Thermo Scientific ITQ™ Series Quadrupole Ion Trap GC/MS^n

Optimized for Real-World Sample Analysis

Dependable performance in ion trap technology

Unmatched sensitivity in full-scan operation

Advance to the power of MS^n for incredible selectivity in the dirtiest of matrices

External source for maximum productivity, reliability, and classical, library searchable spectra

True Choice and Valuable Investment Protection Options

Thermo Scientific ITQ Series Quadrupole Ion Traps

The most sensitive ion trap mass spectrometers available today

The Thermo Scientific ITQ Series of external ionization ion trap mass spectrometers is the latest generation in our industry-recognized legacy of ion trap instrumentation – GC/MS^n. For unmatched results, day in and day out – whether it's in an environmental lab monitoring the water quality near industrial facilities, a state forensic laboratory tracking clues in a criminal investigation, or a food safety laboratory striving to protect food supplies in a global economy, the ITQ Series fits your laboratory's needs.

- Significantly less chemical background for enhanced detectivity with the proven high temperature ion source
- Precision quantitation day after day with electronic flow control of CI reagent gas
- Maximum up-time with simple ion volume change for rapid routine maintenance
- Superior manufacturing quality control
- Computer independence and networking with Ethernet communication
- Exceptional MS/MS performance with automatic waveform optimization for more efficient ion storage
- Tuning for USEPA-regulated methods and selection of standard libraries for searching and identification
- Versatile analysis modes including simultaneous full-scan MS and MS/MS, MS^n, PPINICI, and Data Dependent scanning

The ITQ Series of GC/MS^n instruments offers your laboratory choices that allow you to match the GC/MS system you select to your lab's needs.

- **The Thermo Scientific ITQ 700™:** The ideal selection for routine, full-scan GC/MS analyses for the laboratory with space and budget limitations.
- **The Thermo Scientific ITQ 900™:** Tap into expanded GC flexibility for versatile injection and detection choices.
- **The Thermo Scientific ITQ 1100™:** The ultimate choice for applications from research to routine, with powerful new tools that expand your lab's capabilities.

The ITQ Series is designed with the ability to upgrade in mind, protecting your investment by adapting to your lab's changing workflows and needs over time. If your needs change, upgrade your instrument to gain access to new features, greater flexibility, more power. Better yet, regardless of your choice, you will have the most sensitive GC-ion trap mass spectrometer available, giving you lower detection limits, even in matrix.

The ITQ Series offers a range of operating modes, from full-scan MS and MS/MS (MS^n), to positive and negative chemical ionization. Dual modes for sequential full scan and MS/MS or positive ion/negative ion chemical ionization (PPINICI™)* allow you to acquire both types of data in a single injection. Smart Thermo Scientific Data Dependent™ scanning allows you to quickly collect data, confirm the identity of compounds, and further reduce sample cleanup costs. Variable damping gas, an option available exclusively on the Thermo Scientific ITQ Series, further improves GC/MS sensitivity up to 5X or more across a broad range of real-world samples.

** Pulsed Positive Ion/Negative Ion Chemical Ionization*

Unsurpassed External Ionization Ion Trap Technology

Every ITQ system features a unique, high temperature external ionization ion source to effectively handle dirty samples and significantly improve response stability. The enhanced source incorporates an external passive collector and utilizes construction materials that are able to withstand higher operating temperatures. With an upper temperature limit of 300 °C, the ITQ source stays cleaner longer, and hundreds of samples can be analyzed before routine source maintenance is required.

Unmatched Full-Scan Sensitivity for Routine GC/MS Applications

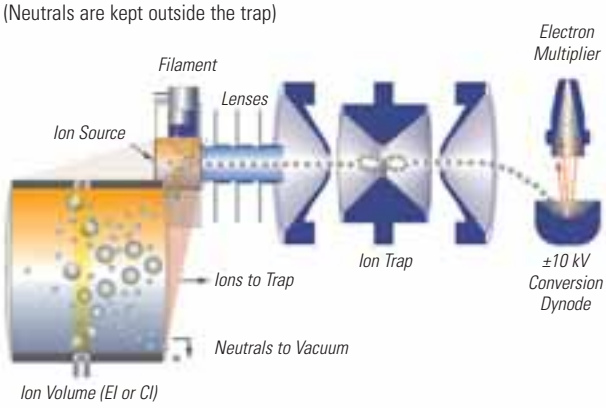
Each ITQ instrument offers the best full-scan electron ionization (EI) sensitivity available today, meaning your laboratory can easily achieve low detection limits, even in matrix. External ionization and advanced tuning algorithms ensure library-searchable mass spectral data that allow for confidence in identification and quantification. Whether it's used for routine environmental analysis, industrial quality control, spectral confirmation, or as a university training instrument, the ITQ Series offers the performance you need for routine methods.

Upgrade to MS^n for Selective Matrix Elimination

Adding the power of mass spectrometry/mass spectrometry (MS^n) to your ITQ system allows your lab to routinely test for compounds that cannot typically be detected with other GC/MS techniques. MS^n provides the ultimate in selectivity for target analytes, eliminating false positives and false negatives. This powerful tool comes standard on the ITQ 1100 system, and is an available option for the ITQ 700 and ITQ 900 instruments. MS^n is applicable to most compounds, and is as simple to use as selected ion monitoring (SIM). The superb selectivity allows detection and quantitation at sub-picogram levels for target analytes in matrices such as plant and animal tissues, soils and sludge, biological fluids, and milk.

- Unequalled performance in difficult matrices
- Setup as simple as selected ion monitoring
- Far higher degree of confidence – eliminates false positives and false negatives

External Ionization
(Neutrals are kept outside the trap)



The external ionization design keeps matrix compounds and neutrals from interfering with the ions of interest.

Where Innovation Meets Productivity and Performance

Innovative Technology Powers the ITQ Series, and Your Productivity

The right system, for right now and into the future

Wider Dynamic Range

Quantitative performance is a vitally important aspect of any GC/MS system. Our engineers have taken the strength of our system and made it even better. Improvements to the algorithms used to trap ions have enhanced linear dynamic range and spectral quality. The quantitation and spectral consistency range extends from femtograms (fg) up to nanograms (ng) and beyond.

Exchange Ion Volumes in Minutes

Removable ion volumes provide added versatility and convenience for all types of analysis. For example, you can easily switch from GC/MS to probe analysis in under three minutes. With the vacuum interlock option, you can exchange the ion volume without breaking vacuum. This allows you to quickly replace a dirty ion volume with a clean one or change to an ion volume optimized for electron ionization (EI), chemical ionization (CI), or the combined EI/CI ion volume, depending on your application. With the versatile EI/CI volume, use digital CI with Data Dependent acquisition to obtain the molecular ion, the MS/MS spectra, and the EI library-searchable spectra – in one injection. Now that's a way to increase your sample throughput – fast!

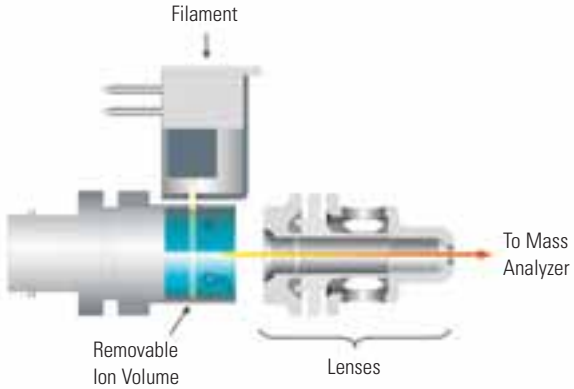
Removable ion volumes allow quick switching from one technique to another, as well as easy changeover to solids probe analysis.

Easy Positive and Negative Chemical Ionization

The reagent gas pressure inside the ion source determines the quantitative reproducibility. These variations are minimized in ITQ systems equipped with chemical ionization (CI) by incorporating electronic flow control of the reagent gas. The method software controls this flow so that any time the data system activates the analytical method, a precise flow of the CI reagent gas is delivered to the mass spectrometer. Calibration curves are stable from day to day and quantitative precision is improved. Positive and negative chemical ionization are easy to set up, and a wide variety of reagent gases are supported through the software. In addition, proprietary Pulsed Positive Ion Negative Ion Chemical Ionization (PPINICI) allows for the acquisition of both positive and negative chemical ionization data in a single injection.

- Digital electronic flow control of reagent gas
- Improved quantitative accuracy and precision
- Reproducible ion ratios

CI in the External Source



ITQ Series Features

- External ionization ion source – standard across the ITQ Series
- Wide spectral/quantitative dynamic range
- Full-scan EI mode for identifying unknowns – library search information
- Removable ion volumes
- ± 10 kV conversion dynode
- Powerful Xcalibur data system

Analytical Versatility

- Three mass range options – match MS capabilities to your analytical needs
- MS^n mode (n≤5) for targeting difficult compounds
- PCI for molecular weight confirmation
- NCI (ECD-MS) for ultimate sensitivity and selectivity
- Simultaneous full-scan MS and MS/MS in a single analysis
- Variable damping gas option for enhanced sensitivity
- PPINICI – hardware/software option with alternating PCI/NCI scans
- Data Dependent scanning option for advanced spectral pattern recognition

Expanded Capabilities

- Vacuum interlock
- Liquid and headspace autosamplers
- DEP/DIP solids probes
- High-capacity, 250 L/s turbopump system
- Two positions available for traditional GC detectors
- Turn-key applications packages

New Advances in Ion Trap Performance and Ease of Use

Easily optimize and improve your MS^n experiments

Continuing with our legacy of innovation, the ITQ Series comes with two new advances in technology, designed to improve data quality and system ease of use. Now, the advantages of MS/MS are more readily achieved.

Automated Collision Energy

For the ITQ, we have introduced new patent-pending Automated Collision Energy (ACE), which greatly simplifies MS^n optimization, making this powerful tool easier and more routine. Determining the collision energy setting required to ensure maximal product ion generation typically means performing a number of separate experiments using different collision energy settings. The results of these experiments would then have to be manually evaluated to determine which setting resulted in the greatest product ion intensities. Any changes – such as to damping gas settings to get more sensitivity – requires a repeat of the process. Plus, the more compounds, the more complex and time-consuming the determination becomes.

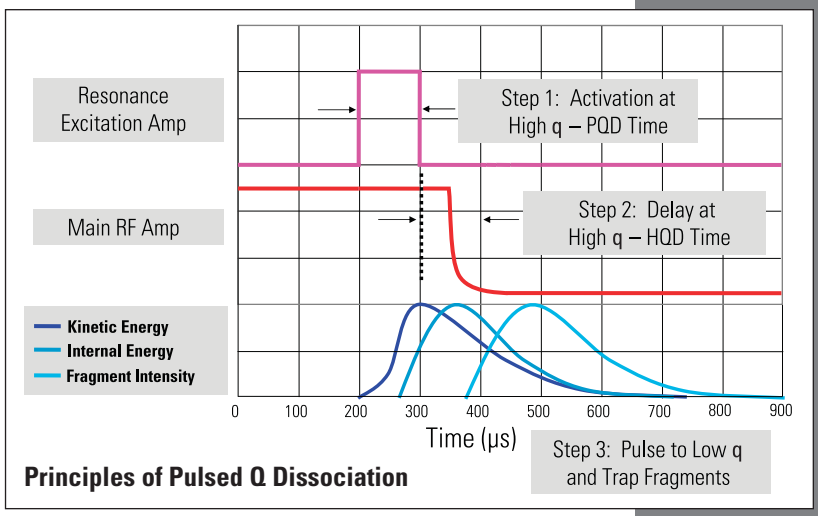
ACE automatically calculates an estimated optimal collision energy based on the operating parameters of the scan. Because of differences in the ease of which ions are fragmented, this calculation is an estimated value. ACE runs three energies in a single scan to ensure optimal fragmentation and product ion production. The optimal energy no longer needs to be determined – ACE covers all of the bases every time you run MS^n. If you want to run at a fixed collision energy, the estimated optimal collision energy calculated by ACE gives you a good starting point.

- Three collision energies in each scan – the estimated optimal plus a lower and higher value
- Easily apply the power of MS^n for routine use
- Simplified starting point for manual methods

Advanced Pulsed Q Dissociation Mode – For Enhanced MS/MS Quality

Our engineers originally developed the patented PQD technique for use in our line of liquid chromatography-linear trap mass spectrometers. Now, for the first time, this advanced technology is available on the ITQ 1100 GC/MS^n system. PQD is used to generate spectral data that are qualitatively similar to data produced using standard collision induced dissociation (CID). The key difference is that PQD increases the overall spectral quality, particularly in low mass range, which lets you see low *m/z* fragments that are usually excluded from CID spectra. PQD also helps you access higher energy dissociation channels. PQD is a novel fragmentation mechanism that involves precursor ion activation at high q, a time delay to allow the precursor to fragment, then a rapid pulse to low q where all fragment ions are trapped. The product ions can then be scanned out of the ion trap and detected.

- Generate information-rich mass spectral data, even in the low mass range
- Eliminates low-mass cutoff
- Produces precise, reproducible fragmentation



Principles of Pulsed Q Dissociation

ITQ 700 and ITQ 900 –
Exceptional GC/MS Value and Performance

Thermo Scientific ITQ 700 GC/MS

The ideal choice for small budgets, tight spaces

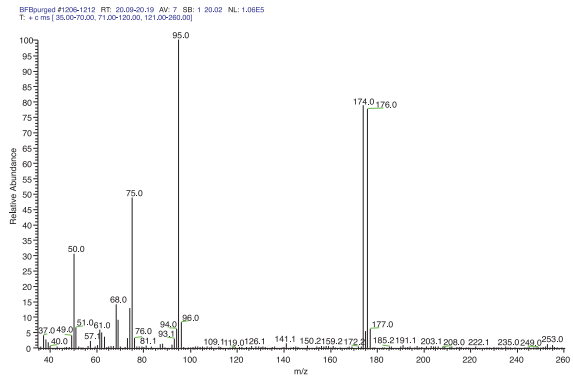
The Thermo Scientific ITQ 700 is fully automated and designed for the analyst who performs routine, high volume GC/MS applications. The optimized external ion source design meets all standard tuning requirements and allows quantitation of samples from the low picogram to the mid-nanogram range. Whether it's used for routine environmental analysis, industrial quality control, spectral confirmation, or as a university training instrument, the ITQ 700 fulfills your lab's needs at an attractive entry-level price.

- Value-packed system for any budget
- Superior software from the MS leader
- Enhanced low mass spectral quality

The ITQ 700 was designed for the laboratory seeking a basic GC/MS system for routine full scan quantitation or basic teaching applications. Featuring the sensitivity of full scan ion trap MS with the small footprint of the Thermo Scientific FOCUS GC, this package is perfect for labs with limited space or budgets. A mass range to 700 amu covers most general GC/MS applications including environmental, QA/QC, forensic, and general teaching and instructional settings.

USEPA 524.2 Tune Report
4-Bromofluorobenzene (25 ng in system)

m/z	Ion Abundance Critera	% Relative Abundance	Pass/Fail
50	From 15 to 40% of m/z 95	30.51	PASS
75	From 30 to 80% of m/z 95	48.84	PASS
95	From 100 to 100% of m/z 95	100.00	PASS
96	From 5 to 9% of m/z 95	8.25	PASS
173	From 0 to 2% of m/z 174	0.35	PASS
174	From 50 to 100% of m/z 95	78.76	PASS
175	From 5 to 9% of m/z 174	6.99	PASS
176	From 95 to 101% of m/z 174	98.36	PASS
177	From 5 to 9% of m/z 176	7.99	PASS



Easily meet BFB and DFTPP tune requirements for EPA methods

ITQ 700 Highlights

Standard Features

- External ionization ion source
- Scan range of 10-700 amu
- Most sensitive EI full scan GC/ion trap MS
- Reliable 70 L/s turbomolecular pump
- Powerful Thermo Scientific Xcalibur™ data system – for instrument operation, data analysis and reporting
- FOCUS GC with split/splitless injector port – full-sized GC performance in a compact package

Upgrade Options

- 250 L/s turbomolecular pump
- Vacuum Probe Interlock – for easy source maintenance without venting
- MS^n with ACE and PQD
- Chemical Ionization – expanded analytical capabilities
- Direct sample probe – analyze samples without chromatographic separation and without venting or moving the GC

Added Value Thermo Scientific Software Options

- QuanLab™ Forms, ToxLab™ Forms, and EnviroLab™ Forms – Software that follows your lab's workflows

Thermo Scientific ITQ 900 GC/MS

Enhanced analytical flexibility with added standard features

The Thermo Scientific ITQ 900 combines the power of ion trap mass spectrometry with the flexibility and capability of the technology leading Thermo Scientific TRACE GC Ultra™ gas chromatograph. The system is the perfect choice for those laboratories performing routine full scan GC/MS but who also desire greater analytical flexibility and performance from the gas chromatograph.

The TRACE GC Ultra offers a full range of injector options: standard split/splitless (SSL), a true Cold-on-Column, Programmable Temperature Vaporization (PTV), plus a complement of traditional GC detectors: FID, ECD, PID, FPD, NPD, PDD including tandem version with the ECD. These GC options give the ITQ 900 added versatility, allowing your lab to expand its capabilities.

In addition, the TRACE GC Ultra provides powerful options like Large Volume PTV injection with back-flush, ideal for detecting trace-level components in complex matrices. The ITQ 900 also features a broader mass range, up to 900 amu, allowing it to detect a wider range of compounds. Tap into even more analytical capability with an upgrade to MS^n, chemical ionization and solids probes.

- Analyze a broader range of targets and unknowns with expanded detector and injector options
- Upgradeable MS options for increased versatility
- Best choice for many routine GC/MS methods, with extended capabilities for more challenging applications

ITQ 900 Highlights

Standard Features

- External ionization ion source
- Scan range of 10-900 amu
- Most sensitive EI full scan GC/ion trap MS
- Reliable 70 L/s turbomolecular pump
- Xcalibur data system – for instrument operation, data analysis and reporting
- TRACE GC Ultra – high-performance GC with multiple detector and injector options for powerful separation and detection capabilities

Upgrade Options

- Vacuum Probe Interlock – for easy source maintenance without venting
- Add GC detectors, plus select from a broad range of injection ports
- 250 L/s turbomolecular pump
- MS^n with ACE and PQD
- Chemical Ionization – expanded analytical capabilities
- Direct sample probe – analyze samples without chromatographic separation and without venting or moving the GC

Added Value Thermo Scientific Software Options

- QuanLab Forms, ToxLab Forms, and EnviroLab Forms – Software that follows your lab's workflows

ITQ 1100 –
GC/MS Power and Performance Unleashed

Thermo Scientific ITQ 1100 GC/MS^n

The ultimate performer, for applications from research to routine

The Thermo Scientific ITQ 1100 is the ultimate ion trap-based GC/MS system, perfect for the laboratory seeking the most powerful and flexible GC/MS platform. This system provides an extended mass range – up to 1100 amu – to increase the number of compounds which can be detected and identified. New advanced MS^n functions – Automated Collision Energy (ACE) and our patented Pulsed Q Dissociation Mode (PQD) are standard on the ITQ 1100. The ITQ 1100 comes standard with a full suite of popular options, including the 250 L/s turbomolecular pump, vacuum probe interlock, MS^n, sequential full scan/MS-MS and Data Dependent Scanning. Available options include the direct insertion probe and chemical ionization.

New Advances Offer Enhanced Performance and Ease of Use

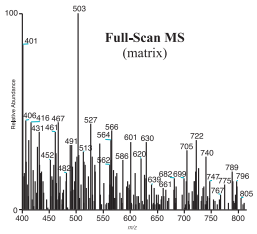
New to the ITQ 1100 system are two advanced modes of operation, each designed to support your lab's needs for advanced benchtop GC/MS capabilities. Automated collision energy (ACE) simplifies the development of MS^n methodologies by automatically determining the proper energy set up for the collision-induced dissociation step. MS/MS experiments are easier to develop, which makes it easier for your lab to apply this powerful technique, even for routine applications. The Thermo Scientific patented Pulsed Q Dissociation Mode (PQD) increases the number of product ions formed during the CID process, yielding greater information for the qualitative MS^n experiment. Both of these advanced functions come with the ITQ 1100 to let your laboratory unlock the true potential of MS/MS, and expand into new markets and application areas.

Restore Performance or Change Modes, Quickly

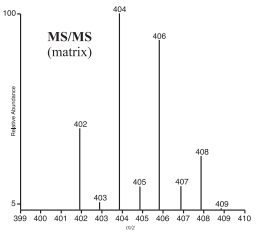
The ITQ 1100 comes standard with a vacuum probe interlock system. This system allows for insertion and removal of the "ion volume" in the source without venting the analyzer. Removable ion volumes provide added versatility and convenience for all types of analysis. With the vacuum interlock option, you can exchange the ion volume without breaking vacuum. Replace dirty ion volumes quickly to restore response factors. With optional chemical ionization, you can switch between EI and CI and back again, without venting the analyzer to make this change. Optimizing data quality for EI and CI work is further enhanced through the use of specially designed ion volumes, each developed to provide optimal performance depending on the ionization mode.

Flame Retardant in Pond Water

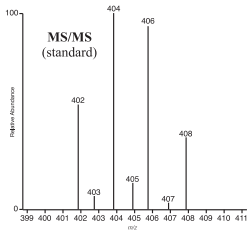
4 ppt 2,2',4,4',6-Pentabromobiphenyl ether in pond water



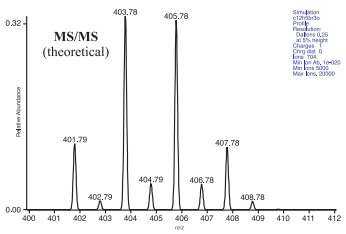
Full-scan spectrum of 4 fg/µL 2,2',4,4',6-PBDE spiked into pond water.



MS/MS product ion of 2,2',4,4',6-PBDE spiked into pond water.



MS/MS product ion of 2,2',4,4',6-PBDE spiked into benzene.

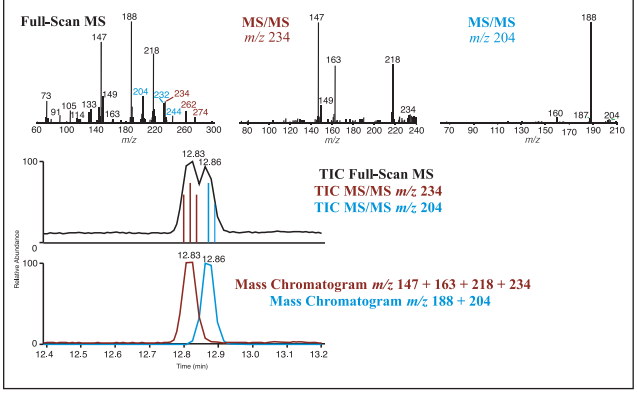


Theoretical product ion cluster of a pentabromodiphenyl ether.

Data Dependent Scanning Facilitates Method Development

Data dependency is a powerful and time-saving tool for dynamic and complex qualitative analyses. Data dependent algorithms probe mass spectra for ions matching given mass selection settings. The list of ions is compiled in an intensity-sorted dependent mass list that is used for MS/MS scans in subsequent events. Data dependency allows MS^n methods to be written without knowing in advance what specific precursor ions may be found during an analysis. Additional data are obtained without spending time running multiple methods. You benefit from library-searchable full-scan MS spectra and additional structural information from the MS^n data.

Methane CI with Data Dependent Scanning



The ion ratio dependence algorithm can be used to locate $[M + H]^+$ ions by the $[M + 29]^+$ and $[M + 41]^+$ methane CI adduct ions. The MS/MS product-ion spectra of $[M + H]^+$ ions reveal the ions necessary to separate co-eluting compounds into separate mass chromatograms.

ITQ 1100 Highlights

Standard Features

- External ionization ion source
- Scan range of 10-1100 amu
- Most sensitive EI full scan GC/ion trap MS
- 250 L/s turbomolecular pump
- MS^n, for MS/MS experiments
- Automated Collision Energy
- Pulsed Q Dissociation Mode
- Vacuum Probe Interlock – for easy source maintenance without venting
- Intelligent Data Dependent Scanning
- Powerful Xcalibur data system – for instrument operation, data analysis and reporting
- TRACE GC Ultra – high-performance GC with multiple detector and injector options for powerful separation and detection capabilities

Upgrade Options

- Chemical Ionization, including PPINICI – expand your analytical capabilities
- Add GC detectors, plus select from a broad range of injection ports

Added Value Software Options

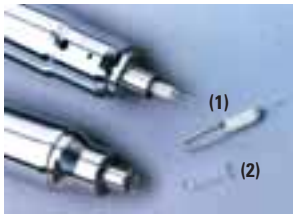
- QuanLab Forms, ToxLab Forms, and EnviroLab Forms – Software that follows your lab's workflows
- Mass Frontier™ – for structural elucidation and fragmentation studies

Advanced Options Boost Performance and Productivity

Solids Probe

Solids probes are most often used for qualitative or semi-quantitative analysis of materials that are difficult, if not impossible to elute chromatographically.

With a GC injection, polar high-molecular weight compounds will often decompose during the volatilization process leaving the analyst with a spectrum containing the desired compound as well as the decomposition products. Our Direct Exposure Probe (DEP) and Direct Insertion Probe (DIP) are especially suited to analysis of thermally labile compounds. Both are controlled by a single, easy-to-use controller.

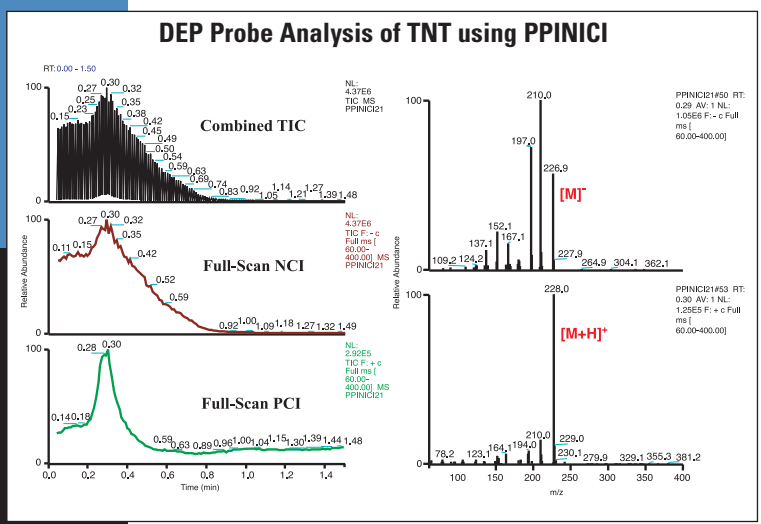


Interchangeable solids probe tips:
(1) Direct Exposure-DEP
(2) Direct Insertion-DIP

ITQ 1100 GC/MS with direct sample probe

Most customers want a simple interface that allows analysis of a solid sample without disturbing the GC setup. With an ITQ system, probe analysis can be performed without disconnecting any part of the gas chromatograph or breaking vacuum.

- Ideal for thermally labile samples
- Convenient, interchangeable probe types



Full-scan Direct Exposure Probe-PPINICI analysis of 2,4,6-TNT

Variable Damping Gas Control

Only the ITQ Series includes a variable damping gas option. This allows you to increase the amount of helium pressure in the ion trap independent of the column carrier gas. The increased helium pressure traps more ions per unit time thereby increasing detectivity, especially in MS^n mode. This option can increase the detected area of compounds 500% or more.

Thermo Scientific TriPlus™ Autosampler – Flexible Sampling Solutions

The TriPlus Autosampler provides unrivaled flexibility in sampling automation, with tremendous productivity for high-throughput labs.

TriPlus Options:

- TriPlus AS for injection of liquid samples
- TriPlus HS for automated headspace sampling
- TriPlus DUO includes both liquid and headspace sampling turrets
- SPME* (Solid Phase Micro Extraction) for quick sample preparation
- Cooled/heated tray option

**Sold under license from Supelco®*

Thermo Scientific AI/AS 3000 Series II Autosampler – Affordable, Powerful Simplicity

The 3000 Series II liquid autosampler combines utmost precision in liquid sampling with simple, self-configuring setup that ensures confident performance in high-throughput and research environments.

AI/AS 3000 Series II Options:

- AI 3000 II Autoinjector – Plug & Inject 8-position modular sampling system
- AS 3000 II Autosampler – 105-position sample tray with integrated control
- AI/AS 3000 II Gemini – Inject into two injection ports on the TRACE GC Ultra simultaneously

Thermo Scientific Xcalibur – A Unified MS Platform

One intuitive platform for GC/MS, LC/MS and Advanced MS instruments provides confident control from method development to reporting

Xcalibur is the the most powerful data system available today, delivering a unique combination of functionality, system control, and ease of use. The software is designed to guide you through your daily analytical tasks. This powerful simplicity combined with the advanced features of the Microsoft® Windows® Operating System and Microsoft Office productivity tools provides an analytical platform second to none.

The ITQ Series generates library-searchable, quality spectra regardless of matrix and concentration. This is a vital asset when dealing with complex unknown samples. Use commercial libraries, NIST, Wiley, Pfleger-Maurer-Weber, or build your own. Xcalibur allows simple exporting of spectra and has powerful editing tools to aid you in quickly generating your own user libraries. Xcalibur also allows you to search multiple libraries simultaneously. Thus, you can easily match your unknown against multiple libraries for confident identification.

Xcalibur provides complete control of the TRACE GC Ultra or FOCUS GC, mass spectrometer and optional liquid and headspace autosamplers. Xcalibur contains a built-in audit trail to ensure compliance with your laboratory's SOP's and Quality programs.

Xcalibur's home page directs you to the six major functions of the program, all from one convenient starting point.

Integrates Layered Applications Including

- Mass Frontier™ – Interpret mass spectral data with tools for fragments, structures, isotope patterns, spectral classification, and more
- EnviroLab Forms – Automated reporting forms package designed for the regulated environmental laboratory
- ToxLab Forms – User-friendly layered application providing automated reports for the toxicological laboratory
- QuanLab Forms – Powerful, general-purpose package for your method development, data analysis and reporting needs