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Evaluation of analytical instrumentation. Part XXVII: a guide to good practice in the purchase of analytical instrumentation

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This guide is designed for those involved in the purchase of analytical instrumentation, including analysts and laboratory staff, purchasing officers and senior managers. It provides recommendations on the stages that are required for the successful evaluation, purchase, installation and reliable operation of analytical instrumentation. The overall intention is to recommend a process where an analyst can make a confident recommendation of instrumentation that meets the desired specification. In addition, guidance is offered to ensure clarity in the roles and responsibilities of those involved in the overall procurement of a major analytical instrument.

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Introduction

The Analytical Methods Committee has received and approved the following report from the Instrumental Analysis Sub-Committee. The report was prepared for the Analytical Methods Committee (AMC) by the author, with contributions and critical review from other members of the Instrumental Analysis Sub-Committee: M. Sargent (Chair), A. R. Godfrey, S. Greenfield, S. J. Hill, S. Hird, R. Lad, P. B. O'Connor, I. Pengelly, M. Saeed, A. Sage and M. West.

The guide provides recommendations on the stages that are required for the successful evaluation, purchase and installation of analytical instrumentation. It is likely to be of most use in circumstances where a substantial investment is to be made. Guidance is offered to ensure clarity in the roles and responsibilities of the analyst (in undertaking an evaluation of performance of available instrumentation and making a recommendation for purchase), the purchasing officer (in negotiating the purchase contract) and the senior manager (in authorising the purchase). In addition to the direct purchase, some aspects of this guide are also relevant to arrangements where instrumentation is to be leased or rented.

The guide is designed to be useful in any major purchase of analytical instrumentation, whether to replace existing equipment or for the provision of instrumentation designed to offer new analytical capabilities. It is not intended for financial administrators, who have an emphasis on fiscal, legal and financial procedures, but rather for the practical analyst who is tasked with evaluating the capabilities of relevant instrumentation and making a recommendation for purchase. These issues include an assessment of the specification and performance of analytical instrumentation that must fulfil a clearly defined analytical role. Other factors include the support and capabilities of the supplier or manufacturer in contributing to the successful installation and operation of the instrumentation.

The approach followed here is that by considering a logical set of issues, a single recommendation for purchase based on rational criteria will be forthcoming. No attempt is made here to cover financial procedures involved in the purchase which will need to comply with the procurement procedures of the individual organisation, and will clearly set a framework within which any analytical recommendation must comply. Individual criteria are set out in this guide for consideration. The analyst may choose to place greater or lesser emphasis on individual recommendations, depending on circumstances, application requirements and experience. It is intended that potential purchasers will find these criteria useful and helpful, but it must be emphasised that any final decision for purchase remains the purchasing organisation's sole responsibility. The criteria are listed in Table 1, which is set out in terms of the key steps to be addressed to facilitate a successful purchase.

Other reports

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

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.

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| Requirements and procedures of the purchasin | ng organisation |
| (1) Making a case | The justification for the purchase of new instrumentation may arise from several causes such as: (i) replacement of obsolete equipment or equipment at the end of its life cycle, (ii) expanding the analytical capability, (iii) developing new analytical capabilities. However, it is normally necessary to develop a case to justify the purchase and to submit that case to the appropriate line manager responsible for that area of activity for approval. It is good practice for an analyst to be aware of instrumentation available on the market. In addition, it may be necessary for the analyst to seek specifications and guide prices from suitable suppliers. However, the analyst should not enter into any commitments or undertake any evaluations, until the case and specification has been approved. |
| (2) Confirming funding and setting the budget | Funding for new instrumentation, especially if a significant investment is to be made, can come from a number of sources, including: (i) the organisation's reserves or capital funds, (ii) financial investment that may involve third parties, (iii) the result of a successful research grant application. It is not appropriate to undertake the formal evaluation and purchase process until funding has been confirmed although it may be useful to undertake an initial investigation at an early stage, especially if the timetable for purchase is tight. Decisions on setting the budget need to take account of a number of factors. If the budget is set too low, this could reduce the choice or even define the purchase. It is recommended that the budget should be considered confidential and is not revealed to any supplier or manufacturer. The purchasing organisation needs to make it clear to the analyst whether the budget is a guide price or an absolute limit that is placed on a purchase. It is recommended that some flexibility is maintained on a budget limit as purchasing managers often take pride in their ability to negotiate discounts, especially in the purchase of high cost pieces of instrumentation or where multiple purchases are involved and circumstances where suppliers may be willing to offer packages that involve extras (that may or may not be relevant to the intended application) in deals that can become quite complex. |
| (3) Agreeing responsibilities | A key stage in the instrument evaluation and purchase process is to agree <i>a priori</i> who is responsible for what activity and what authority they have for decision making. It is normally expected that: (i) the analyst (supported by appropriate colleagues) will be responsible for evaluating the available instrumentation and making a recommendation for purchase, (ii) a purchasing officer will be responsible for negotiating the purchase price and a purchase contract, (iii) a senior officer of the organisation will be responsible for signing off all the details and authorising the purchase. |
| (4) Institutional purchasing policy | All organisations have policies that specify the criteria and procedures that must be followed in the purchase of capital equipment. These policies are designed to ensure that purchases comply with the organisation's accounting procedures, and national and international financial regulations and may involve a formal tendering process. In addition to being familiar with these policies, all actions in assessing instrumentation undertaken by an analyst must comply fully with these organisational requirements. |
| (a) Declarations of interest | It goes without saying that the analyst making the recommendation must have no impediments to making an entirely dispassionate recommendation for any purchases in which he or she is involved. |
| (b) Other institutional issues | A number of issues not directly related to instrument performance may affect purchase decisions. These issues may include: (i) within or cross-organisation standardisation of instrument type or manufacturer, (ii) timing in the calendar year for obtaining authorisation, committing expenditure, and making the full payment. In some cases, it is essential that delivery takes place before the end of a financial year, as organisations may not be allowed to carry over large sums of money into the next financial year. In other cases, funding may become available just before the end of the financial year to use surpluses that have arisen in other budgets. In both these situations, the latest date by which delivery must take place may be a critical issue. |

(5) Identification of suppliers

It is assumed that an experienced analyst is familiar with potential manufacturers/suppliers of the instrumentation being sought. If not, information can be obtained from trade magazines, attending international and national meetings, manufacturer exhibitions, internet searches and by networking with analysts from other laboratories working in the same field.

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| (6) Previous experience of a manufacturer's instrumentation | Where a purchasing organisation already has experience of instrumentation supplied by a manufacturer, a number of issues may contribute positively or negatively to a new purchase recommendation, including (i) to (iv) below. Alternatively, similar information can often be obtained through the sources mentioned in (5) above. |
| (a) Innovation | If a company has a record for the design and manufacture of instrumentation with effective innovative features, this demonstrates a knowledge and understanding of the instrumentation in relation to user requirements. |
| (b) Reliability record | The record of a company for instrument reliability reflects good design and a quality manufacturing capability. |
| (c) Similarity of operation, layout and design (including software) to existing instruments in the laboratory | A similarity in the design and operation of new instrumentation to that already operated by the organisation means that operators can draw on in-house expertise, resulting in reduced costs and time for training. It may also then be possible to maximise use of spares and fittings. These issues may be important for routine or commercial work, but less important in research applications. |
| (d) Confidence in the supplier | Confidence gained from past experience with the supplier or the experience of other users can contribute to a purchase recommendation and demonstrate a benefit of continuing effective working relationships. These experiences may include instrument support including technical, preventative maintenance service contract, engineer dispatch time and availability of instrument parts. |
| (e) Trust in the supplier | Trust in the supplier can cover a range of issues, but one aspect is to avoid purchase of instrumentation that will become out of date soon after delivery in circumstances where the supplier is aware but does not reveal information about the development of a more effective model. Of course, the purchase of an obsolescent model may be an issue for consideration, if performance is satisfactory and the discount large enough. |
| (f) Record of post-purchase upgrades | Especially in the case of complex instrumentation, it is expected that the manufacturer will introduce new components that improve performance in the course of the purchased instrument's operational lifetime. A relevant issue may then be whether the purchased instrument is designed to be upgraded and whether any upgrades (such as software) are covered by a maintenance contract. |
| (7) After sales service(a) Service support | It is essential that to ensure continued operation of an instrument over the planned lifetime, that there is confidence in the availability and quality of service support from the supplier or an approved third-party. |
| (b) Calibration and validation services | The use of calibration and validation services from the supplier or approved third-party is often a requirement if data is to be used in regulatory measurements or in support of accreditation assessments. |
| (c) Availability, cost and delivery of spares and consumables | The range of stock carried by, or quickly available to, the supplier or third-party will influence instrument down-time and affect day-to-day operating costs. |
| (d) Effectiveness of service support | The ability of a service agent to identify and fix faults will reduce instrument down-time, although it is recognised that it may only be possible to judge this criterion based on previous user experience. |
| (e) Maintenance contract | Several of the above issues are formally covered by taking out a maintenance contract once the warranty period has expired. The cost, as well as type and quality of a maintenance contract is likely, for complex instrumentation, to be an issue that influences purchase decisions. Relevant issues include response time (may be linked to the cost option chosen), remote diagnostics, availability of spare parts, expertise of maintenance engineers. Furthermore, it is important to distinguish those items that are regarded as 'consumables' and ancillary equipment that are not included in a maintenance contract (and in some cases excluded during the warranty period), to avoid any unwelcome surprises should additional costs occur. It is also important to clarify liability for the repair of faults that are caused by the failure of services (power, water, gases, air conditioning) that are provided by the purchaser's organisation. These may not be covered by a standard maintenance contract. |

Table 1 (Contd.)

| Issue | Explanation of relevance and/or importance |
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| (8) Technical support from the instrument | |
| (a) Applications advice and development | To maximise the capability of in-house staff to use instruments for new applications (or to optimise existing operations), advice available from the vendor's applications department may be important as well as the willingness of the applications laboratory to develop custom applications relevant to the intended use of the instrument. |
| (b) Technical literature | The range and quality of technical literature, including the instruction manual, application notes and published research papers is likely to help operators to optimise measurements for new and existing applications, raise awareness of other instrumental capabilities and promote the correct use of instrumentation. |
| (c) Telephone and internet assistance | The rapid availability of assistance is likely to reduce the need for service call-outs through support available <i>via</i> telephone or internet, including software updates. It is recognised that it may only be possible to judge this criterion by reference to other user's experiences. |
| (d) Training | To ensure that operators use instruments effectively, training must be available during or following installation of an instrument. This issue is of particular importance in the purchase of instrumentation to be used by previously inexperienced operators. |
| (e) User meetings | Meetings, conferences and technical briefings organised by the manufacturer or third-party for users of the instrument are often the best source of advice for solving problems and developing new applications, and for promoting useful contact with other users. |
| (f) Other issues relevant to the instrument supplier | The assessment of instrument performance may be much easier to undertake if the supplier is willing to loan the instrument for use in the purchaser's laboratory. This option is only likely to be available for certain categories of instrument and there must be a clear understanding of liability for maintenance and damage. |
| (g) Warranty | A one year warranty is standard for many analytical instruments, but purchase decisions may be influenced by the availability of extended warranties (that delay the need to take out a maintenance contract) and details of what the warranty covers. In particular, items classified as 'consumables' are likely to be an additional cost to the purchaser and there are likely to be restrictions that any instrument repairs or investigations can only be undertaken by the manufacturer's engineers, for a warranty to remain valid. |
| Technical assessment of potential instruments | |
| (9) Criteria for the assessment of performance | For simple instruments, it may be possible to assess instrument performance from a range of manufacturers on the basis of published specifications. On the other hand, for very specialised instrumentation, there may only be a single supplier. However, for many instruments, there are competing suppliers of instrumentation. In all these circumstances, it is advisable to run test samples in the manufacturer's application laboratory to evaluate instrument performance and to ensure that results are fit-for-purpose. As an alternative, it may also be advantageous to contact or visit the laboratories of existing users, both to assess instrument performance (but noting that a user's laboratory is sometimes contracted by a supplier to undertake a formal demonstration). In some cases it may also be possible to obtain limited hands-on experience in this way, for example with the instrument software. It is intended that this approach should provide evidence of transparency in contributing to the final purchase decision. It is important that the person making the purchase recommendation should be present, whenever possible, during any demonstration of instrument performance. |
| (a) Purpose of the evaluation | Instrument performance is likely to be one of the issues that will contribute to the final purchase decision. The purpose of the evaluation of instrumentation is to provide evidence that the instrumentation under evaluation is fit for purpose in relation to the proposed application, noting that other criteria will contribute to the final decision (such as purchase cost and an overall assessment of value for money). |

Table 1 (Contd.)

| Issue | Explanation of relevance and/or importance |
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| (b) Choice and evaluation of test material | Test materials should be selected that represent samples which the instrumentation will be used to characterise. The composition of these samples should be known to the purchase evaluator, but not to the applications laboratory, although the applications laboratory will need to know some information about the test samples, such as matrix type. For instrumentation that requires significant user interaction, the user should ideally be present when measurements on test samples are made. Exactly the same materials and instructions should be given to the demonstrators of all instruments to be evaluated. The user may need to use his or her judgement to ensure that results represent a fair assessment of instrument performance, rather than an evaluation of the knowledge and expertise of the applications laboratory. |
| (c) Non-disclosure agreement | In specialised applications, where test materials or test methods have intellectual property value, it may be necessary for the purchaser to require a supplier and/or applications laboratory to sign a non-disclosure agreement to protect the organisation's intellectual property. In some circumstances, the supplier may also ask potential purchasers to sign such an agreement to protect innovative design features of advanced instrumentation. |
| (d) Assessment of other factors | In addition to evaluating instrument performance, the presence of the purchaser in the applications laboratory will also allow an assessment to be made of the ease of instrument operation and the effectiveness of interaction with the operating system. |
| (e) Assessment of evaluation data | When all the instrument evaluations have been completed, the purchaser will need to evaluate the quality of test data against the criteria set for purchase. Instrument performance must clearly be fit for purpose in relation to the proposed application. In circumstances where instrument performance exceeds the specification for the proposed application, the purchaser will need to score the related benefit. In research applications, 'superior' performance may be scored highly. In routine applications, this may be judged to be unnecessary. It is courteous, at this point, to provide some feedback on performance to the participating applications laboratories. |
| (f) Final assessment | A number of factors are likely to be important in making a final recommendation for purchase. These factors are likely to include instrument performance, purchase cost, and other issues summarised in this table. The final recommendation for purchase should be supported by evaluation documentation that shows that a fair, rational and logical process has been followed. |
| (g) Probity | In conducting this evaluation, the purchaser must be aware of and fully comply with the organisation's policy on the acceptance of any benefits-in-kind from the supplier (this may include offers to cover the cost of travel and accommodation when visiting the applications laboratory or users' sites, personal gifts or concessions). In the interests of transparency in demonstrating a fair assessment, all such benefits in kind should be discouraged and may be judged to be illegal. Any negotiations concerning purchase discounts should be conducted by the organisation's purchasing department, following the organisation's standard purchasing rules. |
| (h) Final offer | Following the performance evaluation described above, it is appropriate to give suppliers details of the timetable for final decision making and to request a final written purchase quotation. |
| (i) Purchase decision | On the basis of all the available information (analytical performance, instrument interactivity, final quotation for purchase price and any other relevant criteria), the purchaser will need to make a final decision in relation to the stated application and value for money. The recommendation for purchase should then be passed on to the organisation's purchasing department. This recommendation should include the acceptance criteria and timetable against which the instrument will be assessed on site before full payment will be made, so that these details can be included in the purchase contract. |
| (j) Placing an order | The purchasing department may be able to negotiate further discounts, based on experience and purchasing power. The purchasing contract will usually specify that a deposit will be paid when placing an order, with an agreed delivery date and timescale for paying the balance. The majority of this payment may fall due on delivery, but it is important that some proportion of the purchase cost is withheld until the supplier can provide evidence that following installation, performance meets the agreed specification/acceptance criteria. |

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| Installation and use of the instrument | |
| (10) Installation requirements | It may be possible to install simple instruments in a normal laboratory environment with no special precautions. More specialised instrumentation may require special facilities, without which installation may not be possible or performance may not meet specification. In such circumstances, the installer may make a pre-delivery assessment to ensure that the appropriate environmental conditions and services are available. In other circumstances, the analyst's organization may be given a specification of services that must be provided, before installation can take place. Significant additional costs may be required to meet this specification and failure to do so may lead to disputes with the supplier. Some of the issues, especially applying to larger and more complex instrumentation are as follows. |
| (a) Delivery | Delivery of instrumentation to the laboratory for installation may be an issue if the instrumentation is bulky and heavy and the room is not on the ground floor or adjacent to a loading bay. Dimensions of corridors, accessible doorway spaces, steps and slopes and the capacity of lifts may then be issues that need to be assessed before delivery. |
| (b) Size and shape of room | As well as providing a comfortable environment for the operator, the positioning of large instrumentation may need to ensure that there is easy access to the rear for connecting the instrument to services, allowing sufficient airflow for heat dissipation and avoiding trip hazards due to tailing cables and pipes. For large and sophisticated instrumentation, floor loading and tolerance to vibration (<i>e.g.</i> , from passing traffic) may be issues. |
| (c) Environmental conditions | All instrumentation is likely to have a specified temperature range in which it will operate to specification and sometimes the acceptable humidity range. The most demanding may require full air conditioning to ensure temperature fluctuation remains within the specified range (especially important for instrumentation with a significant heat dissipation capacity). |
| (d) Power requirements | Simple instruments may operate from a standard electrical socket. More complex instruments may need special power supplies (possibly three phase) with the need for particular attention to the quality of the earthing system, avoidance of interference on the supply line and possibly the need to install an uninterruptable power supply system. |
| (e) Other services | Some instrumentation may require the provision of other services, for example cooling water and gas supplies (which may need to be piped in from a caged store outside the building) and exhaust gas extraction. Exceptionally, planning approval may be required should external alterations to the building be required as well as an environmental impact assessment. |
| (f) Installation costs | Depending on the installation requirements, significant additional costs may be incurred in providing appropriate laboratory services. Clarity is required to ensure that the organisation has agreed a budget to meet these additional costs on a time scale that is compatible with the installation timescale. |
| (11) Installation, commissioning and | |
| (a) Delivery and installation timetable | Following the placement of a purchase contract, an outline timetable for delivery and installation should be agreed. |
| (b) Unpacking and configuration | The purchaser may be responsible for arranging transport of the instrument to the laboratory, but unpacking is likely to be the responsibility of the installation engineer, with attempts by the user to do so invalidating the warranty. These responsibilities must be confirmed with the supplier. |
| (c) Connection to services | It will normally be the purchaser's responsibility to organise the connection of the instrument to essential services, but this must be undertaken with the approval of the installation engineer. |
| (d) Training | The competence of users to operate and evaluate the performance of instrumentation is a crucial aspect of the acceptance following commissioning. For simple instrumentation, especially when replacing existing equipment, training might be a simple briefing. For more complex instrumentation, users may be required to attend bespoke courses, and/or receive instruction from the installation engineers. It is very important that training is complete before users' are required to make a judgement of whether instrumentation is operating to specification. |

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| (e) Demonstration of specification and performance | The installation engineer is likely to want to test the instrument to demonstrate that the instrumentation will operate to the manufacturer's specification. This is not the same as the instrumentation operating in an application to the purchaser's satisfaction. The criteria on which instrument acceptance will be based must be agreed between purchaser and supplier as part of the purchase contract. |
| (f) Formal acceptance and payment of final installment | Formal acceptance of the instrument marks the point at which the warranty begins and is likely to trigger the final payment (unless a reliability delay is part of the purchase contract). At the point at which the purchase contract is issued, it is important to specify the evidence on which formal acceptance will be agreed. |
| (g) Dispute resolution | Should there be a dispute between purchaser and supplier that the instrument is not performing to the specification summarised in the purchase contract, it is important that there should be an agreed procedure by which a potential conflict will be resolved. |
| (12) Routine use and exploitation | Having successfully installed and accepted the instrumentation, a clear plan is desirable to show how the instrumentation will be used. This may involve: (i) routine use in applications, replacing end of life cycle or obsolete equipment, (ii) extending existing or developing new applications to exploit the enhanced capabilities of the instrumentation, (iii) attracting 'high' status research applications that will justify the investment that has been made. In these circumstances, briefing on instrument capabilities, training in instrument operation and guidance in the interpretation of results may need to extend beyond the team originally responsible for instrument evaluation and installation, requiring the allocation of additional resources. |
| (13) Evaluation of investment | Especially for instrumentation of high value, an organization is likely to require a review to demonstrate the value for money resulting from this investment. The style of such an evaluation will depend on the nature of the organization, but the focus is likely to be the claims of benefit made in the original case developed to justify the capital outlay. Reviews may be required annually to demonstrate usage, and/or could be more substantial in demonstrating the overall value for money offered by the investment. |

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. Simultaneous Wavelength 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 Highperformance 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.

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

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

Part XV Instrumentation for Gas Chromatography-Ion-Trap Mass Spectrometry, Analyst, 2001, 126, 953.

Part XVI Evaluation of General User NMR Spectrometers. Accred. Qual. Assur. 2006, 11, 130–137.

Part XVII Instrumentation for Inductively Coupled Plasma Atomic Emission Spectrometers. Accred. Qual. Assur 2005, 10, 155–159.

Part XVIII Differential Scanning Calorimetry. Accred. Qual. Assur 2005, 10, 160–163.

Part XIX CHNS Elemental Analysers. Accred. Qual. Assur 2006, 11, 569–576. Part XX Instrumentation for Energy Dispersive X-ray Fluorescence Spectrometry. Accred. Qual. Assur 2006, 11, 610– 624.

Part XXI NIR instrumentation for process control, Accred. Qual. Assur 2006, 11, 236–237.

Part XXII Instrumentation for liquid chromatography/mass spectrometry, Accred. Qual. Assur, 2007, 12, 3–11.

Part XXIII Portable XRF instrumentation, Accred. Qual. Assur, 2008, 13, 453– 464.

Part XXIV Instrumentation for quadrupole ICP-MS. Anal. Methods, 2010, 2, 1206–1221.

Part XXV Differential Scanning Calorimetry. Anal. Methods, 2015, 7, 1240– 1248.

Part XXVI Instrumentation for Voltammetry. Anal. Methods, 2015, 7, 1249– 1260.