The Mass Spec Source

Fall, 2008

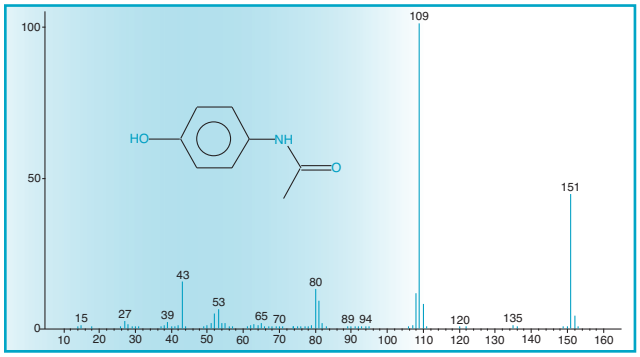
*For Mass Spectrometry and Chromatography*

# NEW! NIST '08

## *NIST/EPA/NIH Mass Spectral Library*

**A Major NEW Release of the world's most widely used, fully evaluated, and trusted mass spectral reference library.**

*NIST '08 is a collection of electron ionization (EI) mass spectra. It also includes MS/MS spectra, GC data, and software for mass spectral analysis*




## NIST '08 Components

### NIST Data Libraries

#### Electron Ionization (EI) Mass Spectral Library:

**220,460 spectra of 192,108 compounds,** with identification and chemical structures **(new salts database included).**

#### Gas Chromatography (GC) Data Library:

**224,038 retention indices of 44,008 compounds (21,847 in the EI library),** with corresponding **GC column conditions and literature citations** on both non-polar and polar columns.

#### MS/MS Spectral Library:

**14,802 spectra of 5,308 precursor ions** (3,898 positive ions and 1,410 negative ions).

### NIST Mass Spectral Software:

#### NIST MS Search Program

Searching and Browsing of the database, which now includes the display of compound derivatives in the database with replicated spectra.

#### MS Interpretation Program

Assists in mass spectra analysis and interpretation. Includes ability to predict fragmentation based on structure input.

#### AMDIS

Extracts noise-free component spectra from GC/MS data of mixtures by deconvolution.

*(cont. on Pg. 2)*

## FEATURE

**NEW - SSIG-17/18 Ionization Gauge** . . . . . .6

A new, improved Bayard Alpert ionization gauges specifically designed for long life and reliability.

**NEW - Turbomolecular Pump Repair Kits** . . . . . .7

Turbomolecular pump repair kits are available from Eagle Instrument Services. Are you tired of simple bearing replacements causing downtime while you ship your turbo pumps out for repair? Now there is a solution! **Turbo Kits.**

## Celestron® Handheld Digital Microscope (HDM)


New state-of-the-art technology in microscopes means you don't need a traditional microscope to view and/or image specimens or objects. **Details on Pg.5**

## CONTENTS

# NIST Data Libraries

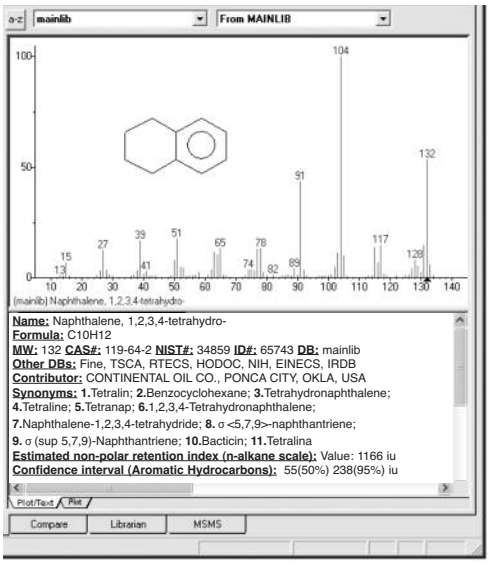
## Summary:

The NIST '08 Mass Spectral Database, the successor to the NIST '05, is a collection of electron ionization (EI) mass spectra. It also contains MS/MS spectra, GC data, and software for mass spectral analysis. The NIST Database is known for its high quality. It is the product of a two decade, comprehensive evaluation and expansion of the world's most widely used mass spectral reference library by a team of experienced mass spectrometrists in which each spectrum was examined for correctness.

## These data libraries are included:

### 1. Electron Ionization (EI) Mass Spectral Library:

**220,460 spectra of 192,108 compounds,** with name, list of synonyms, CAS registry number, molecular formula/weight, chemical structure, contributor name, list of peaks, and estimated GC retention index. The size **increased 15% over NIST '05**, with continued improvement in library quality. Thousands of spectra of common derivatives and contaminants have been reexamined. It now also includes a separable library of 717 spectra of 672 low-volatile salts (nist-salts). Libraries are provided in NIST format, usable with the NIST search software and certain data systems. Other formats, including Agilent ChemStation .L are also available.




EI Library Example Spectrum

1. Value: 1153.9 iu; Column Type: Capillary; Column Class: Standard non-polar; Active Phase: Petrocol DH; Column Length: 50 m; Carrier Gas: He; Column Diameter: 0.25 mm; Phase Thickness: 0.5 um; Data Type: Linear RI; Program Type: Ramp; Start T: 35 C; End T: 200 C; Heat Rate: 3 K/min; Start Time: 10 min; End Time: 10 min; Source: Censullo, A.C.; Jones, D.R.; Wills, M.T., Speciation of the volatile organic compounds (VOCs) in solventborne aerosol coatings by solid phase microextraction-gas chromatography, J. Coat. Technol., 75(936), 2003, 47-53

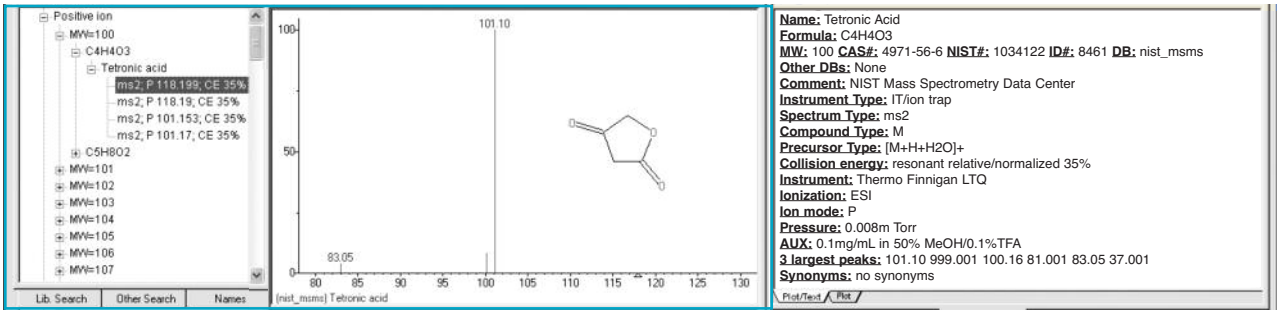
GC Library Example Data

### 2. Gas Chromatography (GC) Data Library:

**224,038 retention indices,** with corresponding **GC column conditions and literature citations,** on both non-polar and polar columns, **for 44,008 compounds (21,847 in the EI library)**. The size increased 50% over NIST '05, and it now includes polar columns.

### 3. MS/MS Spectral Library:

**14,802 spectra of 5,308 precursor ions** (3,898 positive ions and 1,410 negative ions). The size increased 250% over NIST '05, with contaminants and metabolites forming a large fraction of the new spectra. Spectra were primarily measured on ion-trap and collision cell instruments using electrospray ionization, though other methods are represented.

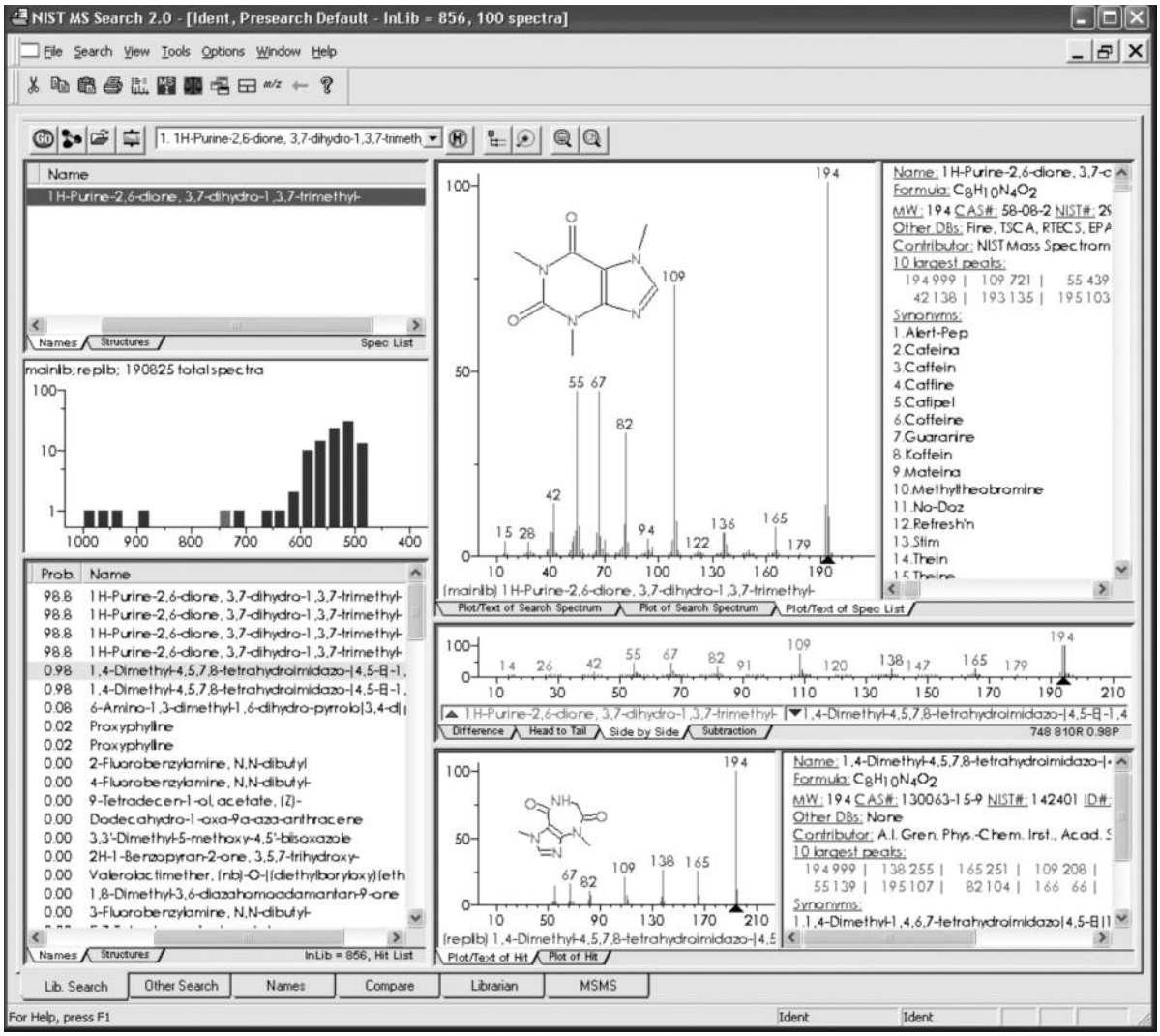



MS/MS Library Example Data

**A more detailed list of changes is available at**
**http://www.sisweb.com/nist#whatsnew**

# NIST MS Search Program

The NIST '08 Database can be browsed and searched using the included NIST MS Search software (below).



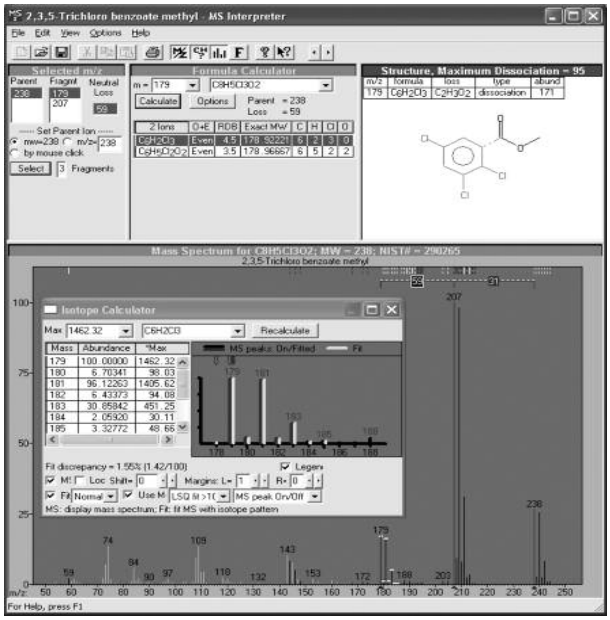

**NIST MS Search Software showing comparison of caffeine spectra (top) with list of Database matches sorted by probability (lower left). Spectra can be compared side-by-side (center), and data on spectra compounds can be examined (upper and lower right).**

## Features:

- **Browsing:** Browse all spectra in the NIST Database or user created databases. Data include MS peaks, structures, formulas, CAS registry number, synonyms, estimated and measured GC retention indices, and GC column data.
- **Spectral searching:** Given user provided (unknown) spectra, search for the best matching spectra in the NIST or user libraries. Searches may add a variety of constraints (name, elements present, common compound, etc.). Searching is also possible from various mass spectral data systems from Agilent, Thermo Finnigan, Varian, and others.
- **Structure searching:** Find all chemical structures similar to the structure of the search spectrum, using the structural data from the NIST MS database or from user structures drawn in most chemical drawing packages.
- **Datasystem interfaces:** Directly transfer data between a number of commercial data systems.
- **Compare views:** Visually compare two spectra in a variety of ways.
- **MS/MS browsing window and MS/MS library:** The MS/MS identity search is a new type of search for searching for MS/MS spectra in MS/MS libraries.

# NIST Mass Spectrum Interpreter

NIST '08 also includes a Mass Spectrum Interpreter utility to assist the evaluation of mass spectra. You can examine neutral losses, isotope patterns and possible chemical formulas, along with computer-assisted chemical structure/spectra analysis.

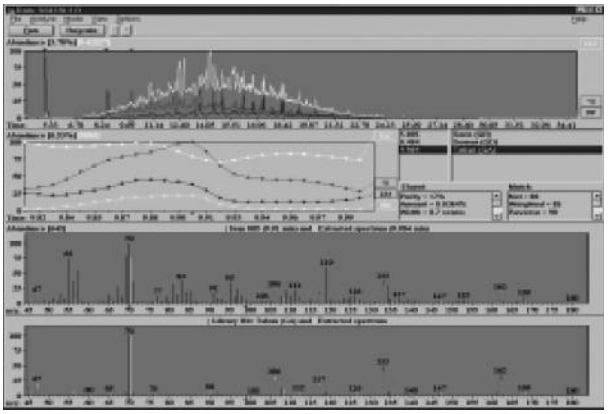



## Features:

- **Spectrum-structure consistency:** After importing a structure and a mass spectrum, each peak is marked as either consistent or inconsistent with fragmentation rules, and molecular formulas of consistent peaks are highlighted.
- **Neutral loss analysis:** Examine fragmentation stating from the molecular ion or any secondary ion.
- **Isotopic cluster analysis:** Calculate theoretical isotopic profiles and compare with spectra.
- **Chemical formula for each peak:** Rapidly find possible elemental formulas for any peak or neutral loss in a spectrum.
- **Interfaced to the NIST MS Search software.**

# Automated MS Deconvolution and Identification System (AMDIS)

NIST '08 also bundles the AMDIS utility, which extracts the spectrum of each component in a mixture analyzed by GC/MS or LC/MS and identifies target compounds.



- **GC/MS deconvolution:** Preprocesses GC/MS or LC/MS data, automatically reconstructing spectra from complex mixtures. Selected compounds can then be sent to the NIST MS Search software for library searching.
- **Chemical Identification:** Can also act as a "black box" chemical identifier, displaying all chemical identifications that meet a user-selectable degree or confidence. Identification can be aided by internal standards and retention times.
- **Interfaced to the NIST MS Search software.**

| Part No. | Description | Price |
|---|---|---|
| 641010 | NIST 08 Library & Search Program, Standard Version | |
| 641010UG | NIST 08 Library & Search Program, Standard Version (Upgrade) | |
| 641010HP | NIST 08 Library & Search Program, Agilent ChemStation Version | |
| 641010HPUG | NIST 08 Library & Search Program, Agilent ChemStation Version (Upgrade) | |

***For Additional Information Please Visit Our Web Site At http://www.sisweb.com/nist***

# New Celestron® Handheld Digital Microscope (HDM)

## *A Breakthrough in Microscope Technology*

### Specifications


- New state-of-the-art technology in microscopes means you don't need a traditional microscope to view and/or image specimens or objects.
- Image what you see with the click of a button for snapshots or video with the provided software or use your own photoimaging software programs.
- Built-in digital camera for viewing and imaging - resolution 0.3mp using a 1/4" CMOS chip (640 x 480 pixels)
- Video Frame Rate - 15 or 30fps
- 20X (Ion power) or 400X (high power) to choose from.
- Field of View - 2.1 degrees (7.5mm)@ 20X smf 0.4 degrees (1.0mm) @ 400X
- Built-in LED illumination provides bright and sharp viewing and imaging.
- Operating Range & Storage Temperature - 5° to 122 °F (-15° to 50°C)
- Powered by a USB 2.0 Cable from your PC or Laptop
- Very portable - 5" x 13/8" (127mm x 35mm) and weighs just 3 oz. (85 grams).
- Warranty - two year limited
- CE/FCC/RoHS Compliant
- Software Included

Powered by a USB 2.0 Cable from your PC or Laptop

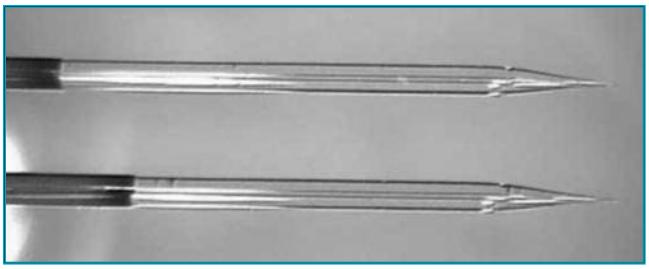
### What are some applications for the HDM?

- Dynamic tuning/monitoring electrospray
- Monitoring MALDI targets
- Forensic work
- Examine circuit boards and welds

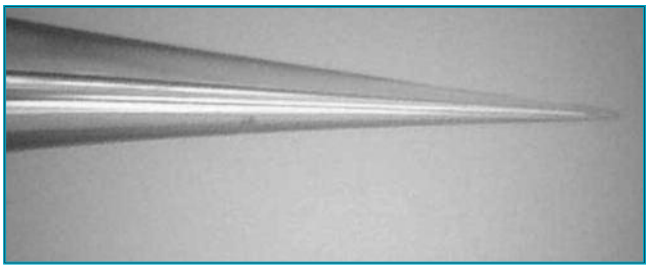
### Computer Requirements

- Operating Systems - Microsoft Windows 98/2000/ME/XP and Vista
  Apple MacIntosh OSX version 10.3 and newer driver can be downloaded from our website. **(www.sisweb.com)**
- CD or DVD Drive
- USB Port Available

***Custom Mounts Available***



**Electrospray Tip - 20x**



**Electrospray Tip - 400x**

| Part No. | Description | Price |
|---|---|---|
| 44300 | Celestron® Handheld Digital Camera | |

# NEW SSIG-17/18 Ionization Gauge

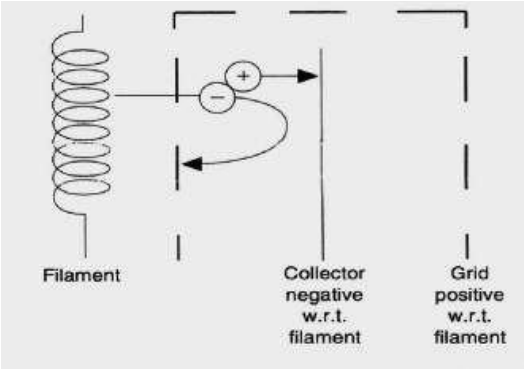
## Specifications

- Bayard Alpert Gauge
- Nude Head
- Conflat® Flange
- Low X-Ray Limit to 3 x 10-11 mbar
- High Reliability
- Long Life
- Robust, Efficient Design
- Twin Filaments: Tungsten or Thoria-coated Iridium
- Bakeable to 400°C

SSIG17 & SSIG-18 are new, improved Bayard Alpert ionization gauges specifically designed for long life and reliability. As well as using high specification materials, the surface area of the grid structure has been reduced, and the collector plus collector shield are of an improved design. Compared to standard BA gauges, these improvements mean that the SSIG-17/18 has a lower x-ray limit that enables pressure measurement down to 3 x 10-11 mbar.

At higher pressure operation (up o 10-2 mbar), the rugged, robust characteristics of the gauge construction ensure a long-life of reliable, repeatable pressure measurement. Whatever the application the very competitive price of the SSIG17/18 ion gauge make it a must for all vacuum systems.

## Principle of Operation



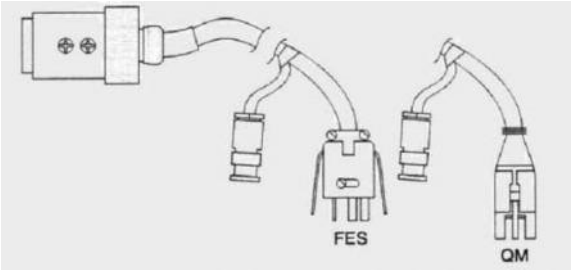

A hot cathode ionization gauge comprises three electrodes: a filament, grid and collector. Electrons are produced from the filament by thermionic emission. A positive potential on the grid attracts the electrons away from the filament, causing them to oscillate through the fine structure many times, until eventually they collide with the grid. Alternatively, the electrons collide with gas molecules producing a positively charged ion, which are collected at a negative electrode (Collector) at the center of the grid structure. The current depends upon the number of ions which is directly proportional to the pressure in the gauge.

## X-Ray Limit

The low pressure limit of the gauge is restricted by the 'x-ray limit'. Electrons hitting the grid produce soft x-rays which in turn produce photoelectron emission ('photoelectric noise') from the collector. Since the measurement electronics cannot distinguish between collecting a positive ion or losing a photoelectron, a theoretical minimum detectable pressure is set. The effect is small and is kept to a minimum by careful design of the gauge.

## Gauge Leads

To connect a SSIG-17/18 ion gauge head to a controller, a lead is required. Bakeable leads are available for both gauges, which means that the gauge can be operated (and pressure monitored) while the system is being baked. Also, the gauge heads can be degassed while the system remains hot.The standard lead is 3 meters long (connections shown below), but any length can be supplied to order.




## Gauge Calibration

Ionization gauges have different sensitivities for different gases and are usually calibrated for nitrogen. Many users accepted the inaccurate pressure measurement for a gas mixture and rely on the long-term reproducibility for the gauge.

For accurate pressure measurements, the gauge head should be calibrated for the type of gas being measured.

The sensitivity of a gauge is defined as:

$$S = \frac{\text{Collector current (A)}}{\text{Grid current (A) x Pressure (mbar)}}$$

| Part No. | Description | Price |
|---|---|---|
| SSIG-17 | Twin Tungsten Ionization Gauge | |
| SSIG-18 | Twin Thoriated Iridium Gauge | |
| SSIG-CABLE | Bakeable Cable | |

# Highlights from the SIS Catalog

## Turbomolecular Pump Repair Kits

Turbomolecular pump repair kits ar available from Eagle Instrument Services. Are you tired of simple bearing replacements causing downtime while you ship your turbo pumps out for repair? Now there is a solution! **Turbo Kits.** Specially designed parts and manuals for easy bearing and seal replacements without the hassle or downtime of sending your pumps out for repair. We work closely with some of the leading manufacturers to ensure that our kits are supplied with the best possible parts.

Each repair kit comes with top grade bearings, seals, O-Rings and where appropriate wicks and felts. The tool kit has the CD Manual, instructions and special tools needed to replace the bearings.

### Turbo Kits*

| Brand | Part No. | Pump Model | Price |
|---|---|---|---|
| Pfeiffer | B050RK | TPH/U-050 | |
| | B060RK | TPH/U-060/062 | |
| | B170RK | TPH/U-170 | |
| | B330RK | TPH/U-330/270 | |
| | B510RK | TPH/U-510 | |
| | B062RK | TPH/U-062 | |
| Leybold | L150RK | TMP-150/151 | |
| | L360RK | TMP-360/361 | |
| | L450RK | TMP-450 | |
| | L600RK | TMP-600 | |
| | L1000RK | TMP-1000 | |
| Varian | V60RK | V60 | |
| | V70RK | V70 | |
| | V250RK | V250 | |
| | V300RK | V300 | |
| | V301RK | V301 | |
| | V550RK | V550 | |
| | V801RK | V801 | |
| Edwards | EXT70 | EXT-70 | |



* Additional Pump Kits are available from SIS.

### Tool Kits

Each tool kit contains all the special tools and standard tools necessary to repair your turbo molecular pump plus a CD and instructions.

| Brand | Part No. | Pump Model | Price |
|---|---|---|---|
| Pfeiffer | EB050TK | TPH/U-050 | |
| | EB060TK | TPH/U-060/062 | |
| | EB170TK | TPH/U-110/170 | |
| | EB330TK | TPH/U-330/510 | |
| | B062TK | TPH/U-062 | |
| Leybold | EL150TK | TMP-150/151 | |
| | EL360TK | TMP-360/361 | |
| | EL450TK | TMP-450 | |
| Varian | EV60TK | V60/70 | |
| | EV250TK | V250 | |
| Edwards | EXT70TK | EXT-70 | |

## ESCAL

### New Calibration Compound for Mass Spectrometers

Scientific Instrument Services introduces a new calibration mixture for electrospray ion sources. This mixture covers a wide mass range from 195 to 1922. It is already in the proper concentration to run directly in an electrospray source without dilution. The mixture consists of caffeine, MRFA (met-arg-phe-ala) peptide, and perfluoroalkylphosphazine.

| Part No. | Description | Price each |
|---|---|---|
| ESCA | 5 ML BTL OF ESCAL | |

**ESCAL Mass Spec Peaks - ESI (+)**

| Exact Mass | Composition |
|---|---|
| 195.08765 | C8H11N4O2 |
| 524.26469 | C23H38N7O5S |
| 1022.00342 | C20H19O6N3P3F28 |
| 1121.99702 | C22H19O6N3P3F32 |
| 1221.99702 | C24H19O6N3P3F36 |
| 1321.98425 | C26H19O6N3P3F40 |
| 1421.97786 | C28H19O6N3P3F44 |
| 1521.97148 | C30H19O6N3P3F48 |
| 1621.96509 | C32H19O6N3P3F52 |
| 1721.95870 | C34H19O6N3P3F56 |
| 1821.95232 | C36H19O6N3P3F60 |
| 1921.94593 | C38H19O6N3P3F64 |

## Ion Transfer Tube for LTQ™, LTQFT, LTQFT Ultra and Orbitrap Mass Spectrometers

This is a direct replacement for the Thermo p/n 97055-20198 ion transfer tube used on the LTQ, LTQFT, LTQFT Ultra, and Orbitrap Mass Spectrometers. The ion transfer tube allows ions from the ESI, APCI, APPI sources to enter the LTQ Linear ion Trap. The LTQ will lose sensitivity over time as contaminates build up inside the tube. It is recommended to replace this guide at least quarterly to insure ultimate instrument sensitivity. Replacement takes only seconds and sensitivity is restored.

| Part No. | Thermo No. | Description | Price |
|---|---|---|---|
| SIS-20198 | 97055-20198 | Ion Transfer Tube | |

# DID YOU KNOW?

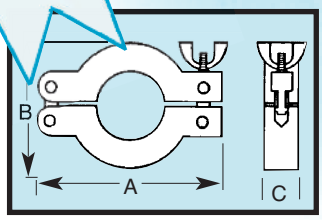
If your company uses VWR or Thermo Fisher Scientific for your supplies, you can still order them from SIS. Just specify the item and reference SIS to your VWR or Thermo Fisher representative. They will order the components through us and you will still be able to benefit from our vast array of quality items.

SALE

SALE

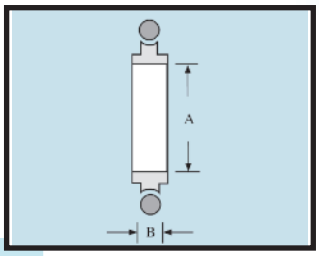
## Special Until 12/31/2008

### Save 20% on the following items



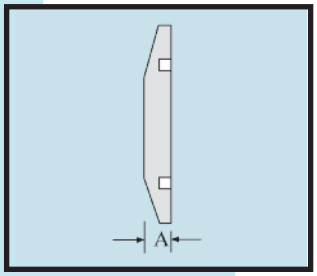

### Clamps

| Part No. | Tube Size | A | B | C | NW Flange Size | List Price | Sale Price |
|---|---|---|---|---|---|---|---|
| QF16-075-CW | .5" & .75" | 2.45" | 1.67" | .65" | 16 | | |
| QF25-100-CW | 1" | 2.86" | 2.16" | .65" | 25 | | |
| QF40-150-CW | 1.5" | 3.53" | 2.73" | .65" | 40 | | |
| QF50-200-CW | 2" | 4.80" | 3.70" | .65" | 50 | | |




### Centering Rings

| Part No. | A | B | NW Flange Size | List Price | Sale Price |
|---|---|---|---|---|---|
| QF10-050-ARV | .39" | .21" | 10 | | |
| QF16-075-ARV | .63" | .21" | 16 | | |
| QF25-100-ARV | .98" | .21" | 25 | | |
| QF40-150-ARV | 1 .53" | .21" | 40 | | |
| QF50-200-ARV | 1.97" | .21" | 50 | | |




### Blank Flanges

| Part No. | A | NW Flange | List Price | Sale Price |
|---|---|---|---|---|
| QF10-050-AB | .20" | 10 | | |
| QF16-075-AB | .20" | 16 | | |
| QF25-100-AB | .20" | 25 | | |
| QF40-150-AB | .20" | 40 | | |
| QF50-200-AB | .20" | 50 | | |

Scientific Instrument Services
1027 Old York Rd.
Ringoes, NJ 08551

**RETURN POSTAGE GUARANTEED**

**INSERT INDICIA**