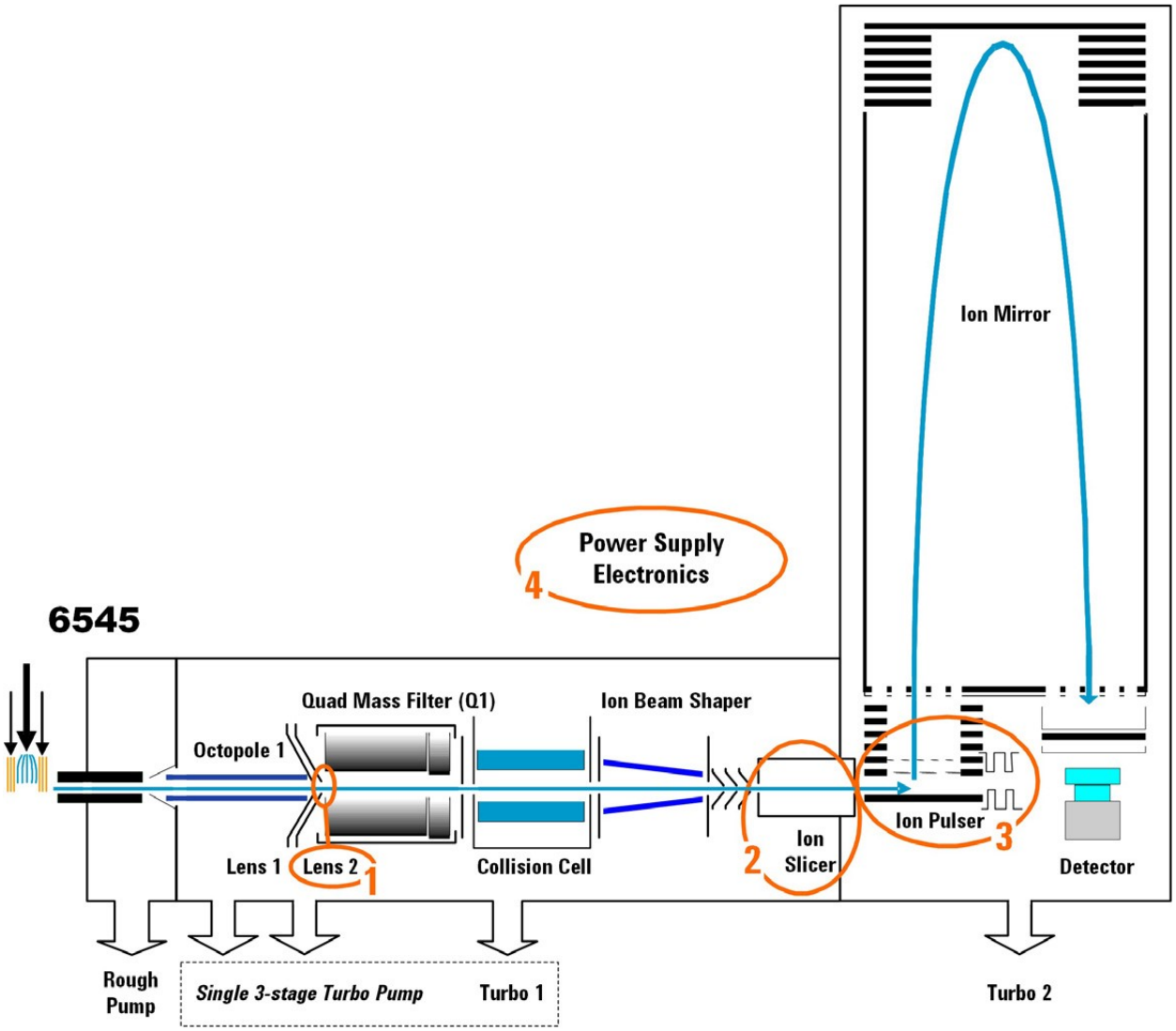
The Agilent 6545 Q-TOF mass spectrometer

The Agilent 6545 Q-TOF mass spectrometer, which is shown in the following picture, is a state-of-the-art quadrupole time-of-flight (Q-TOF) mass spectrometer that performs both high resolution mass spectrometry (HRMS) and high-resolution tandem mass spectrometry (HRMS/MS). It consists of a quadrupole mass analyzer, a hexapole collision cell, and a high resolution TOF mass analyzer. During HRMS analysis, the quadrupole mass analyzer and the hexapole collision cell are simply used as ion guides to transport ions. During HRMS/MS analysis, the quadrupole mass analyzer selects precursor ions that are fragmented in the hexapole collision cell into product ions, which are then impelled to the TOF mass analyzer, at an angle perpendicular to the original path.

The following Figure shows the ion optics of the Agilent 6545 Q-TOF mass spectrometer, with major improvements over the Agilent 6540 Q-TOF mass spectrometer identified.



1. **Enhanced Wide Bore Lens 2.**
   Identical to the lens 2 design used in the 6560, a larger orifice is used in the 6545. Ions are still conditioned via DC and RF voltages prior to quad transmission or isolation, but ions will not get in close proximity to the lens surface. The possible risk of ion deposition on the surface is greatly reduced, leading to an increased robustness of the system under high ion current conditions.
2. **Slicer design.**
   The slicer design on the 6545 is identical to the 6550. It has 2 different sizes of the opening: a larger one for high sensitivity applications, and a smaller one for high resolution applications. The positions can be changed in the Tune Context and are saved as part of the tune file. In total, 10 positions are usable: 4 positions for the high sensitivity, and 6 positions for high resolution.

3. **Improved pulser design.**
   Thermal and long-term stability of the pulser is optimized by better process control of the delay time, leading to less variations in mass accuracy.
4. **Improved Power Supplies.**
   In comparison to the 6540, changes were made to the feed-through as well as the type of power supply for better thermal and other environmental stability. As a consequence, better resolution is achieved with this change.

The following Table shows the specification of the Agilent 6545 Q-TOF mass spectrometer.

Parameter	Measure	Specification
Sensitivity, MS mode, electrospray on-column, 400 µL/min flow rate	1 pg LC/MS injection of reserpine. Signal-to-noise for the reserpine $(M+H)^+$ at *m/z* 609.2807 while maintaining a resolution of 40,000 at *m/z* 2,722 in 4 GHZ mode	500:1 RMS
Sensitivity, MS/MS mode, electrospray on-column, 400 µL/min flow rate	1 pg LC/MS injection of reserpine. Signal-to-noise for most intense product ions (174, 195, 397, and 448 *m/z*) while maintaining a resolution of 40,000 at *m/z* 2,722 in 4 GHZ mode	1,500:1 RMS
Mass resolving power	Measured at *m/z* 2,722 after automatic tuning procedure	Greater than 45,000 FWHM at *m/z* 2,722
Mass accuracy – MS mode, electrospray on-column, 400 µL/min	Measured at the $(M+H)^+$ ion of reserpine (*m/z* 609.2807) using an internal mass reference	Less than 0.8 ppm RMS as measured from 10 repeat injections
Mass accuracy – MS/MS mode, electrospray on-column, 400 µL/min	Product ion *m/z* 397 for reserpine	Less than 2 ppm RMS on *m/z* 397 as measured from 10 repeat injections
Mass accuracy temperature stability, MS mode	Temperature: 15 to 35 °C (59 to 95 °F) at constant temperature	Maintain 1 ppm mass accuracy (variations < 3 °C from calibration temperature)
Dynamic range	Intrascan dynamic range on coeluting components	Up to 5 decades
Mass range		*m/z* 100–10,000 extended mass range *m/z* 50–1,700 or 50–3,200 for both high resolution and extended dynamic range modes Quadrupole up to *m/z* 4,000
Spectral acquisition rate, MS mode	*m/z* 50 to 1,700 in MS mode while maintaining a resolution of 40,000 at *m/z* 2,722 in 4 GHZ mode	50 spectra/second
Spectral acquisition rate, MS/MS mode	*m/z* 50 to 1,700 in MS/MS mode while maintaining a resolution of 40,000 at *m/z* 2,722 in 4 GHZ mode	30 MS/MS spectra/second
Positive to negative swithing	Complete cycle switching from positive to negative and positive modes allows for stabilization time	1.5 seconds