Accred Qual Assur (2007) 12: 3–11
DOI 10.1007/s00769-006-0188-7

GENERAL PAPER

Evaluation of analytical instrumentation. Part XXII

features are considered to be of greater importance they are marked I. Those features of greatest importance are marked as VI (very important). A scale should be chosen for the weighting factor that allows the user to discriminate according to needs, e.g., × 1 to × 3 or × 1 to × 10.

3. (ST) Sub-total. Multiplying PS by WF obtains this.
4. In some circumstances, where there is a fundamental incompatibility between a feature of the instrument and the intended application, it may be necessary to exclude an instrument completely from further consideration.

With these requirements in mind, the user should then evaluate the instruments available on the market, taking into account the following 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 and may then become important. However, in some specialized cases, only one or two instruments will have the ability or necessary features to be used in the intended application.

The guidelines are intended to be used as a checklist of features to be considered, mostly of the instrument itself, but also of service requirements and any existing relationship between the user and the manufacturer. The relative importance of these features will depend on a number of factors, which in some circumstances could be subjective. However, if all the points have been considered, the choice should be informed.

The committee considers that instrumentation for energy

charge (*m/z*) ratio of ionised molecules. The analyte must

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score		
Electrospray (ESI/API)	Score highest for instrumentation that will accept the widest range of eluent flow rate. This will be achieved by use of a source heater with a wide variable temperature control and with nebulizer gas with a wide range of flow rates.	I	HPLC columns used in LC/MS range from ‘analytical’ at approx. 1 mL/min. flow rates, through ‘microbore’ at L/min, to capillary at sub L/min flow rates (see nanospray).	PS WF ST		
Nanospray	Score highest for instrumentation which has provision of a nanospray source, essential for capillary HPLC capability, where applicable. Alternatively, score for system where					

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score		
MS/MS instruments	Ion-trap and FTMS instruments are able to perform MS/MS experiments. Quadrupole, sector and TOF analysers must be combined, either with similar mass analysers or as hybrid instruments. Many MS/MS experiment setups possible. Application will dictate type, but focus here on most used for LC/MS only.					
Quadrupole/quadrupole	Coupled quadrupole mass analysers *via* 'collision cell' where fragmentations are usually induced by collision with inert gas. The collision cell is itself a quadrupole or higher multi- pole, but with radio frequency (rf) only, transmitting all ions, not mass filtering.	I	Most widely used for small molecule LC/MS and quantitation. Several different scan modes. MS1 and MS2 separate analysers can be scanned simultaneously for constant neutral loss/gain (CNL/CNG). MS2 static with MS1 scanning for precursor ion scan. High sensitivity for single/multiple reaction monitoring (SRM /MRM), with MS1 and MS2 both static. Relatively low cost.	PS WF ST		
Quadrupole/TOF	MS2 quadrupole replaced with TOF mass analyser. Score for *m/z* range of both analysers, sensitivity and mass accuracy/resolution (TOF).	I	Good combination, especially for proteomics, with high sensitivity and resolution. TOF as obligatory scanning analyser excludes some scans where MS1 is static. However, software manipulation allows equivalent dynamic experiments.	PS WF ST		
Detector Choice of detectors	Detectors in modern instruments are generally based on electron multipliers and two classes of					

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