

Packaging - Processing

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**Thermo Scientific DFS High Resolution GC/MS is the highest performance magnetic sector mass spectrometer ever built for target compound analysis.**

**The DFS is as simple and straightforward in operation as your benchtop MS systems.**

## DFS High Resolution GC/MS

High Performance Magnetic Sector GC/MS



- **Lowest LOQs** - The unparalleled high resolution capabilities of the DFS provide the highest specificity for trace and target compound analysis for unambiguous compound identification and deliver superior signal to noise characteristics for reliable peak integration and quantitation.
- **Ease of operation** - The DFS is operated like and feels like a benchtop GC/MS. The automated universal mass calibration is unique and provides the full versatility for all scan modes and ionization techniques.
- **Highest sample throughput** - The DFS offers your lab unattended automatic operation with full method versatility. Two GCs can be optionally installed in parallel for maximum flexibility on column separations. Thermo Scientific TriPlus™ XT Autosampler serves both GCs from common sample trays.

### DFS Mass Spectrometer

The DFS is a high resolution magnetic sector mass spectrometer like none before. Several new technologies have been incorporated in this revolutionary design. All of these combined provide the most powerful high resolution GC/MS ever. The DFS high resolution GC/MS operates under Thermo Scientific Xcalibur™, the premier data system, for complete system control and automated data processing.

## Hardware Specifications

### Ion Source

The ion source has been designed with special emphasis on sensitivity and durability for increased productivity, low maintenance and increased uptime.

- Plug-in ion source with 1 push operation
- Exchange of ion volume and filament without venting by a pneumatically actuated vacuum interlock
- Response optimized EI volume with special filament, optimized box design for quick exchange including built in ion extraction lens for ease of maintenance
- Optimized long lifetime filaments for EI and CI
- Each ionization volume carries its own special filament for the ionization technique
- One ion source for all techniques EI, CI (PCI/NCI)
- GC interface control independent of source temperature

### Reference Inlet

The independent reference compound inlet system is continuously flow adjustable and can be individually evacuated. It allows syringe introduction of liquid or gaseous samples.

### Vacuum Interlock

The DFS is equipped with a vacuum interlock for quick exchange of ionization volumes and filaments without venting.

- Pneumatically actuated
- Faulty operation is virtually eliminated by system control

### Tuning

The DSF enables the reliable, routine use of AUTOTUNE in all ionization modes without restrictions, including slit control and automated resolution setting. All tuning lenses are part of the ion source.

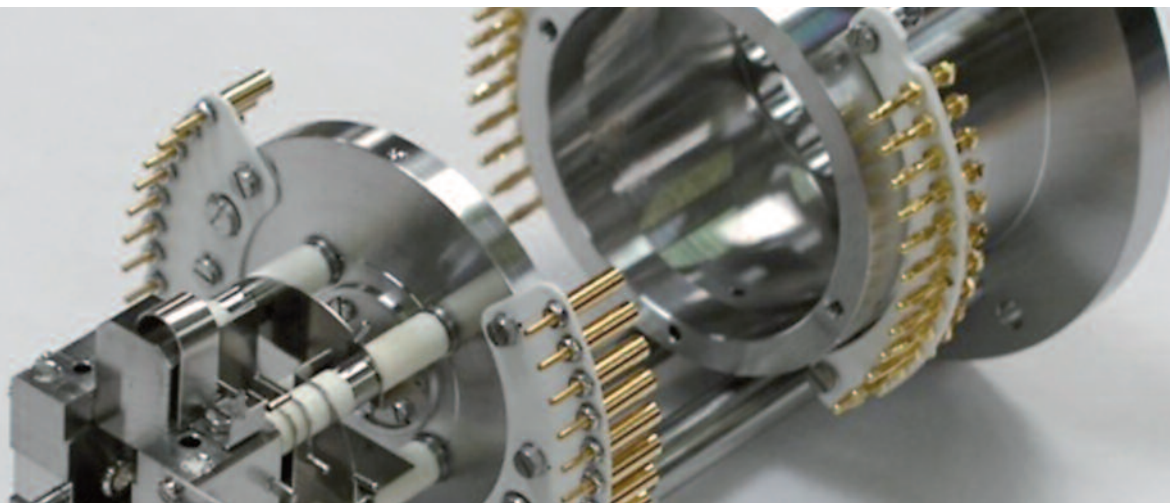
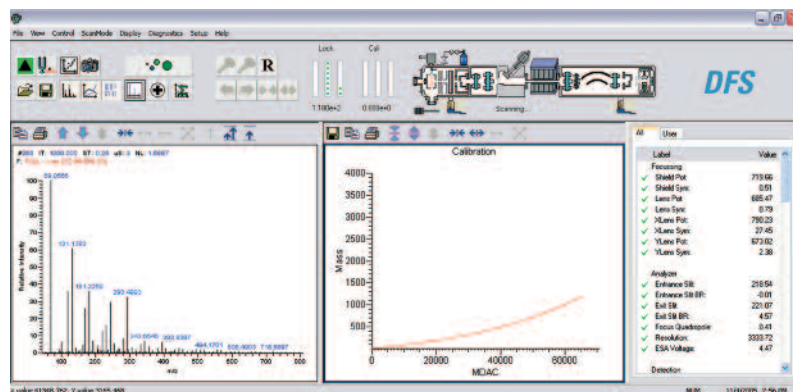
The DFS provides TunePlus™, the renowned user interface for Thermo Scientific ion trap, quadrupole GC/MS and LC/MS instruments. For the first time, a magnetic sector mass spectrometer uses the same concept, making tuning, experiment and sequence set-up intuitive and simple. High resolution MID is an integral part of this user interface.

### Mass Calibration

Thermo Fisher Scientific invented the field calibration method of scanning magnetic mass spectrometers. The DFS offers full data system control of field calibration scanning.

The mass scale needs to be calibrated only once. The operator can change mass range and scan speed without the need for recalibration. It is the same approach and handling as known from benchtop GC/MS systems.

- Constant mass calibration based on magnetic field measurement
- Calibration independent of mass range, scan speed, scan mode (including linked scan MS/MS), ion polarity and ionization technique
- No recalibration required after change of ion volume or ionization technique



## Analyzer

The newly designed DFS analyzer is the first with virtually no image aberrations. It is perfectly double focusing, employing an ultra high precision toroidal electrostatic analyzer and a carefully refined magnetic analyzer. This directly translates into stability and ruggedness.

- Novel ion optics design is based on the proven reverse Nier-Johnson geometry
- Mass independent focus with uniform resolution throughout the mass range
- Ion optics optimized for an acceleration voltage of 5 kV
- All ionization techniques operational with full acceleration voltage
- High precision, data system controlled, continuously variable Tantalum entrance and exit slits for fast response and long lifetime
- Low hysteresis, radially laminated H-type magnet of special metal alloy with mass independent focal length, deflection radius 350 mm, deflection angle 65°
- Innovative Rogowsky magnet entrance pole pieces for optimum sensitivity regardless of ionization method
- Novel electrostatic analyzer (ESA) using a computer optimized toroidal design for highest mass precision and ion transmission with virtually no image errors
- All focusing and detection elements housed in a single monoblock vacuum chamber
- Entire DFS analyzer assembled on an integrated shock mounted platform for isolation from floor vibration

## Performance Characteristics

- Resolution (static) > 60,000 (10% valley)
- Scan rates 0.1 to 10,000 seconds/decade (continuously variable)
- Mass accuracy < 2 ppm
- Sensitivity EI GC/MS  
S/N > 800:1 for 100 fg 2378 TCDD at m/z 322, R = 10,000
- Mass range 2 - 6000 Da;  
2 - 1200 Da at full acc. voltage

## Detection System

The long lifetime secondary electron multiplier of the DFS always provides optimal signal amplification for all ionization modes including negative CI.

- Long lifetime off axis secondary electron multiplier detection system
- Post-acceleration/conversion dynode, variable to  $\pm 20$  kV (Thermo Fisher Scientific patent)
- Quick change mount on an individual flange

## Vacuum System

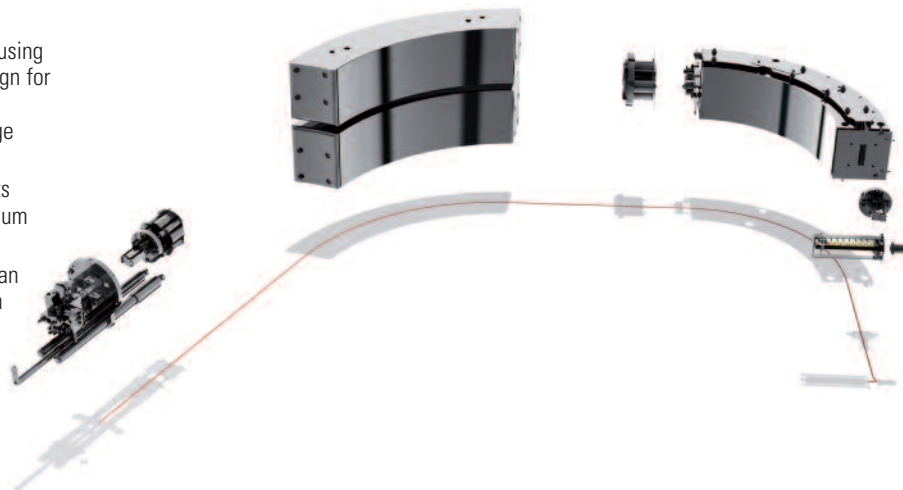
The clean high vacuum background produced by turbomolecular pumps enables the DFS to achieve lower detection limits routinely.

- Directly coupled high speed differential pumping system with three turbo molecular pumps
- Push-button control
- Automated protection system

## Electronics Cabinet

Integrated electronics cabinet for low space requirements. Optimized air flow for efficient cooling of magnet power supply. Effective potential decoupling between digital electronics and mass spectrometer high voltage and power supplies.

- Universal input/output for Ready/Start communication with external devices using programmable signal logic
- Analog in
- Digital in/out



## Direct Inlet Options

### Direct Probe Base Unit (optional)

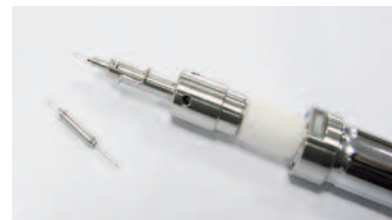
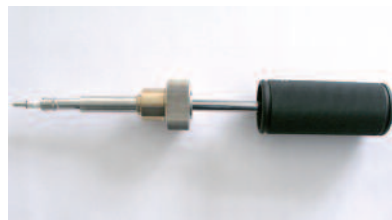
- Port for direct insertion probe
- Required to attach any of the following probe options
- Contains exchange lock and probe electronics

### Water Cooled DI Probe (DI / DIP) (optional)

- Direct insertion probe
- Data system controlled, liquid cooled
- Using disposable aluminum crucibles
- Heating rates: 20 °C to 200 °C in 30 s, 200 °C to 300 °C in 30 s
- Temperature range from 10 °C above ambient
- Maximum temperature 350 °C

### DCI Probe (optional)

- Direct chemical ionization probe
- Full data system control
- Using reusable filaments
- Ultra fast heating rates of > 500 °C/s
- Maximum temperature 1600 °C
- High temperature tip for DCI probe (optional)
- Using reusable quartz crucibles
- Maximum temperature 800 °C



## Software Specifications

### Xcalibur Data System

Xcalibur is the uniform software platform for system control of the Thermo Scientific GC/MS and LC/MS systems.

The DFS comprises the complete Xcalibur instrument control software package for high and low resolution operation, multiple ion detection MID, selection of positive or negative ions, linked scans, peak matching, and full control of analyzer and inlet systems supporting the following capabilities:

- INTENSITY AUTOTUNE independent from resolution
- RESOLUTION AUTOTUNE with computer controlled slit setting
- Control of standard and optional inlet systems
- Xcalibur accurate mass program CMASS for accurate mass conversion and averaging
- Complete Xcalibur application software, incorporating all mass spectrometry processing tasks such as chromatogram and spectrum display, integrated NIST library search, elemental composition and isotopic pattern calculation
- QuanBrowser, the comprehensive quantification package
- Instrument diagnostics
- MS data import and export using the ANDI/netCDF formats, conversion from Finnigan MassLab data file formats, ASCII text export
- Standardized output to LIMS systems

### TargetQuan (optional)

The special Xcalibur DFS software package for automated data evaluation on target compounds including:

- Dioxin method setup
- Support of instrument and quantitation
- Response file and reporting programs
- Data evaluation for isotope dilution methods as well as relative response factors
- Compliant with the published EPA methods for dioxin measurements and data evaluation according e.g. EPA 1613, EPA 8280, EPA 8290, EPA 23, EPA 513, EN 1948 and equivalent JIS methods
- Compliant with the requirement for TEQ low-med-upper bound reporting
- Standardized output to LIMS systems

### Library Options

- NIST Library
- Wiley Library
- Pflieger-Maurer-Weber Library
- Thermo Scientific Pesticide Library

### Software Licenses

The DFS Xcalibur software licenses are supplied for instrument control as well as reprocessing.

New instrument software releases are supplied free of charge within 12 month after delivery.

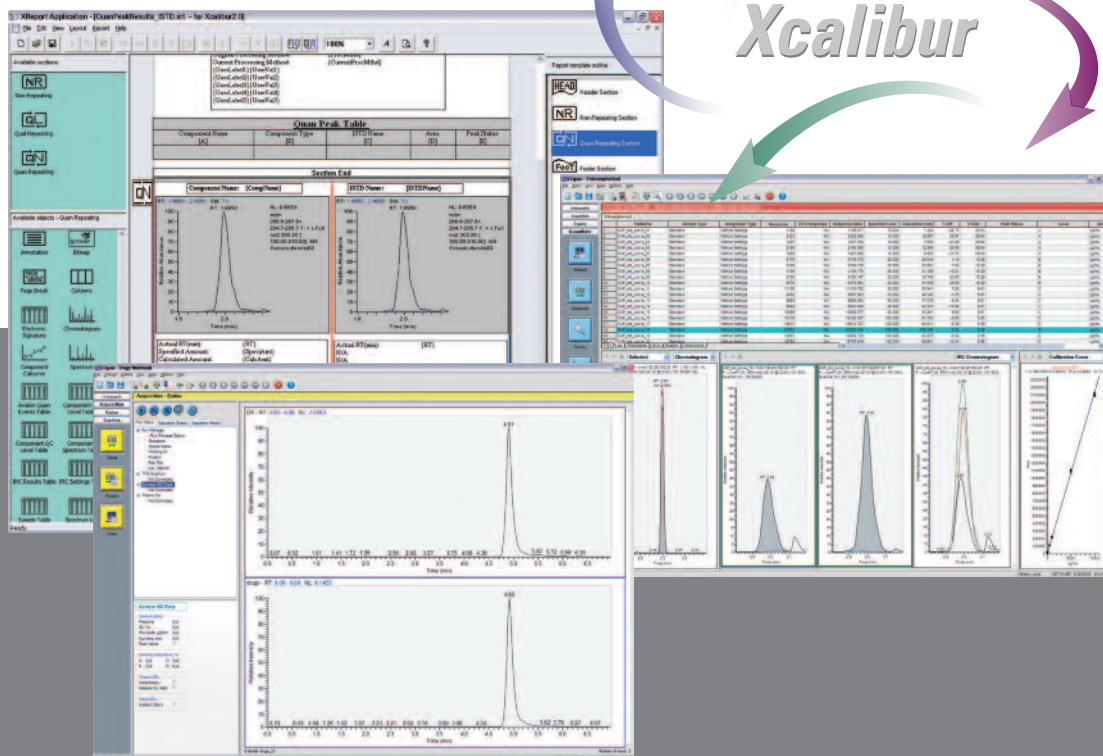
## Data System

Personal Computer in the following minimum configuration\*:

Dell Optiplex™ GX 620 or equivalent

- INTEL® PENTIUM® 4 Processor, 2,8 GHz
- 1024 MB 400 MHz DDR2-SDRAM
- 3,5" Floppy Disk Drive
- 160 GB SATA Hard Disk
- DVD-RW Drive
- DVI-Add in card
- 1 parallel port
- 2 serial ports
- 6 USB 2.0 ports
- Network chip Intel 10/100/1000 MHz on board
- Microsoft® XP professional operating system (English)
- MS Office 2003 small business edition (English)
- High resolution 19" TFT color monitor
- Laser Printer, BW, 1200x1200 dpi, up to 25 pages/min

\* Minimum data system specifications may change without prior notice in case of technological improvement. Call for latest configuration.



## Gas Chromatography Options

### Thermo Scientific TRACE GC Ultra™

The TRACE GC Ultra comprises capabilities like leak check and column characterization, flow and pressure programming, gas saver operation.

An automatic calibration test measures and stores column parameters therefore avoiding the need of entering unknown or unsure column parameters.

The DFS source is connected via a direct coupling GC/MS interface with uniform temperature distribution and precise temperature control up to 350 °C.

GC oven, injector and interface temperatures and valve timing can be controlled and displayed by the Xcalibur data system.

### Column Oven

- Temperature range to 450 °C
- Program rates: 0.1 to 120 °C/min
- Fast cool-down in 250 seconds from 450 °C to 50 °C
- Fast heat-up in 420 seconds 50 °C to 450 °C
- Usable space: 27 x 27 x 17 cm (H x W x D)

### Oven Cryogenic System for liquid CO<sub>2</sub> (optional)

- Permits subambient oven operation down to - 55 °C
- Includes all parts for direct connection to a liquid CO<sub>2</sub> cylinder (not included)

### Oven Cryogenic System for liquid nitrogen (optional)

- Permits subambient oven operation up to - 99 °C
- Includes all mechanical parts to supply liquid nitrogen into the oven and solenoid valve ending with a 1/4" Swagelok nut. (liquid nitrogen reservoir not included)

### Digital Pressure/Flow Control

- Integrated pressure and mass flow controller
- Built-in capability to measure true column resistance
- Pressure regulation range from 10 to 1000 kPa (145 psi) in steps of 1 kPa (0,1 psi)
- Up to three pressure/flow programming ramps
- Compensation for ambient variation of pressure and temperature
- Column flow regulation from 0.1 mL/min to 100 mL/min in 0.1 mL/min increments

### Capillary Injectors

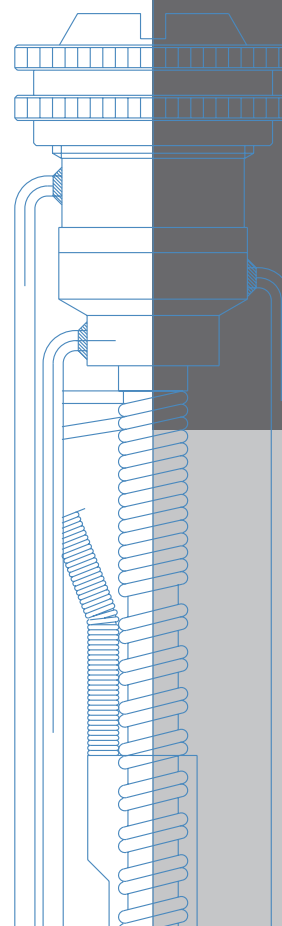
All split/splitless and PTV™ injectors are compatible with TriPlus Autosampler and include:

- A high precision mass flow controller for split from 10 to 500 mL/min
- A fixed calibrated flow regulator in the purge line at 5 mL/min
- The carrier gas saver feature programmable in time

### Optimized Geometry Split/Splitless injector (standard 1st injector)

This new geometry with optimized thermal profile for either split or splitless injection virtually eliminates discrimination for heavy compounds and ensures wide linearity. Temperature settings from 50 °C to 400 °C in 1 °C increments.

Large volume injection capability up to 50 µL, available on a standard TRACE GC Ultra SSL injector, greatly extends sensitivity of conventional methods in a simple and effective fashion.



**B.E.S.T. PTV Injector (optional 2nd injector)**

This injector features very low thermal mass components and can therefore achieve very fast heating and cooling rates for a virtually discrimination free sample transfer in any situation, even when high boiling samples are involved.

- Maximum temperature of 400 °C
- Heating rate up to 14.5 °C/s (870 °C/min)
- 3 temperature programmable ramps with 4 plateaus
- 3 pressure/flow programmable ramps with 4 plateaus
- Air-cooled down to few degrees above ambient temperature

**Large Volume B.E.S.T. PTV injector (optional 2nd injector)**

This injector preserves the capabilities of the standard PTV injector but with the facility to accept large volume sample injection.

- Up to 80 µL can be injected “at once” by slow, programmable injection depending of syringe volume
- Includes a two way heated solvent split valve, a 50 mm long needle syringe for large volume injections (250 µL capacity) and a pre-packed, deactivated silcosteel liner in the standard outfit

**Cold On-Column Injector for TriPlus Automated Operation (optional 2nd injector)**

This injector allows the liquid sample to be introduced directly into the capillary column inside the oven in a zone under oven temperature control. The injector can be fully automated only by the TriPlus Autosampler throughout a special lever actuated by a dedicated motor.

**Liquid CO<sub>2</sub> Cooling for PTV Injector (optional)**

This option permits the BEST PTV injector to be programmed down to - 30 °C and should be used when very volatile samples are introduced through the PTV. Included are all parts for direct connection to a liquid CO<sub>2</sub> cylinder (not included).

**Liquid nitrogen cooling for PTV injector (optional)**

This option permits the BEST PTV injector to be programmed down to - 50 °C and should be used when very volatile samples are introduced through the PTV. It includes all mechanical parts and solenoid valve to supply liquid nitrogen into the injector (liquid nitrogen reservoir not included).

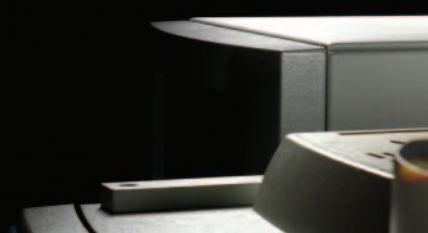
**Autosampler Options**

**TriPlus Liquid Autosampler (optional)**

The TriPlus liquid autosampler for GC sample injection is fully controlled by the Xcalibur software, is used for single sample analysis as well as batch measurements for unprecedented workload capacity.

The special DFS autosampler version TriPlus XT can be serving autonomously two TRACE GC Ultra systems serving a maximum of three injectors in parallel.

- Can be combined with any injector and parameter settings (SSL, PTV, On-column)
- Multiple types of injection techniques including large sample volume introduction (up to 450 µL)
- Syringe recognition with a snap-on connection for fast and safe replacement. Uses standard 10 µL syringes
- Injection volumes can be finely selected in steps of 0.1 µL
- Combined solvent cleaning capability allows any possible 4-solvent combination sequence to be programmed
- Standard sample tray for 150 vial positions
- Up to two sample trays for a maximum capacity of 300 vials (1, 2, 2.5 mL optional)
- Liquid and headspace sampling tray types can be combined
- Manual injections without disconnecting the unit from the GC
- Cooled / Heated tray option for the handling of very volatile solvents and very viscous samples at ambient temperature, programmable temperature range for each tray is from 4 to 70 °C



### TriPlus Headspace Injection (optional)

The TriPlus headspace option adds automated headspace analysis capability for the TriPlus liquid autosampler:

- Exchangeable syringe sizes: 1, 2.5, 5 mL, gas-tight, side hole
- Injection volumes: 0.1 – 5 mL
- Syringe temperature range: 40 – 150 °C
- Inert gas flushing on barrel hole prevents cross contamination
- Incubation oven capacity: 6 vials
- Incubation oven temperature range: ambient or 40 °C – 150 °C, 1 °C resolution (electrically heated)
- Agitation by mechanical shaking within 0 – 600 seconds



### TriPlus Bar Code Reader (optional)

The TriPlus bar code reader option implements a rotating bar code reader including:

- Bar code reader for automatic sample identification, suitable for 2, 2.5, 10, and 20 mL vials
- 2 mL screw-top vials (set of 10)
- Magnetic caps suitable for 2 mL vials complete with 9 mm caps and septa (set of 10)

The system allows random orientation of the vials with its capability to automatically rotate the vial reading position. Also available as upgrade kit.



### Additional Primary Tray 1-150 (optional)

The additional primary sample tray option includes:

- 1 tray holder
- 1 sample tray with 1 – 150 position labeling; suitable for 1, 2, 2.5 mL vials
- 150 x 2 mL vials, screw caps and septa

Also available as upgrade kit.

### Secondary Tray 151-300 (optional)

The additional secondary sample tray option includes:

- 1 tray holder
- 1 sample tray suitable for 1, 2, 2.5 mL vials
- 150 x 2 mL vials, screw caps and septa

Also available as upgrade kit.

### Standard Washing Station, 5 x 10 mL

This option allows multiple solvent rinsing (up to 4 different solvents within the same cleaning phase), to entirely eliminate any cross contamination effect. A waste vial with drain tube is also available as an option. This option includes:

- Solvent vials holder
- 5 x 10 mL solvent vials, with snap caps and teflon faced septa

Also available as upgrade kit.

### Washing Station 2 x 100 mL (optional)

This option for the TriPlus liquid autosampler allows reducing the frequency of solvent bottles re-filling, and enhancing the waste volume handling through a drain tube.

This option includes:

- 100 mL bottles holder
- 2 x 100 mL solvent bottles
- 1 x 10 mL waste vial provided with a drain tube
- Snap caps with Teflon faced septa (set of 5) for solvent bottles, suitable for low boiling point solvents
- Aluminum crimp-top caps with ring shaped silicon septa (set of 5) for solvent bottles, suitable for medium and high boiling point solvents

Also available as upgrade kit.



## Installation Requirements\*

### Recirculating Water Chiller

The DFS package includes the Merlin M33PD2 type recirculating chiller for stable and precise cooling of magnet and turbo molecular pumps. The cooler is controlled by a temperature sensor mounted on the DFS magnet.

- Precise temperature control and temperature stability of up to  $\pm 0.1$  °C
- Adjustable high and low temperature safeties with audible alarm
- Environmentally-friendly CFC-free air-cooled refrigeration system

## Supplies

### Power

The DFS is designed to operate at a nominal voltage of 230 V AC, 50/60 Hz. The minimum and maximum voltage tolerances are in compliance with IEC 950, Amend 2, 1993. Approximate consumption values for regular operation are:

- 0,9 kW for GC operation
- 1,9 kW for MS operation
- 1,6 kW for chiller

The maximum possible power consumption of the DFS is about 12 kW, including data system, GC(s), and water chiller.

### Helium

For GC carrier gas: 99.996%, ultra-high purity. Total hydrocarbons should be less than 2.0 ppm.

### Compressed Air

Compressed air with a pressure of 6 bar (87 psi) is required to operate the pneumatic valves of the instrument. A suitable compressor can be ordered from Thermo Fisher Scientific (Part No. 026 1850).

## Space Requirement

### DFS Mass Spectrometer

- HxD 140.6 cm (55.4") x 156.8 cm (62.5")
- Width with one GC installed 161.1 cm (63.5")
- Width with two GCs installed 209.1 cm (82.4")
- MS console with analyzer and magnet 900 kg (2000 lb)
- Data system 130 kg (< 290 lb)
- GC with console 60 kg (130 lb)
- Recirculating cooler Merlin M33 PD2 54 kg (120 lb)

### TRACE GC Ultra

- HxDxW: 44.4 cm x 64.8 mm x 61.0 cm
- Weight: 60 kg (130 lb)

### TriPlus AS/HS Autosampler

Overall dimensions on the GC:

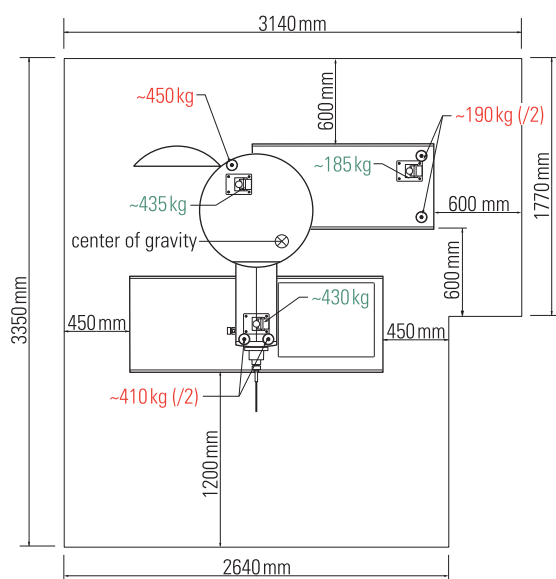
- Length (X axis) 87 cm  
The extended X model length is 122 cm
- Width (Y axis) 77 cm  
(20 cm of which are protruding the rear)
- Turret height (Z axis) 50 cm
- Height approx. 68 cm

**CPU:** 42 x 18 x 44.5 cm (16.5 x 7 x 17")

**Monitor:** 42 x 40 x 43 cm (16.5 x 16 x 17")

**Keyboard:** 2.5 x 47 x 18 cm (1 x 18 x 7")

## Recommended Instrument Clearances and Weight Distribution



## Environment

### Room Temperature

Laboratory room temperature must be maintained between 15 °C and 26 °C (59 and 79 F). The optimum operation temperature is between 18 °C and 21 °C (65 and 70 F).

### Air Conditioning Load

The average power dissipation during analysis operation for a basic DFS system, including gas chromatograph and data system, is approximately 4.7 kW (4.5 BTU/s). For dual GC configuration, the average air conditioning load amounts approximately to 4.9 kW (4.7 BTU/s).

### Humidity

The relative humidity of the operating environment must be between 30 and 70%, with no condensation.

\*Detailed installation requirements are provided in the DFS Preinstallation Requirements Guide PN/1194630

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