Agilent 5977 Series EI Source Selection Guide

Technical Overview

Introduction

The Agilent GC/MSD system has long been a mainstay productivity tool in laboratories performing environmental, forensic toxicology, food, fine chemical, and other analyses. Each generation of the system has improved the data quality, ease of use, and cost of operation, helping laboratory managers meet their performance goals during challenging economic times.

The ion source of an MSD instrument is critical to its performance. The efficiency of ionization and focusing of the ion beam into the quadrupole determine the sensitivity of the instrument. Many of today's MSD applications are run in electron ionization (EI) mode, requiring EI sources that optimize instrument performance. Agilent is the leader in the development of ion source technology that provides the high sensitivity and reliability needed for today's MSD applications.

The Agilent 5977 Series GC/MSD offers four EI source options:

- The traditional stainless steel source provides performance most similar to previous Agilent MSD instruments at an economic price.
- The inert source enables high sensitivity for active compounds that are most likely to interact with non-inert surfaces.
- The Extractor EI source provides higher sensitivity than previous sources, while also being inert.
- The High Efficiency source delivers unparalleled sensitivity for ultra-trace level applications.

This technical overview provides a guide for selection of the ion source most appropriate to the user's application.

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High Efficiency Ion Source (HES)

This state-of-the-art ion source incorporates a novel design not seen in previous EI source generations. The source increases the ionization efficiency in the ion body and maximizes the ions transferred into the quadrupole analyzer, providing unparalleled sensitivity for ultra-trace analysis. Advantages and benefits of using this ultra-efficient source include:

- Lower and improved detection limits
- Minimized maintenance frequency (for example, liner replacement and column trimming) by injecting less sample

The components of the HES are made of an inert material with temperature programmable capabilities up to 350 °C, resulting in robust performance for a wide variety of compounds in the low fg to sub-ng level.

Extractor Ion Source

This innovative ion source has an extractor lens in place of the draw-out plate used in previous EI source designs, and is made of an inert material. It is programmable up to 350 °C to deliver enhanced response for active compounds and late eluters.

The extractor lens provides additional focus of the ion beam into the mass analyzer. A potential is applied to the extractor lens, which pulls the ions out of the ionization chamber, adding to the push provided by the repeller voltage (Figure 1). The result is a significant increase in the number of ions analyzed, improving the true sensitivity of the instrument.

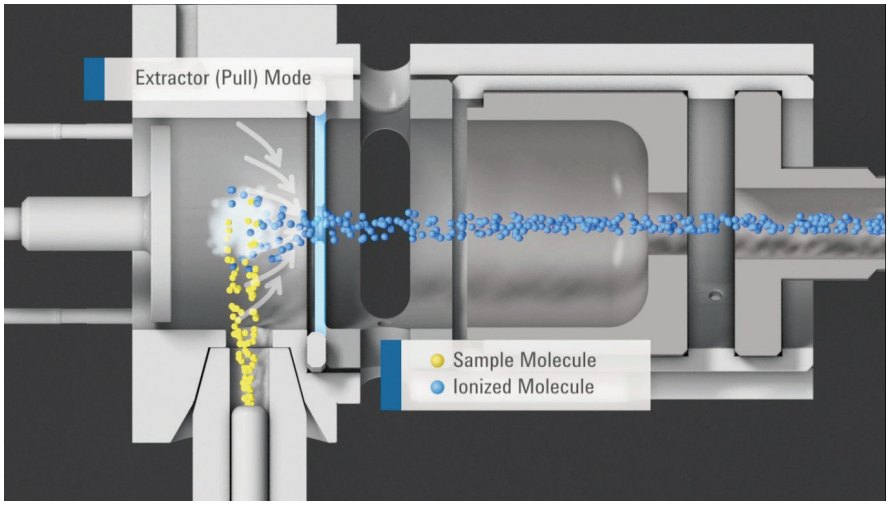

Figure 1. The Extractor EI Source for the Agilent 5977 GC/MSD, illustrating the pull mode, which increases the number of ions introduced into the chamber.

There are three available aperture sizes for the Extractor source, as well as the two other sources: 3, 6, and 9 mm (Table 1). Generally, the 3 mm aperture provides the best sensitivity. Selecting one of the larger aperture sizes enables the analysis of higher concentrations of target compounds. Increasing aperture diameters also reduces the residence or interaction time, and provides higher effective inertness for fragile compounds.

Table 1. Extractor Lens Aperture Diameters Available for the Agilent 5977 Series Ion Sources

	Extractor lens aperture diameter		
EI source	**3 mm†**	**6 mm**	**9 mm**
Stainless steel	05971-20134*	–**	–
Inert	G2589-20100	G2589-20045	–
Extractor	G3870-20444	G3870-20448	G3870-20449
HES	G7002-20061	–	–

† Standard configurations for all sources comes with the 3 mm extractor lens aperture diameter

* Part number

** It is mechanically possible to install the 6 mm drawout lens of the inert source into the stainless steel source

The Extractor EI source can be operated in the higher sensitivity mode of extraction tuning, or in standard mode, in which it behaves in the same way as the standard stainless and inert sources. The ability to change between extractor and repeller-only mode is controlled by the software and does not require any physical changes. A video description of the Extractor EI Source is available at http://www.chem.agilent.com/chem/resolve.

Inert Ion Source

To ensure accurate quantification and high sensitivity, the entire GC/MSD flow path, including the detector surfaces, must be highly inert. The inert ion source is made of the same inert material used in the Extractor and HES EI sources, and is programmable to 350 °C, enabling trace-level detection and SVOC and VOC analyses (Table 2).

Table 2. Source Selection for Various Applications

Application	**Source(s)**	**Draw-out/Extractor lens (mm)‡**	**Tune**
Ultra-trace level (low fg–sub ng) (mid fg–low ng)	HES, Extractor	3	HES_Atune, Etune
Trace level (fg-ng)	Extractor, Inert	3	Etune, Atune
Mid–high level (pg–high ng)	Extractor, Inert, Stainless steel	6,9	Atune
Obtain spectra closest to older instruments	Stainless steel	3	Stune
VOC P&T–(BFB)	Extractor, Inert	6	BFB Autotune
SVOC (DFTPP)	Extractor, Inert	6	DFTPP

‡ See Table 1 for extractor lenses available for each source.

Stainless Steel Ion Source

The most cost-effective source for picogram to high-nanogram sensitivity and for obtaining spectra most similar to legacy instruments is the stainless steel ion source, which is programmable up to 350 °C (Table 2).

Source Tune, Gain, and Flow Guidance

Choosing the most appropriate source configuration and tune can have a significant effect on the success of an application (Tables 2 and 3). The guidelines outlined here are meant to be general suggestions as starting points. Application-specific method development should be performed to ensure the best operating conditions. This is particularly important with the most sensitive sources, the HES and the Extractor source. Since these ion sources generate up to 10 times more ions, the gain needs to be modified accordingly (more likely lower the gain) to maintain method performance or improve it. Read and understand "A Quick-Start Guide to Optimizing Detector Gain for GC/MSD" (5991-2105EN) before attempting to optimize any method or gain configuration. Table 4 gives a description of the various tune modes and their use.

Table 3. Source Configurations and Supported Tunes

EI Source	HES Atune	Etune	Atune	BFB Atune	Lomass	Stune	DFTPP	BFB
Stainless steel	–	–*	✓	–	✓	✓	✓	‡
Inert	–	–*	✓	✓†	✓	✓	✓	‡
Extractor	–	✓	✓	✓†	✓	✓	✓	‡
HES	✓	–	–	–	–	–	–	–

* Etune can be executed from the tune menu with a non-extractor source but will produce only an Atune

† BFB_Atune requires the use of the 6 mm draw-out plate/extraction lens

‡ BFB_Atune is the preferred tune. See Application Note 5991-0029EN.

Table 4. Description of the Tune Options for the Agilent 5977 Series Ion Sources

Tune menu items (default tune file names as *.U)	Description
Tune MSD	Performs the type of tune that is embedded in the active tune.
QuickTune	Provides fine tuning to ensure acceptable response, resolution, and accurate mass assignment.
Autotune (Atune.U)	The standard repeller-based tune of the Agilent 5973 inert MSD and Agilent 5975 Series.
Extraction Source Tune (Etune.U)	Used with the Extractor source to provide high sensitivity. Equivalent to Atune when used with inert or stainless sources.
HES Autotune (HES_Atune.U)	The only tune available for the High Efficiency Source novel design, which is optimized to provide the highest sensitivity.
BFB Autotune (BFB_Atune.U)	Used in conjunction with Atune to meet USEPA BFB tuning criteria. Requires the use of a 6-mm draw-out/extraction lens, and operates in standard repeller-based tuning mode.
Low Mass Autotune (Lomass.U)	Identical to Autotune, except it tunes on masses 69, 131, and 219 instead of 69, 219, and 502. Intended for low molecular weight applications and natural gases under 250 daltons.
Standard Spectra Tune (Stune.U)	Ensures standard response over the full mass range. Specifically, PFTBA mass 69 is the base peak, mass 219 is between 35 and 99%, and mass 502 is >1%. This is a lower sensitivity tune used to better match legacy libraries created using the Agilent 5971 or 5972 MSDs.
DFTPP (DFTPP.U)	A specific target tune used for USEPA semivolatile analysis (8270 methods).
BFB (BFB.U)	A specific legacy target tune used for VOC analysis. It does not provide the same sensitivity and stability as BFB Autotune. Provides continuity for established SOPs and for users with a preference for target tuning. See Application Note 5991-0029EN for a description of the recommended procedure for VOC analysis.

Additionally, selection of an adequate carrier gas flow into the source and vacuum chamber is critical for application success. By selecting an appropriate carrier gas flow, the overall mass spectrometer performance and chromatographic performance are optimized. It is recommended that applications using GC/MS systems are set at a constant flow not to exceed 1.5 mL/min. For example, to be at an adequate carrier gas linear velocity of ~40 cm/s (for He), a 30 m × 0.25 mm, 0.25 µm column requires 1.2 mL/min, whereas a 20 m × 0.18 mm, 0.18 µm column requires 0.8 mL/min.

EI Tune Options

In the **Tune** menu, and in the **Tune and Vacuum Control** view, there are several options for tune selection. The top two options are mechanisms to run part or the entire active tune. The remaining menu options are tunes for specific purposes, and are described in Table 4.

Available EI Sources for the Agilent 5977 Series GC/MS

Table 5. EI Source Parts List

EI source	Benefit	Product number (spare parts)
Stainless steel	Inexpensive	G2591D
Inert	Reduced activity	G2591B
Extractor	Reduced activity, high and low sensitivity	G2591C
HES	Reduced activity, highest sensitivity	G7008C

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