer is used to introduce the LC eluate, the capillary nebulizer is used to introduce internal mass reference. With internal mass calibration, the mass accuracy of the Agilent 6545 Q-TOF LC/MS system is less than 0.8 ppm.

APCI.

APCI is a gas-phase chemical ionization process. The APCI technique passes the LC eluate through a nebulizing needle, which creates a fine spray. The spray is passed through a heated ceramic tube, where the droplets are fully vaporized, as shown **Figure 3**. The resulting gas/vapor mixture is then passed over a corona discharge needle, where the solvent vapor is ionized to create reagent gas ions. These ions in turn ionize the sample molecules via a chemical ionization process. The sample ions are then introduced into the capillary. APCI requires that the analyte be in the gas phase for ionization to occur. To vaporize the solvent and analyte, the APCI source is typically operated at vaporizer temperatures of 400 to 500°C.

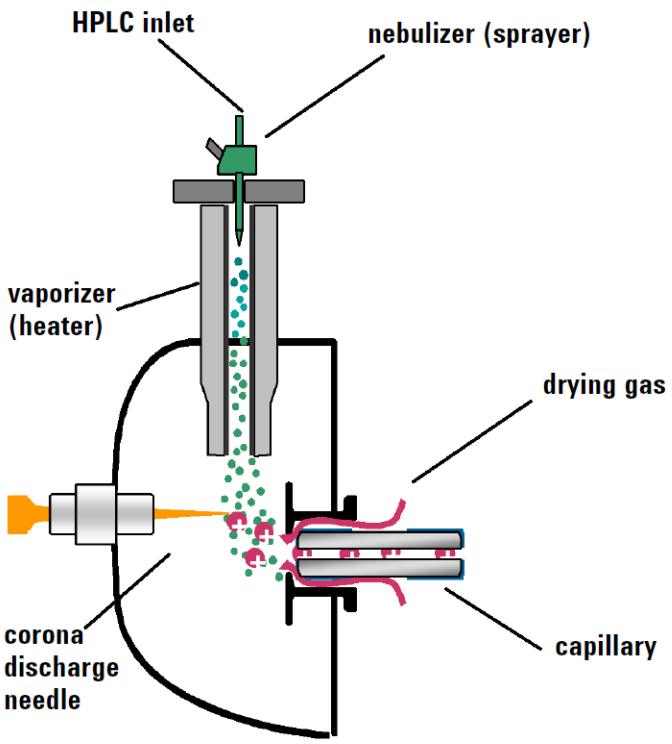

Figure 3. The Agilent APCI

GC-APCI.

While the non-volatile relatively polar compounds are usually analyzed by LC/MS, the more volatile non-polar compounds require GC/MS analysis. Adding GC-APCI capability to the Agilent 6545 Q-TOF mass spectrometer provides the flexibility to perform high mass accuracy and high resolution quantitative and qualitative analysis of both non-volatile relatively polar and more volatile non-polar compounds on a single instrument, therefore saving time, money and bench space.