The Analyst
AMC PAPER

# Report by the Analytical Methods Committee

# Evaluation of analytical instrumentation

# Part XIII. Instrumentation for UV–visible–NIR spectrometry

**Analytical Methods Committee†**

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*Received 1st December 1999*

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

## Introduction

The following 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 was undertaken by a working party chaired by Dr C. Burgess with Dr D. G. Jones to whom the committee expresses its thanks.

The purchase of analytical instrumentation is an important function of many laboratory managers, who may be called upon to choose between a wide range 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 also hoped that this evaluation will, to some extent, also help manufacturers to supply the instrument best suited to their customers' needs. It is perhaps pertinent to note that a number of teachers have found the reports to be 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 features that are on offer by the manufacturers.

The XIIIth report of the Sub-Committee deals with ultraviolet, visible and near-infrared spectrometry.

### 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 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 a 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 features will be by proportion, *e.g.*, from 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 is indicated as follows: VI (very important); I (important), 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 total exclusion of an instrument.
3. (ST) Sub-total. This is obtained by multiplying PS by WF.

Ultraviolet, visible and near-infrared spectrometry (UV–VIS–NIR) is a well established analytical technique with applications in many areas. An often bewildering range of instrumentation is available from a large number of different manufacturers. Systems range from simple filter based instruments for colorimetry to dual monochromator systems with variable spectral bandwidths and microcomputer-based controllers for multicomponent deconvolution. NIR instruments based upon AOTF (acousto-optical tuneable filter) technology are not included in this paper. In addition, the highly specialised dual wavelength instruments are not covered. 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. The performance of any UV–VIS–NIR method depends primarily on the nature of the spectroscopic parameters necessary to yield satisfactory data and the nature of the sample matrix.

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. The study of chiro-optical phenomena in this spectral range lies outside the scope of this report and will be subject to a separate investigation.

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 assay.

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

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DOI: 10.1039/a909502k

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, UV–VIS–NIR spectrometers are safe in normal use, but care should be taken when handling flammable solvents. In addition, eye protection should be worn when aligning or changing UV lamps.

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

## Previous reports in this series from the Analytical Methods Committee

### Evaluation of Analytical Instrumentation


Part I Atomic Absorption Spectrophotometers, Primarily for use with Flames, *Anal. Proc.*, 1984, **21**, 45. Revised 1997. *Analyst*, 1998, **123**, 1407.

Part II Atomic Absorption Spectrophotometers, Primarily for use with Electrothermal Atomizers, *Anal. Proc.*, 1985, **22**. Revised 1997. *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 Instrumentation for Inductively Coupled Plasma Mass Spectrometry, *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.


**Instrumental criteria sub-committee evaluation form**

| Type of instrument UV–Visible–NIR spectrometer | | | | | | |
|---|---|---|---|---|---|---|
| Manufacturer: | | | | | | |
| Model No.: | | | | | | |
| Feature | Definition and/or test procedures and guidance for assessment | Importance | Reason | Score | | |
| **Non-instrumental criteria** | | | | | | |
| *Selection of manufacturer* | Laboratories in possession of other spectrometers should score highest for the manufacturer with the best past record based on the following sub-features: | | | | | |
| (*a*) Previous instruments | | | | | | |
| (*i*) Innovation | Company's record for developing instruments with innovative features. | I | The manufacturer should be alert to developments in optical design and detector technology. | PS<br>WF<br>ST | | |
| (*ii*) Reliability record | Company's record for instrument reliability. | I | Indicates history of sound design/ manufacturing concepts. | PS<br>WF<br>ST | | |
| (*iii*) Similarity of operation, layout and design to existing instruments in the laboratory | For routine purposes this may be important. However, this may be less important for research application. | I | Similarity of layout means that operators can draw on in-house expertise, resulting in reduced training costs and time. It may also maximise the use of spares and fittings. | PS<br>WF<br>ST | | |
| (*iv*) Confidence in the supplier | Confidence gained from past personal experience. | I/NVI | Good working relationship already in place. | PS<br>WF<br>ST | | |
| (*b*) Servicing | Score according to manufacturers' claims and past record, judged by the sub-features (*i*)–(*v*) below: | | | | | |
| (*i*) Service contract | Availability of suitable service contracts from the supplier, agent or third party contractor. | VI | Suggests long term commitment to user. Often ensures preferential service and guarantees a specific response time to call-outs. | PS<br>WF<br>ST | | |
| (*ii*) Availability and delivery of spares | Range of stock carried by, or quickly available to, the manufacturer/agent/ contractor. | I(VI) | Rapid delivery of spares reduces downtime. | PS<br>WF<br>ST | | |
| (*iii*) Call-out time | Availability of adequate service such as the time for the engineer to reach the laboratory following a call. | I | Keeps laboratory in operation by reducing down time [see also (*i*)]. | PS<br>WF<br>ST | | |

| Feature | Definition and/or test procedures and guidance for assessment | Importance | Reason | Score | | |
|---|---|---|---|---|---|---|
| (*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. | I | Ability to repair on-site avoids return visit or removal of equipment for off-site repair so reduces down time and may reduce sevice cost. | PS<br>WF<br>ST | | |
| (*v*) Cost of call-out and spares | It *may* be inappropriate to score this feature if in-house servicing is contemplated. | | The proximity of the service centre may be a factor in travel costs. | PS<br>WF<br>ST | | |
| (*c*) Technical support | As in (*b*) score in consideration of the quality of the sub-features (*i*)–(*vi*) below. | VI for new user | | | | |
| (*i*) Applications department | The advice and training available from the manufacturer's applications department. | I(NVI) | This helps in-house staff with new applications problems. | PS<br>WF<br>ST | | |
| (*ii*) Technical literature | The range and quality of technical literature including the operating manual. | I(NVI) | Guidance on optimum use of instrument suggests manufacturer's awareness of applications. | PS<br>WF<br>ST | | |
| (*iii*) Telephone assistance | Willingness of the manufacturer/supplier/contractor to give effective advice over the telephone. This can normally only be evaluated by reference to existing users. | I(NVI) | Rapidly available technical help reduces the number of call-outs and enhances productivity. | PS<br>WF<br>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<br>WF<br>ST | | |
| (*v*) Installation | Full installation requirements, including site requirements were applicable. | I | Specifying the essential services required before hand will save time. | PS<br>WF<br>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<br>WF<br>ST | | |
| **Instrumental criteria**<br>1. *General features*<br>(*a*) Facilities required for: | | | | | | |
| (*i*) Access and location of connections and controls on instruments | Score according to convenient access taking into account the proposed location of the instrument. | I | Depending on bench position and layout, connections and controls may limit accessibility for servicing and installation particularly at the rear of the instrument. | PS<br>WF<br>ST | | |
| (*ii*) Power requirements | Many systems require multiple power inputs. Score maximum for instruments with the minimum of separate power leads. | NVI | Excessive numbers of power cables when combined with other services create hazards and make servicing more difficult. | PS<br>WF<br>ST | | |
| (*iii*) Size of equipment | Score according to convenience of installation, talking into account the proposed location of the instrument. | I(VI) | Dimensions may be critical if space is limited. | PS<br>WF<br>ST | | |
| 2. *Spectral sources* | Spectral sources need to be available to cover the appropriate wavelength range required within 180–2500 nm. | | | | | |
| (*a*) Source selection | Score highest for availability of appropriate sources and additionally for those with lowest noise and drift. | VI | Sources in commercially available instruments are usually confined to deuterium; 180–350 nm and tungsten–halogen, 340–2500 nm. Minimising source noise and drift increases the quality of the spectral data. | PS<br>WF<br>ST | | |
| (*b*) Ease of lamp replacement and alignment | Score highest for easiest replacement and alignment. | I | Routine lamp replacement is necessary. Ease of fitting and alignment makes for less down time. | PS<br>WF<br>ST | | |
| (*c*) Cost of lamp replacement | Score highest for lowest cost source replacement consistent with noise and drift requirements. | I | Minimises running costs. | PS<br>WF<br>ST | | |
| 3. *Instrument factors* | The choice of optical geometry and measurement mode(s) are important factors in obtaining a meaningful signal for a given application. | | | | | |

| Feature | Definition and/or test procedures and guidance for assessment | Importance | Reason | Score | | |
|---|---|---|---|---|---|---|
| (*a*) Optical geometry | Score highest for the optical geometry most appropriate for the application, *i.e.*, single beam or double beam. | VI | Single beam instruments are often the lowest cost option and are generally used for single wavelength measurements. For spectral scanning, double beam instruments are preferred when using dispersive optics. Reverse confocal optics and interferometers are encountered only in specialised applications. | PS<br>WF<br>ST | | |
| (*b*) Measurement mode | The majority of instruments operate in the absorbance/transmittance mode. Score additionally if concentration modes or specialist modes (*e.g.*, tristimulus values) are required. | NVI | Many simple instruments allow a conversion factor to be entered to convert absorbance values directly to a concentration. More sophisticated instruments can output absorbance data in a variety of colour data formats including tristimulus coordinates, CIE LAB units, *etc.* | PS<br>WF<br>ST | | |
| 4. *Sample compartment* | | | | | | |
| (*a*) Size | Score maximum for the availability of adequate space for cuvette holders and, if appropriate, accessories. | I | Convenience of interchangeability of cuvettes and/or accessories increases productivity and reduces potential sources of error. | PS<br>WF<br>ST | | |
| (*b*) Temperature stability | Score highest for sample compartments which are least sensitive to temperature changes during routine operation. | I(VI) | In the absence of thermostatic control, many solutions exhibit significant spectral changes with temperature. Spectrometers with sample compartments close to spectral sources and/or electronics are more likely to suffer heating effects. | PS<br>WF<br>ST | | |
| (*c*) Accessibility | Score highest for spectrometers which allow ready access to accessory slots and service inlets to the sample compartment. | NVI | For spectrometers which require water thermostated cuvettes or sample changers, for example, ease of access is important for efficient operation. | PS<br>WF<br>ST | | |
| (*d*) Gas purge | Score only if the presence of this feature is required. | I | For work below 200 nm, it becomes increasingly necessary to purge the optical path with dry particulate free argon to remove oxygen which absorbs significantly in this region. | PS<br>WF<br>ST | | |
| 5. *Sample presentation* | | | | | | |
| (*a*) Cuvette | | | | | | |
| (*i*) Design and size | Score highest for cuvette holders which allow positive and reproducible positioning. Score additionally for the ability to accommodate a range of cuvette sizes and types *e.g.*, flow through, microcell, if appropriate. | VI | It is essential to present the cuvette reproducibly centred and normal to the incident beam to minimise any optical effects due to non-parallelism of the cuvette faces and inter-reflection errors. | PS<br>WF<br>ST | | |
| (*ii*) Thermostatic control | Score highest for systems with cuvette thermostating accessories. For kinetic and/or temperature jump applications, Peltier controllers are highly desirable. | VI | Many solutions exhibit significant spectral changes with temperature. Temperature control of the sample within ±1 °C is normal for multi-component deconvolution work. However, ±0.1 °C may be required for, *e.g.*, kinetic studies. | PS<br>WF<br>ST | | |
| (*iii*) Autochanger | Score only if the application requires multiple cuvette operation. | VI | Some applications, *e.g.*, tablet dissolution or multi-sample kinetics, require programmable automatic cuvette changing. | PS<br>WF<br>ST | | |
| (*b*) Skipper (flow cell) systems | Score for the presence of this accessory if required. | I(VI) | When a large number of samples are required to be measured, the use of a flow cell and peristaltic pump make the sample handling much easier and the quality of the data more consistent. | PS<br>WF<br>ST | | |
| (*c*) Reflectance accessories | Score for the availability of diffuse or specular reflectance accessories and integrating spheres which enable solid and semi-solid samples to be measured. Score only if appropriate. | I(VI) | The vast majority of measurements are made in solution. However translucent and solid samples are increasingly being examined using transflectance or reflectance techniques. | PS<br>WF<br>ST | | |

| Feature | Definition and/or test procedures and guidance for assessment | Importance | Reason | Score | | |
|---|---|---|---|---|---|---|
| (*d*) Fibre optic probes | A variety of fibre optic probes for transmittance, transflectance and reflectance are available for remote measurement of liquid and solid samples. Score for the availability and suitability of each of these according to the application. | I(VI) | For many in-process control applications, the use of a probe allows measurement to be made rapidly and remotely from the spectrometer. Due consideration should be given to the optical performance of the fibre in the spectral region of interest. | PS<br>WF<br>ST | | |
| *6. Wavelength selection devices* | A range of wavelength selection devices are available in the UV–VIS–NIR spectral region. Some of the more technical aspects have been covered in Part IV of this series of papers. | VI | | | | |
| (*a*) Filters | These are used in the simplest type of single beam colorimeters and photometers. Score highest for those with the largest number of filter options and smallest bandwidth. | I | A combination of interference and blocking filters can provide adequate monochromation for simple colorimetric measurements. | PS<br>WF<br>ST | | |
| (*b*) Single grating monochromators with fixed or variable slit | The majority of spectrophotometers are of this type. Score highest for those systems which have the slit widths required and additionally for scanning capability if required. | I | For spectral bandwidths of 2–10 nm, a single grating monochromator will provide adequate monochromation for qualitative scanning and quantitative single wavelength applications provided that the stray radiant energy requirements are not stringent. See below. | PS<br>WF<br>ST | | |
| (*b*) Double monochromators | For the most exacting work particularly below 220 nm, the stray radiant energy performance is critical. Score highest for systems with the best stray radiant energy performance. Score additionally for the widest range of scanning speeds and spectral bandwidths. | I | Stray radiant energy causes deviations from the Beer–Lambert law. For consistent work above an absorbance of 2 the use of a double monochromator instrument is almost obligatory. | PS<br>WF<br>ST | | |
| (*d*) Polychromators | See Part III of this series of papers and Section 8(b) for details. | I | Polychromators utilise the advantage of photodiode array detectors. | PS<br>WF<br>ST | | |
| *7. Detectors* | At low absorbance, spectrometer performance is limited by instrument noise primarily from the detector and associated circuitry. | VI | | | | |
| (*a*) Single channel | Single channel detectors are used in conjunction with a conventional monochromator. Score highest for detectors meeting the sensitivity, noise and drift requirements for the spectral measurement. | VI | | PS<br>WF<br>ST | | |
| | (*i*) Silicon photodiode; 200–700 nm. | | Silicon photodiodes are satisfactory for most UV–VIS applications where noise and sensitivity are not critical. | | | |
| | (*ii*) Photomultiplier tube; 180–900 nm. | | The photomultiplier is still the detector of choice for most UV–VIS applications as it has much better sensitivity, dynamic range and noise performance than the silicon photodiode. The range can be extended into the NIR region. | | | |
| | (*iii*) NIR detectors; 750–2500 nm | VI | Beyond 1000 nm, lead sulfide, InGaAs and mercury telluride detectors are required. Lead sulfide detectors, however, have poor signal to noise performance particularly in the 800–1000 nm region. | | | |
| (*b*) Multi-channel charge transfer detectors | Multi-channel detectors are found in polychromators. Here the dispersion and detection of the radiation attenuated by the sample are combined and all wavelengths monitored essentially simultaneously. Score for the highest number of diodes per nm and the best signal to noise, drift and sensitivity. | VI | These detectors are currently based on photodiode arrays. CCD and CID based detectors are being developed. Users need to be aware of the limitations of array technology, *e.g.*, shadowing and the effects of the electronic data massage necessary during the readout cycle. | PS<br>WF<br>ST | | |

| Feature | Definition and/or test procedures and guidance for assessment | Importance | Reason | Score | | |
|---|---|---|---|---|---|---|
| *8. Spectral performance* | | | | | | |
| (*a*) Range | Score for the appropriate spectral range(s) needed, *e.g.*, UV 180–400 nm; visible 350–900 nm; NIR 750–2500 nm. Note that these boundaries are somewhat arbitrary and that some instruments will span the total range. | VI | The information content of the analytical signal is dependent upon the spectral region chosen. | PS<br>WF<br>ST | | |
| (*b*) Accuracy and reproducibility | Score for an accurate and reproducible wavelength scale. Standard materials such as rare earth oxides (solutions and glasses) and YAG crystals are available from national laboratories (*e.g.*, NPL and NIST) for calibration purposes. The wavelength accuracy may be checked using observed positions of atomic lines, *e.g.*, $D_2$ at 486 nm and 656 nm or other suitable line sources in the UV–visible region. | VI | For consistent and reliable spectral data, the wavelength scale must be accurate and precise. | PS<br>WF<br>ST | | |
| (*c*) Resolution | The ability of a monochromator to accurately discern the spectral features of a sample is dependent upon the natural half bandwidth of the chromophore and its spectral bandwidth (SBW). SBW affects the observed band shape, intensity and position of the band maxima or minima. The resolution may be checked using observed half heights of atomic lines, *e.g.*, $D_2$ at 486 nm and 656 nm or other suitable line sources in the UV–visible region. Polystyrene may be used in the NIR.<br><br>Score for the most appropriate spectral bandwidth required. | VI | The majority of absorption bands of chromophores in the UV–VIS–NIR region are relatively broad and have natural half band widths of 50 nm or more. It has been shown that for a pure gaussian band if the ratio of the NBW/SBW is approximately 1/8 then the observed absorbance value is $>99\%$ of the true value.† For the majority of applications, therefore, a SBW of about 2 nm is sufficient. However, for benzenoid chromophores and gas spectra SBWs of down to 0.1 nm may be needed. However, in the NIR, the bands are usually even broader than those in the UV–visible and larger spectral band widths are used, *e.g.*, 4–8 nm. | PS<br>WF<br>ST | | |
| (*d*) Stray radiant energy (SRE) | Score highest for the lowest SRE value in the wavelength range of interest. The SRE level may be measured using cut-off filters or solution filters using alkali metal halides.‡ | I(VI) | SRE levels limit the linear photometric range of the spectrometer. For reliable sample absorbances over an absorbance of 2 a double monochromator instrument is usually required. | PS<br>WF<br>ST | | |
| *9. Photometric performance* | Score highest for the performance demanded by the application. | | | | | |
| (*a*) Accuracy and reproducibility | The ordinate scale of the spectrometer must be accurate and precise. Standard materials such as potassium dichromate are available from NIST for solution calibration purposes. Various calibrated artifacts, glass filters, silica on quartz filters, *etc.*, are available from National laboratories (*e.g.*, NPL and NIST). In addition, solid reflectance standards are available. | VI | For consistent and reliable spectral data, the ordinate scale must be checked at regular intervals. | PS<br>WF<br>ST | | |
| (*b*) Baseline flatness, noise and drift | Score for the highest signal to noise ratio and least drift. Score additionally for scanning instruments with the flattest base line. Methods for determining these parameters are available.§ | I(VI) | Stability of instrument performance is essential if consistent spectral data are to be generated. | PS<br>WF<br>ST | | |

† P. Torkington, *Appl. Spectrosc.*, 1980, **34**, 189.
‡ ASTM, *E 387-84 Standard test method for estimating stray radiant power ratio of spectrophotometers by the opaque filter method; Annual Book of ASTM Standards 1966*, American Society for Testing and Materials, West Conshohocken, PA, 1995, 03.06, pp. 714–723.
§ ASTM, *E 275-93 Standard practice for describing and measuring the performance of ultraviolet, visible and near-infrared spectrophotometers; Annual Book of ASTM Standards 1996*, American Society for Testing and Materials, West Conshohocken, PA, 1993, 03.06, pp. 682–692.

| Feature | Definition and/or test procedures and guidance for assessment | Importance | Reason | Score | | |
|---|---|---|---|---|---|---|
| *10. Instrument control and data collection* | | | | | | |
| (*a*) On-board computer | Score highly for a simple low cost effective routine instrument which has on-board software and is controlled from an integral keyboard. Score additionally for the facility to export data to an external computer (for further data manipulation if this is needed). | VI | Simplifies the operation and ideally should be able to provide simple method storage and limited data manipulation routines, *e.g.*, linear quantitation using standards. | PS<br>WF<br>ST | | |
| (*b*) Data output | For routine analyses score for an instrument that can output data to a printer/plotter or as an ASCII or industry standard file for external processing. A scanning instrument may output an analogue signal to a chart recorder or data logger. | I | A digital output is preferred so that if necessary further data processing may be easily performed. | PS<br>WF<br>ST | | |
| (*c*) External control of instrument parameters | For non-routine analyses or research, score highest for a comprehensive software package to control the spectrometer and collect the data. | VI | Ensures that the same analyses are always performed under identical preset conditions. This is vital if the system is in a regulated laboratory. Manufacturer supplied software will have to be validated. It is rarely cost effective to write one's own software. | PS<br>WF<br>ST | | |
| (*d*) 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 instruments are used in regulated laboratories, it is vital that the system performs diagnostic checks on power up. This information must be recorded. | PS<br>WF<br>ST | | |
| *11. Data manipulation* | | | | | | |
| (*a*) Data collection software | Define the requirements before scoring these items. Most manufacturers offer software packages with routines for setting the instrument parameters and collecting the data. The choice of how the software runs can be a very personal choice. Make sure that the features offered are fully evaluated. The ease with which the data can be acquired and reports generated are of prime importance. Score only for the availability of essential routines. | VI | Control and data collection software options are essential for data integrity and must include all of the required routines. Software packages from the manufacturer are expensive, but the effort it will take to write and validate one's own software would prove to be extremely time-consuming and therefore more expensive. | PS<br>WF<br>ST | | |
| (*i*) Fixed wavelength or multiple data collection | Score highest if all parameters can be set and stored with the spectral data to ensure that all future analyses can be performed under the same instrumental conditions. | VI | Deviations must be flagged by the software. Essential for many regulatory requirements, *e.g.*, GLP, GMP and all regulated industries. | PS<br>WF<br>ST | | |
| (*ii*) Spectral data over a selected wavelength range | Score highest if all parameters can be set and stored with the spectral data to ensure that all future analyses can be performed under the same instrumental conditions. | VI | Deviations must be flagged by the software. Essential for many regulatory requirements, *e.g.*, GLP, GMP and all regulated industries. | PS<br>WF<br>ST | | |
| (*iii*) Time dependent data collection | Score highest if all parameters can be set and stored with the spectral data to ensure that all future analyses can be performed under the same instrumental conditions. | VI | Deviations must be flagged by the software. Essential for many regulatory requirements, *e.g.*, GLP, GMP and all regulated industries. | PS<br>WF<br>ST | | |
| (*iv*) Storage of data files | Score maximum for a system where all data collection parameters are also stored with the ASCII data. | VI | ASCII data can be exported to and manipulated by many software packages. This expands the scope of data manipulation and chemometric routines available to the user. | PS<br>WF<br>ST | | |
| (*v*) Display software routines | Score maximum for a comprehensive set of spectral display routines. | VI | Simple versatile spectral display routines are vital. Pseudo 3D contour plotting shows additional useful features especially if studying time related data. | PS<br>WF<br>ST | | |

| Feature | Definition and/or test procedures and guidance for assessment | Importance | Reason | Score | | |
|---|---|---|---|---|---|---|
| (*b*) Data handling | | | | | | |
| (*i*) Software to perform all arithmetic functions, *e.g.*, area, smoothing, derivatives, averaging, calculations on single points or spectra | Score according to the availability of these routines especially if spectral comparison measurements are to be made or multi-component calculations envisaged. For accessories score additionally for the ability to transform data, *e.g.*, Kubelka–Munk functions for reflectance data, colour co-ordinates. | VI | The software enables routines to transform raw data without having to use third party software. This is particularly important for regulatory requirements, *e.g.*, GLP, GMP and all regulated industries. | PS<br>WF<br>ST | | |
| (*ii*) Quantitative analysis routines using single wavelength data or spectra for multi-component work | Score according to the availability of several routines for, *e.g.*, single wavelength quantification. Score additionally if spectral data can be exported to be used in multi-component analysis software also. | I(VI) | Linear and other non-linear functions should be provided for single wavelength quantitative analysis as well as kinetic models, especially for biochemical assays. | PS<br>WF<br>ST | | |
| (*iii*) Software to control any accessory and collect associated data | Score maximum for the availability of routines to control and collect data directly from accessories, *e.g.*, Peltier temperature data, vial numbers from autosamplers. | I | Simplifies the measurements and ensures that all data are compatible when doing the calculations. | PS<br>WF<br>ST | | |
| (*iv*) Specific application routines and the ability to customise and record the parameters | Score maximum if this feature is present and appropriate. | (VI) | This facility enables routines to be made so that less experienced staff can perform the analysis under optimum conditions routinely. | PS<br>WF<br>ST | | |
| (*v*) Routines for checking the sensitivity of the spectrometer | Score maximum for the availability of routines and the appropriate 'standard' samples to make these check measurements. | VI | Keeping track of the instrument sensitivity is vital. For example, these measurements will show up a lamp nearing the useful end of its life. | PS<br>WF<br>ST | | |
| (*vi*) Validation software | Score maximum for a system to comply with the regulating authorities' standards with validation routines as a standard feature. | (VI) | Essential in many laboratories for regulatory requirements, *e.g.*, GLP, GMP and all regulated industries. | PS<br>WF<br>ST | | |
| *12. Hardware and output requirements* | | | | | | |
| (*a*) Computer | Score for compatibility with either existing or company selected computer. | VI | There may be a company requirement for uniformity. Speed and ability to upgrade are important. | PS<br>WF<br>ST | | |
| (*b*) Output devices | Score maximum for a system which uses a standard printer, *e.g.*, laser, inkjet, dot matrix. | VI | This facility has become very important for uniformity. | PS<br>WF<br>ST | | |
| (c) Data storage | Score for possibility to store data on suitable media for future retrieval and use. | VI | This is very important as is the provision of a hard copy. Date and acquisition parameters must also be archived. | PS<br>WF<br>ST | | |
| (*d*) Data output from simple instruments | Score if printed data output from a digital readout on the instrument or analogue output to a recorder is needed. Score if this feature is required. | I | It is beneficial if the system can be coupled to a standard printer to produce a hard copy. | PS<br>WF<br>ST | | |
| (*e*) Ability to be networked | | I(VI) | In many laboratories the instrument is run from a PC and at a suitable time the data is transferred to a server. | PS<br>WF<br>ST | | |
| | | | | Sum of sub-totals | | |
| *13. Value for money* (Points per £) | Sum of the previous sub-totals divided by the purchase price of the instrument. Subject to proportional scoring and weighting factors, including ST in grand total. | I | 'Simple' instruments are often good value for money, whereas those with unnecessary refinements are often more costly. | PS<br>WF<br>ST | | |
| | | | | Grand total | | |

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