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Report by the Analytical Methods Committee

Evaluation of analytical instrumentation. Part XV. Instrumentation for gas chromatography-ion-trap mass spectrometry

Analytical Methods Committee†

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The Analytical Methods Committee has received and approved the following report from the Instrument Criteria Sub-Committee.

Introduction

This report was compiled by the above Sub-Committee of the AMC which consisted of Professor S Greenfield (Chairman), Dr M Barnard, Dr C Burgess, Professor S J Hill, Dr K E Jarvis, Dr M Sargent and Mr D C M Squirrell with Mr C A Watson as Honorary Secretary. The initial input of the features for consideration and the reasons for their consideration was undertaken by a working party Chaired by Dr M Sargent with Dr A Edge, Dr G O'Connor and Dr K S Webb, to whom the committee express their thanks.

The purchase of analytical instrumentation is an important function of many laboratory managers, who may be called upon to choose between a wide variety of competing systems which are not always easily comparable. The objectives of the Instrumental Criteria Sub-Committee are to tabulate a number of features of analytical instruments which should be considered when making a comparison between various systems. As is explained below, it is then possible to score these features in a rational manner, which allows a scientific comparison to be made between instruments and as an aid to equipment qualification.

The overall object is to assist purchasers in obtaining the best instrument for their analytical requirements. It is hoped that this evaluation will, to some extent, also help manufacturers to supply the instrument best suited to their customer's needs. It is perhaps pertinent to note that a number of teachers have found the reports of use as teaching aids.

No attempt has been made to lay down a specification. In fact, the Committee considers that it would be invidious to do so: rather it has tried to encourage the purchasers to make up their own minds as to the importance of the various features of the equipment that is on offer by the manufacturers.

The XVth report of the Sub-Committee deals with gas chromatography-ion-trap mass spectrometry (GC-ion-trap MS)

Notes on the use of this document

Column 1. The features of interest
Column 2. What the feature is and how it can be evaluated.
Column 3. The Sub-Committee has indicated the relative importance of each feature and expects the users to decide on a weighting factor according to their own application.
Column 4. Here the Sub-Committee has given reasons for its opinion as to the importance of each feature.
Column 5. It is suggested that scores are given for each feature of each instrument and that these scores are modified by the weighting factor and sub-totals obtained. The addition of the sub-totals will give the final score for each instrument.

Notes on scoring

1. (PS) Proportional scoring. It will be assumed, unless otherwise stated, that the scoring of features will be by proportion, *e.g.*, Worst/0 to Best/100.

2. (WF) Weighting factor. This will depend on individual requirements. An indication of the Sub-Committee's opinion of the relative importance of each feature will be indicated as follows: VI (very important), I (important) and NVI (not very important). A scale is chosen for the weighting factor which allows the user to discriminate according to needs, *e.g.*, ×1 to ×3 or ×1 to ×10. The factor could amount to the total exclusion of the instrument.

3. (ST) Sub-total. This is obtained by multiplying PS by WF.

This report deals with bench-top ion-trap detector mass spectrometers used with gas chromatography. It does not address the purchase of traditional magnetic sector mass spectrometers nor quadrupole mass spectrometers. Even so, there is a wide selection of ion-trap MS equipment on the market and considerable variability in both the design and the operating characteristics. In addition, the instrumentation is essentially a hybrid, offering scope for varying the gas chromatographic facilities coupled to a specific design of mass spectrometer. Selection of a suitable instrument for purchase is, therefore, not an easy task and the purpose of these notes is to provide some guidance to areas which should be considered so that the choice is based on a full consideration of the available options. However, the performance of any gas-chromatographic method depends primarily on the separation conditions and thus on the nature of the column material, stationary phase and carrier gas and whether a packed or open-tubular column is used. The mass spectrometer detection systems range in complexity and as a result price. A number of alternative instruments may thus be suitable.

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The first task in the selection of an instrument is to examine the range of analyses that it will be expected to perform. Care should be taken not to specify these requirements too closely as uses change with time. The analytical scientist should also not try to envisage every potential application or the selection criteria may become too detailed.

With these requirements in mind, the user should then evaluate the instruments available on the market while bearing in mind the guidelines and any financial limitations. In many instances it will quickly become clear that a number of different instruments could be satisfactory and non-instrumental criteria may then be important. However, in some specialised cases only one or two instruments will have the ability or necessary features to carry out the analysis.

The guidelines are intended to be used as a check list of features to be considered, mostly of the instrument itself, but some also of its service requirements and of the relationship of the user with the manufacturer. Their relative importance will depend on the installation requirements of the instrument as well as the uses to which it will be put. Therefore, to some extent, the selection process will inevitably be subjective, but if all the points have been considered it should be an informed choice.

The Committee consider that, in general, GC-ion-trap mass spectrometers are safe in normal use, but care should be taken when handling flammable and/or high pressure gases. In addition, a high voltage may be present on some parts of the mass spectrometer and detector.

Finally, as many laboratories are now working to established quality standards, some consideration should be given to third party certification of the manufacturer to quality standards such as the ISO 9000 series. Such certification should extend to the service organisation.

The Analytical Methods Committee have published the following reports in the series:

Evaluation of analytical instrumentation

Part I Atomic-absorption Spectrophotometers, Primarily for use with Flames, *Anal. Proc.*, 1984, **21**, 45. Revised in *Analyst*, 1998, **123**, 1407.

Part II Atomic-absorption Spectrophotometers, Primarily for use with Electrothermal Atomisers, *Anal. Proc.*, 1985, **22**, 128. Revised in *Analyst*, 1998, **123**, 1415.

Part III Polychromators for use in Emission Spectrometry with ICP Sources, *Anal. Proc.*, 1986, **23**, 109.

Part IV Monochromators for use in Emission Spectrometry with ICP Sources, *Anal. Proc.*, 1987, **24**, 3.

Part V Inductively Coupled Plasma Sources for use in Emission Spectrometry, *Anal. Proc.*, 1987, **24**, 266.

Part VI Wavelength Dispersive X-ray Spectrometers, *Anal. Proc.*, 1990, **27**, 324.

Part VII Energy Dispersive X-ray Spectrometers, *Anal. Proc.*, 1991, **28**, 312.

Part VIII Instrumentation for Gas–Liquid Chromatography, *Anal. Proc.*, 1993, **30**, 296.

Part IX Instrumentation for High Performance Liquid Chromatography, *Analyst*, 1997, **122**, 387.

Part X Inductively Coupled Plasma-Mass Spectrometers, *Analyst*, 1997, **122**, 393.

Part XI Instrumentation for Molecular Fluorescence Spectrometry, *Analyst*, 1998, **123**, 1649.

Part XII Instrumentation for Capillary Electrophoresis, *Analyst*, 2000, **125**, 361

Part XIII Instrumentation for UV-VIS-NIR Spectrometry, *Analyst*, 2000, **125**, 367

Part XIV Instrumentation for Fourier Transform Infrared Spectrometry, *Analyst*, 2000 **125**, 375

Instrumental criteria sub-committee instrument evaluation form

Type of instrument: GC-ion-trap mass spectrometer								
Manufacturer:								
Model No:								
Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
Non-instrumental criteria *Selection of manufacturer*								
(*a*) Previous instruments	Laboratories in possession of other GC-MS systems should score highest for the manufacturer with the best past record based on the following sub-features:							
(*i*) Innovation	Company's record for developing instruments with innovative features.	I	The manufacturer should be alert to developments in technology and chromatography.	PS WF ST				
(*ii*) Reliability record	Company's record for instrument reliability.	I	Indicates history of sound design/ manufacturing concepts.	PS WF ST				
(*iii*) Upgrading compatibility. Inter-changeability of column and other components.	The ease with which columns, injectors, and pneumatic modules can be changed between different instruments.	I	Common column fitting methods allow columns to be transferred between instruments, giving greater flexibility. Open tubular columns are usually interchangeable. Also common spares and components such as amplifiers can be interchanged.	PS WF ST				
	Availability and ease of software upgrades and compatibility with earlier versions.	I	Greatly extends the life of modern instruments, important that old data files remain accessible.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*iv*) Similarity of layout and design to instruments existing in laboratory		NVI	Similarity of layout means that operators can draw on in-house expertise, resulting in reduced training costs and time. It can also maximise the use of spares and fittings.	PS WF ST				
(*v*) Confidence in supplier	Confidence gained from past experience.	I	Good working relationship already in place.	PS WF ST				
(*b*) Servicing	Score according to manufacturers claims and past record, judged by the sub-features (*i*)–(*v*) below:							
(*i*) Service contract	The availability of a suitable service contract from the manufacturer or agent. Reliability of manufacturer in keeping to scheduled service calls.	I	Suggests long commitment to user. Often ensures preferential service and can guarantee a specific response time to call-outs.	PS WF ST				
(*ii*) Availability and delivery of spares	Range of stock carried by the manufacturer and delivery time.	VI	Rapid delivery of spares reduces downtime.	PS WF ST				
(*iii*) Call-out time	The time for an engineer to reach the laboratory following a call.	VI	Keeps laboratory in operation by reducing down time (see also (*i*)).	PS WF ST				
(*iv*) Effectiveness of service engineers	The ability of the service engineers as judged from previous experience and reports of others, including the carrying of adequate spares.	VI	Ability to repair on-site avoids return visit or removal of equipment to supplier and reduces service time, costs and downtime.	PS WF ST				
(*v*) Cost of call-out and spares	It *may* not be appropriate to score this feature.	NVI	The proximity of service centre may be a factor in travel costs.	PS WF ST				
(*c*) Technical support	As in (*b*) score in consideration of the quality of sub-features (*i*)–(*vi*) below:							
(*i*) Applications department	The advice and training available from the manufacturer's applications department.	VI for new user	This helps in-house staff with new application problems.	PS WF ST				
(*ii*) Technical literature	The range and quality of technical literature including the operating manual. Also availability of updates and routine provision for existing users.	VI for new user	Guidance on optimum use of instrument suggests manufacturer's awareness of applications.	PS WF ST				
(*iii*) Telephone assistance	Willingness of the manufacturer to give effective advice on problems over the telephone. This can normally only be evaluated by reference to existing users.	I	Rapidly available technical help reduces the number of call-outs.	PS WF ST				
(*iv*) Training	This includes initial training when setting up the instrumentation and follow up courses for more advanced users.	VI	A comprehensive training scheme will ensure that operators and instrumentation are working effectively.	PS WF ST				
(*v*) Installation	Full installation requirements, including site requirements where applicable.	I	Specifying the fittings, gases required before installation will save time.	PS WF ST				
(*vi*) User group	Informal newsletters, meetings, *etc*. organised by manufacturer or third party.	I	Other users are often the best source of advice on problems, solutions and applications.	PS WF ST				
Instrumental criteria 1. *General features* (*a*) Facilities required for:								
(*i*) Location of connections and controls on instrument	Score according to convenience, taking into account the proposed location for the instrument.	I	Depending on bench positioning and layout, these may limit accessibility for servicing and installation, particularly at rear of instrument.	PS WF ST				
(*ii*) Connections to mass spectrometer	Score for the ability to link the chromatograph to the spectrometer with heated transfer line if not purchased as a combined unit.	I	Heated line avoids cold spots.	PS WF ST				
(*iii*) Snap-on coded fittings on gas lines.	Score for provision of snap-on fittings and clarity of coding.	I	Coded supplies should be more secure and reduce risk of incorrect connections.	PS WF ST				
(*iv*) Power and heat dissipation	The ability to remove heat particularly during oven cooling cycles. Score highest for instrument most suited to proposed location.	I	The oven generates considerable heat during operation. Air conditioning or ventilation may be needed. Depending on the design of the oven exhaust vent an area of bench may need to be left free for heat dissipation.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*v*) Dimensions	Score according to compatibility of dimensions (width and depth) with space available.	I	Availability of suitable bench space. This may be important in some circumstances.	PS WF ST				
2. *Gas supplies*								
(*a*) Gas control	Score maximum for a control system which gives the most stable gas flows under the required operating conditions.	VI	Control is needed to give a constant gas flow, upon which adequate precision and reproducibility are partially dependent.	PS WF ST				
(*i*) Flow controllers	Score maximum for the provision of the most accurate and precise mass-flow controllers.	VI	Useful for packed and wide-bore open tubular columns where back pressure variation may occur.	PS WF ST				
(*ii*) Pressure controllers	Score maximum for the provision of the most accurate and precise pressure controllers.	VI	Useful with open-tubular columns.	PS WF ST				
(*iii*) Electronic control	Score for availability of electronic control of both flow and pressure.	VI	Electronic control is more precise and reproducible than manual control. This is particularly desirable if the settings will be changed frequently.					
(*iv*) Controlled temperature	Score additionally if the flow controllers are contained within a controlled temperature environment.	I	A controlled temperature environment will increase the stability of the system.	PS WF ST				
(*b*) Gas supply features								
(*i*) Carrier leak detector	Score zero if this feature is not present when combustible gases are to be used.	VI	Vital for safety if hydrogen is used as carrier gas to avoid build-up of gas in the oven in the case of a leak. Also to avoid wasting gas.	PS WF ST				
(*ii*) Detector 'make up gas'	Score if ancillary detectors are to be purchased.	I	Need to maintain a suitable gas flow through the detector when capillary columns are used.	PS WF ST				
(*iii*) Gas purity requirements	Score highest if operating specification can be achieved without ultra-pure gases.	I	Ultra-pure gases/gas purifiers are expensive.	PS WF ST				
(*iv*) Auto purge facility	Score for well-designed system.	I	Carrier gas may be wasted if it is of poor design, *e.g.* purge is left on indefinitely after a run.	PS WF ST				
(*c*) Connections								
(*i*) Gas supply lines	Score according to availability and ease of fitting of non-permeable gas lines. Also use of standard (or consistent) gas fittings.	I	Plastics can age with use and if exposed to sunlight. Metal tubing is more robust and essential if hydrogen is used. Different fittings on GC and MS complicates servicing and modification.	PS WF ST				
(*ii*) Gas purifiers	Score according to availability, stated efficiency, and ease of fitting of on-line traps, such as activated carbon or molecular sieves, into gas supply lines.	VI	Removal of oxygen and water from carrier gas is desirable for some sensitive stationary phases or for operation at high sensitivity. Oil may also need to be removed from air lines if a compressor is used.	PS WF ST				
3. *Injection ports*								
(*a*) General								
(*i*) Ease of cleaning	Score according to ease by which units can be dismantled and reassembled for cleaning.	I	The need to remove involatile residues.	PS WF ST				
(*ii*) Replaceable liners	Score for provision of replaceable liners for injection ports.	VI	Replacement of the liner removes involatile residues and reduces contamination.	PS WF ST				
(*iii*) Septum replacement	Score according to ease of removal and replacement of septa.	VI	Frequent changes of septa are necessary for satisfactory operation.	PS WF ST				
(*iv*) Septum purge	Score additionally for provision of bleed of carrier gas from just below septum.	I	Removes volatiles arising from degradation of the septum and reduces background peaks. Particularly needed for temperature programmed separation on open-tubular columns.	PS WF ST				
(*b*) Heaters								
(*i*) Injector heater control	Score highest for most stable control of temperature of injector heater unit. Score additionally for an independent temperature read out.	I	Injector temperature can affect volatilisation and sample stability on injection.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*ii*) Programmable cooling/ heating of injection zone	Score for availability of a programmable unit for temperature control of the injection zone.	I	Can be used in split/splitless injection (particularly important for capillary chromatography) to focus the sample. Also useful for on-column injection to raise the temperature rapidly after the start of a run.	PS WF ST				
(*iii*) Independent injector oven	Score for the provision of a separate oven for the sample injection ports.	I	The temperature of the injection port should not be altered by variation of column oven temperature if repeatable subsequent injections are to be obtained.	PS WF ST				
(*iv*) Heater temperature range	Score maximum for provision of the widest range normally required.	I	Normal applications need up to 350 °C. Some high temperature applications may need up to 450 °C.	PS WF ST				
(*c*) Types of injection port								
(*i*) Capillary or open-tubular column injectors	For capillary (open tubular) columns score for provision of both split/ splitless and on-column injection facilities. Score additionally according to ease of changing ports and provision of manual or automatic operation.	VI	Choice enables wider range of analytes to be examined. *Split*—mainly used for samples with limited volatility range. Wide ranging samples may suffer some discrimination. Ability to set split ratio is required for quantitative results. *On-column*—needed for thermally sensitive samples and to avoid discrimination effects with a wide range of volatility samples.	PS WF ST				
(*ii*) Gas sampling valves	Fixed volume loops which can be switched into the carrier gas line. Score according to availability and ease of connection.	I (depending on application)	Needed for gaseous samples as syringe injections can give poor repeatability.	PS WF ST				
(*iii*) Large volume injections	Score highest for instrument which accommodates volumes greater than 100 μl.	I	This is particularly useful for the determination of very low concentration species in a clean matrix, as it greatly reduces the sample preparation time.	PS WF ST				
(*iv*) Programmable volatilisation temperature	Score for availability of a programmable injection port which preferentially removes low boiling point components, typically the solvent, by using a very rapid heating ramp.	VI	This is essential for reducing excessive solvent peaks.	PS WF ST				
4. *Column ovens*								
(*a*) Oven design	Score according to the convenience afforded by internal dimensions, location of components, *etc*.	I	Sufficient space is required to enable work in the oven to install and replace columns.	PS WF ST				
(*b*) Oven temperature								
(*i*) Hysteresis	Score maximum for smallest temperature lag during heating and cooling cycles.	I	Slow response can limit programming and cooling rates and prolong re-equilibration time.	PS WF ST				
(*ii*) Maximum temperature	Most ovens operate satisfactorily up to 350 °C. If higher temperatures are required score additionally if oven will operate up to 450 °C.	VI	Some high temperature separations using special columns may need up to 450 °C.	PS WF ST				
(*iii*) Thermal fuse/ electronic cut-out	Score for provision of thermal fuse or electronic cut-out to turn off oven heater in case of controller failure.	VI	Safety device to protect columns (and injector) from excessive heating.	PS WF ST				
(*iv*) Near-ambient operation	Most ovens operate satisfactorily down to 10 °C above ambient. For the examination of volatile samples score additionally for satisfactory control at near-ambient temperature.	I	Enables repeatable analysis of volatile samples. Some ovens have minimum usable temperatures for reproducible control.	PS WF ST				
(*v*) Sub-ambient capability	If required, score additionally for availability of an add-on cooling system.	I	Needed for some gas samples and for highly volatile samples.	PS WF ST				
(*vi*) Temperature gradients across oven	Score maximum for minimum temperature gradients within oven.	I	Gradients due to poor air mixing in the oven can produce poor peak shapes with open-tubular columns because of their low thermal mass.	PS WF ST				
(*vii*) Oven cooling	Score maximum for fastest effective cooling cycle.	I	Saves time between runs.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*c*) Oven programmers								
(*i*) Temperature/ gradient settings	Score highest for provision of digital control rather than analogue control for temperature gradient settings.	I	Digitally controlled temperature programmes are easier to reproduce.	PS WF ST				
(*ii*) Number of steps available	Score according to the numbers of separate delay periods and temperature ramps that can be programmed.	I (for complex samples)	The more steps available, the greater the flexibility. Desirable for complex samples, particularly to flush off involatiles. Most samples will only need a limited number of steps in the programme.	PS WF ST				
(*iii*) Heating rate	Score highest for the maximum ramp rate that the oven can achieve over the temperature range required.	I	High rates are needed for cold on-column injections or with short columns. Also needed when chromatograph is linked to autosampler to coordinate injection with temperature programme and data collection.	PS WF ST				
(*iv*) External control programme	If an external computer system is likely to be used, score for ability to control all necessary temperatures.	VI	An external computer may be useful for special purposes or remote operation.	PS WF ST				
(*v*) Reproducibility of programmed temperature	Score highest for the best reproducibility in temperature control on resetting programme.	VI	Programme reproducibility is more important than accuracy. Needed to ensure consistency of results.	PS WF ST				
(*d*) Column installation								
(*Column materials and stationary phases are outside the scope of this evaluation.*)								
(*i*) Column fittings	Score according to ease of changing columns.	I	Self evident.	PS WF ST				
(*ii*) Inter-changeability	Score for the ability to interchange between open-tubular, and wide-bore columns. When narrow open-tubular columns are to be used, score additionally for minimum dead volume in mass spectrometer interface.	I	Gives maximum flexibility in use of system, bearing in mind that most instruments are dedicated to one mode. Presence of large dead volumes degrades separation efficiency and may cause discrimination effects.	PS WF ST				
(*iii*) Ability to use wide-bore columns	If the application calls for the use of wide-bore columns, score additionally for the provision of this feature.	NVI	Allows greater column loadings.	PS WF ST				
5. *Autosampler*								
(*a*) General	Score for availability of the sub-features (*i*)–(*iv*) listed below.							
(*i*) Interfacing compatibility of micro-controller with the GC-MS computer system	Score for the ability of the autosampler to be controlled by the mass spectrometer system.	VI	Needed for reliable and flexible automatic operation and data collection. Some units operate only from their in-built controller which may have limited facilities.	PS WF ST				
(*ii*) Inter-changeability between sample injection ports	Score for ability of autosampler to inject into each of the available ports.	I	Needed in dual-column instruments so that either column position can be used.	PS WF ST				
(*iii*) Carousel sample capacity	Score for the maximum number of sample positions.	I	A large number of sample positions means that more samples can be analysed unattended.	PS WF ST				
(*iv*) Carousel temperature	Score for availability of temperature control for samples awaiting injection.	I	Permits pre-column derivatisation or cooling for thermally labile or volatile samples.	PS WF ST				
(*b*) Injection system								
(*i*) Injection volumes	Score maximum for greatest range of injection volumes that can be programmed.	I	If different volumes can be programmed for each injection this increases versatility so that different levels of analyte concentration can be handled.	PS WF ST				
(*ii*) Minimum sample size	Score maximum for system requiring minimum amount of sample in vial to flush needle and make injection.	VI	Sample size may be limited. Amount can be dependent on position of needle tip in vial and hence shape of vial.	PS WF ST				
(*iii*) Sample carry-over	Score highest for the system which minimises contamination of the next injection. Score additionally if needle wash is available.	VI	Avoidance of cross-contamination. Intermediate blank samples may otherwise be needed which will, however, increase analysis time.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*iv*) Injection modes available	Score for provision of hot needle–cold needle injection and for on-column injection.	I	Use of hot or cold needle and on-column injection can improve chromatographic separation and reproducibility.	PS WF ST				
(*v*) Needle residence time	Score maximum for shortest needle residence time in injection port.	I	To minimise sample degradation of sensitive samples within the needle during injection.	PS WF ST				
(*vi*) Automatic one-shot injection	Score for facility to inject a single sample automatically.	VI	Can be used to improve repeatability compared with manual operation.	PS WF ST				
(*vii*) Manual injection	Score for facility for manual injection without removing auto-injection.	VI	Improves flexibility of the instrument for non-routine samples.	PS WF ST				
(*viii*) Multiple injections	Score for facility to make a number of injections from a single sample vial.	VI	Used to improve the precision of measurements.	PS WF ST				
(*ix*) Needle depth	Score for the facility to alter the depth of the needle within the sample vial.	I	Allows liquid extraction from different sample volumes to be performed within the sample vial.	PS WF ST				
(*x*) Variable needle draw time	Score for sufficient range according to application.	I	Essential for the analysis of viscous samples.					
(*xi*) Variable injection speed	Score for sufficient range according to application.	I	Different times needed for on-column and split/splitless injection.	PS WF ST				
(*c*) Autosampler controller								
(*i*) Control programme	Score according to ability to programme operation of the autosampler. Score additionally if control can be effected *via* an external computer and if different conditions can be used for specified samples.	I	Improves versatility of operation. Enables use of wash solutions on repeating standard reference solutions within run.	PS WF ST				
(*ii*) Carousel control	Score for ability to select individual sample locations and/or use bar code reading.	I	Provides flexible batch analysis and positive sample identification.	PS WF ST				
6. *Mass Spectrometer*								
(*a*) Vacuum and interface system								
(*i*) Time to evacuate the mass spectrometer or bring it up to atmospheric pressure	Score highest for instrumentation that can be either evacuated or brought up to atmospheric pressure the fastest. Score higher for more robust systems.	I	Cleaning of internal components of the mass spectrometer requires that the system be brought up to atmospheric pressure for cleaning. Re-evacuation of the system to allow the use of the instrumentation can delay analysis.	PS WF ST				
(*ii*) Protection provision	Score for availability of devices which in the event of failure of mains power prevent excessive pressure in the source or the failure of the water supply (if appropriate).	I	Avoids instrument down-time and repair costs.	PS WF ST				
(*b*) Ionisation sources								
(*i*) Electron ionisation (EI)	Score highest for a greater range of electron energies.	VI	Fragmentation patterns are obtained by bombarding the eluant molecules with electrons. The fragmentation pattern is dependent on the energy of the incoming electrons. A greater range of structural information is obtained with electron impact compared with CI.	PS WF ST				
(*ii*) Chemical ionisation (CI)	Score according to the variety of available compounds that can be used for the ionisation process.	VI	CI is caused by firing low molecular weight ions at the eluent molecules. CI directly determines the molecular weight of the eluting compound. CI also gives greater sensitivity, which allows for lower concentrations to be determined.	PS WF ST				
(*iii*) Positive and negative ionisation	Score highest for the ability to do both positive and negative ionisation.	VI	CI and EI can be performed by either positively charged ions or negatively charged ions. Different ionisation modes are needed for some compounds, giving the mass spectrometer greater sensitivity.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*iv*) Changing between CI and EI	Score highest for instrumentation that allows the sources to be changed without having to re-evacuate the mass spectrometer. Score additionally for instrument that allows a combination of CI and EI in one chromatographic run paying particular attention to the reliability of the check valve system.	VI	EI and CI require different sources. These can either be combined on the same unit or be independent. Any leak or malfunction will cause serious operating/performance problems.	PS WF ST				
(*c*) Mass analyser								
(*i*) Mass range	Score for the size of the range between the maximum and minimum mass detected. Most systems operate with *m*/*z* (mass/charge) values between about 800 and 10.	VI	The greater the mass range the greater the variety of samples that can be analysed. A low mass limit is required for permanent gas analysis.	PS WF ST				
(*ii*) Mass resolution	Score for the smallest discernible difference in mass that is detectable by the mass spectrometer. The mass resolution at half height width (50% valley) typically varies from several hundred for low resolution to several thousands for high resolution, benchtop instruments.	VI	Important for distinguishing between ions having a very small difference in *m*/*z* (mass/charge) *e.g.*, isomers. This is particularly important for selective ion monitoring as it ensures that only the target ions are being monitored.	PS WF ST				
(*iii*) Scan rate of the mass spectrometer	Atomic mass units (u) per second. Score highest for instruments with the highest scan rate applicable over the entire mass range, and in multiple ion detection modes.	I	Fast scan rates generally improve the precision, and also allow for faster chromatography.	PS WF ST				
(*iv*) Background signal	Score for the lowest signal resulting from the detection of stray ions. These can either be present within the mass spectrometer, due to very small leaks or due to extraneous material eluting from the column such as stationary phase.	VI	The magnitude of and variations in the background signal will affect detection limits and the precision for small signals.	PS WF ST				
(*d*) Detector								
(*i*) Choice of detectors	A number of detectors are now compatible with ion trap-MS. The most common types are discrete and continuous dynode electron multipliers. Score for an instrument that is compatible with many types of detector.	I	Not all detectors offer the same attributes. The final choice of detector should rest with the user and will depend on the individual laboratories need for sensitivity, robustness, ability to cope with dirty samples and price. The design of the multiplier can affect its ability to cope with large volumes of dirty samples. Also the surface area of the emissive coating in the detector may affect the sensitivity.	PS WF ST				
(*ii*) Dark current	Score for lowest dark current.	I	Dark current is the residual current measured by the detector with no ions being detected. It is caused by noise in the detector electronics.	PS WF ST				
(*iii*) Linear dynamic range	Score maximum for the detection system (*i.e.*, detector and electronics) offering the widest linear dynamic range.	VI	Permits measurement of the widest range of analyte concentration.	PS WF ST				
(*iv*) Sensitivity	Counts per unit concentration at a specified mass. The response from a solution containing a range of compounds across the mass range should be used to evaluate the relative sensitivity. Score maximum for the instrument demonstrating the highest sensitivity taking into account the proposed application. Confirm that sensitivity is adequate across entire mass range.	I	High sensitivity coupled with a low and stable background will result in the lowest detection limit. Some instruments show wide variability across mass range.	PS WF ST				
(*v*) Life time (in use)	Score for longest life time at maximum operating voltage, according to the manufacturer's specification.	VI	The gain of a detector will diminish with use due to contamination or erosion of the detector surface.	PS WF ST				
(*vi*) Life time (storage)	Detectors are consumable items. Score maximumum for the longest shelf life after purchase, as stated by the manufacturer.	I	Many detectors are air and moisture sensitive. They are shipped in sealed bags and have a shelf life of <5 months. Storage for longer periods requires a nitrogen atmosphere at reduced pressure.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*vii*) Ease of replacement	Score according to ease of replacement.	VI	Most multipliers are small and therefore difficult to work with. The problem is reduced for simple slot in type devices constructed on ceramic plates.	PS WF ST				
(*viii*) Detector efficiency	This describes the percentage of incident radiation converted into secondary emissions at a given voltage. Score for the most efficient.	I	The higher the efficiency the greater the sensitivity and detector lifetime.	PS WF ST				
(*e*) Operating characteristics								
(*i*) Tuning	Score for the ability to use an internal or external source to calibrate the instrumentation.	I	Provides increased flexibility of operation.	PS WF ST				
	Score additionally for automatic tuning which generates a report of the settings which have been applied.	I	Knowledge of automatic tune settings reveals anomalies and is needed for QC purposes.	PS WF ST				
(*ii*) Instrument stability	Score highest for a stable response over both short term (minutes) and long term (hours).	VI	Any drift in instrument response will degrade the quality of analytical results. Significant drift will necessitate frequent recalibration.	PS WF ST				
(*iii*) Selective ion mode	The capability of acquiring data by repetitively monitoring a number of mass peaks selected by the operator anywhere within the instrument's mass response range. Score zero if this feature is absent.	VI	Operation in this mode maximises the data acquisition rate on mass peaks of interest. This improves the signal, increasing the sensitivity of the instrument to the selected ions.	PS WF ST				
(*iv*) Isotope ratio measurement	The ability to calculate the abundance of one isotope relative to another. If relevant to the type of application, score for the availability of specialised software that allows data to be acquired and processed to maximise precision.	VI (if applicable)	To measure natural abundance ratios or for isotope dilution mass spectrometry (IDMS) determinations.	PS WF ST				
(*v*) Reference inlet	Score for the availability of an inlet for introducing mass spectrometer calibration compounds into the instrument. Score additionally if both gas and liquids can be used.	VI (if applicable)	Ensures that mass spectrometer is optimally calibrated for a particular application. A range of calibration materials may be needed for pyrolysis GC.	PS WF ST				
(*vi*) Detector overload protection	Score zero if this feature is absent.	VI	Overloading of the detector and associated electronic circuits by exposure to an excessively high ion count rate can reduce the operating life of some detector types, particularly electron multiplier detectors. Furthermore, in these circumstances, the detector may take some time to recover its normal operating characteristics.	PS WF ST				
(*f*) Tandem MS (MS-MS) capabilities	Ion trap facilitates the use of MS-MS as it has the ability to store selected ions inside the trap. The trapped ions can then be fragmented allowing further elucidation of the structure of the compound of interest. This feature is provided by software control. Test reproducibility especially in qualitative mode, if applicable, and score accordingly.	VI (if applicable)	This technique is particularly useful for 'dirty' samples as it allows the determination of residual components even on co-eluting peaks. The difference in the fragmentation pattern allows a distinction to be made between different ions of the same mass. Good MS-MS quantitation is difficult to achieve.	PS WF ST				
(*g*) General maintenance								
(*i*) Column coupling	Score highest if the connector between the column and the mass spectrometer allows the column to be changed without the need to re-evacuate the mass spectrometer.	I	Saves instrument downtime.	PS WF ST				
(*ii*) Access to the ionisation source	Score highest for an ionisation source that is readily accessible.	VI	The source requires cleaning due to particulate build-up from samples. Easy access reduces the time for this cleaning.	PS WF ST				
(*iii*) Ion trap construction	Score highest for simple construction and ease of dismantling.	I	Ion traps are small and difficult to clean and maintain.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
7. *Software*								
(*a*) General aspects								
(*i*) PC-based software for overall control and data processing	Score for availability of this feature, as well as individual control of the GC and the MS.	I	Most instruments utilise a PC for overall instrument operation and control but also incorporate separate microprocessor controllers for the GC and the MS. Availability of both allows maximum flexibility of operation.					
(*ii*) Ease of use	Score according to the ease which a new user can learn to use the software.	VI	This reduces the time spent learning how to use the instrumentation and also reduces operator errors.	PS WF ST				
(*iii*) Availability of validatable software	Score for software that has been developed under a recognised quality system and fully documented.	VI (where applicable)	Essential for laboratories operating in a regulatory environment.	PS WF ST				
(*iv*) Processing of results	Score for the degree of automation by which results can be processed and reported. Score additionally for full access to the raw data which has been automatically processed.	I	This reduces manual intervention saving operator time. Allows manual checking and/or rework of calculations.	PS WF ST				
(*v*) Network capabilities	Score highest if the PC controller allows networking.	I (where applicable)	This allows data to be reviewed from remote terminals. Also valuable for archiving data. Ability to process spectra whilst collecting data. This saves on time.	PS WF ST				
(*vi*) Multi-tasking	Score for software which allows previous results to be processed whilst a run is on-going. Score highest for software which allows data to be collected and analysed concurrently.	VI	Ability to process spectra whilst collecting data. This saves on time.	PS WF ST				
(*b*) Instrument control								
(*i*) Control flexibility	Score for the amount of control that the software gives the user over the instrumentation.	VI	Allows full optimisation of the instrument.	PS WF ST				
	Score additionally for ability to lock the settings in routine use.		Prevents accidental or unauthorised changes.					
(*ii*) Instrument performance diagnostics	Score maximum for an instrument which self checks on power up and has a simple validation routine programmed into the software.	VI	As more systems are used in regulated laboratories it is vital that the system performs diagnostic checks on power up This information must be recorded.	PS WF ST				
(*iii*) Instrument malfunction protection	The procedure adopted by the software when there is an instrument malfunction. Score highest for the greatest degree of flexibility associated with a range of potential malfunctions.	VI	This permits automatic shutdown or allows the user to decide if it is safe to continue.	PS WF ST				
(*c*) Data analysis								
(*i*) Mass spectral data interpretation	Score highest for the widest range and most applicable data manipulation.	VI	By addition or subtraction of spectra (*e.g.*, background noise) the mass spectra can be enhanced. Other manipulations of the raw data can further enhance the interpretation of the mass spectra.	PS WF ST				
(*ii*) Ease of use of chemometric software	Score highest for the most comprehensive features for the analysis of the raw data using chemometric techniques.	VI (if applicable)	This feature permits greatest flexibility for data interpretation and analysis. This would include integration of the raw data, determination of the shape of peaks, quantification using standard calibration curves, *etc*.					
(*iii*) Export of data	Score for ability to transfer data to other software using standard data formats (*e.g.*, ASCII)	VI (if applicable)	Many useful data analysis facilities are available using separate chemometrics or other statistical packages.	PS WF ST				
(*iv*) Available library searches	The number of available mass spectra libraries that are available for the analysis of the mass spectra. Confirm that all relevant aspects of the software are compatible with these libraries. Score highest for the most applicable libraries.	VI	Interpretation of spectra can be a time consuming affair. The use of commercial libraries greatly reduces the time spent interpreting spectra. Certain libraries are targeted at a particular range of compounds.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
8. *Additional features and accessories*	These features may be required for specific analytes or applications, and enquiries should be made as to the availability of suitable accessories. These features should only be scored when appropriate.							
(*a*) Column switching	Score for the ability to transfer eluent gas flow to second column and to reverse flow through column.	I	Can be used to facilitate heart-cut and back flush methods for complex samples.	PS WF ST				
(*b*) Headspace sampling unit	Score for the availability of this feature.	I	Extraction and injection of headspace vapour from above solid or liquid complex matrices. This is used for volatile analytes in comparatively less volatile matrices.	PS WF ST				
(*c*) Headspace analysis	Score if automated headspace analysis is required. Score according to the flexibility of the headspace analyser. Score higher for a combined shaker and heater system.	I (depending on application)	Useful introduction technique as it reduces sample preparation time.	PS WF ST				
	Score for the availability of this feature.	I	Ability to thermally degrade sample rapidly in inlet carrier gas flow is used to analyse involatile samples as characteristic volatile fragments.	PS WF ST				
(*e*) Thermal desorption unit.	Score for the ability to interface the chromatograph to a thermal desorption unit.	I	Thermal desorption units are often required for the analysis of volatile analytes in solid matrices including toxins from entrapped environmental air samples.	PS WF ST Sum of sub totals				
9. *Value for money* (points per £)	Sum of the previous sub-totals divided by the price of the instrument. This sub-total should be subject to proportional scoring and weighting factors and included in grand total.	VI	'Simple' instruments are often good value for money, whereas those with unnecessary refinements are more costly.	PS WF ST				
				Grand total				