WHITE PAPER

UV/VIS AND UV/VIS/NIR SPECTROSCOPY

Major Considerations in Choosing a High Performance UV/Vis or UV/Vis/NIR System

While UV/Vis and UV/Vis/NIR spectroscopy are well established analytical techniques being effectively applied across a broad spectrum of well-known industries, high performance UV/Vis spectroscopy has expanded into new applications, especially in the life sciences. Yet even in the traditional application areas such as materials characterization, optics, coatings, glass, pharmaceutical QA/QC, and color control, UV/Vis spectroscopy has become more sophisticated, providing higher quality results faster and easier than ever.

In choosing a UV/Vis system or one with added NIR capabilities, there are many considerations. Traditional specifications such as wavelength range or sensitivity are critically important. Yet other elements such as ease of operation, speed of analysis, sampling flexibility, maintenance and long-term durability may be important in meeting current and future needs.

The remainder of this document will examine these issues and present some newly available options that can provide a stronger foundation for choosing your next UV/Vis or UV/Vis/NIR system.

Instruments have to work harder

Many UV/Vis systems today are low-priced units purpose-designed for repetitive tasks in specific application areas. For labs that face easier samples and a narrow range of simple measurements, these low-cost units may be a cost-effective choice. On the other hand, some labs performing repetitive tasks also require high performance instruments, especially for solid samples. As analyses have expanded in scope and complexity, other considerations have entered the equation, including the need for NIR measurement capability and increasingly automated accessories.

Key Benefits

- Current and future applications
- Performance criteria
- Sampling flexibility
- Accessories that meet your needs
- Higher productivity and ease of use
- Software designed to follow best practices
- Quality maintenance and service

PerkinElmer®
precisely.

Many labs are also facing pressures of doing more with less. Often there is no longer a UV/Vis expert, and so personnel are expected to perform a wider variety of functions, which has led to a need for "smarter" instruments and software. Productivity and flexibility have grown in importance, and the need for high-performance instruments that can meet these challenges has grown likewise. As a capital purchase, a new instrument needs to work harder than ever.

With fewer trained UV/Vis analysts, systems that are easy to use, even for the most sophisticated applications, will quickly produce the return on investment demanded by lab managers. And as labs analyze and develop more sophisticated products with tighter tolerances, the need for fast and reliable results becomes more important than ever.

Broadly speaking, your decision will likely be based upon wavelength range, sensitivity, sample type and size, current and future applications, required accessories, productivity, ease of use, software, time saved for other tasks, flexibility, maintenance, price and total cost of ownership. As no two labs are identical, no single set of criteria will rank the same with all users. With any investment of this magnitude, you need to be satisfied that the instruments under consideration meet or exceed those criteria essential to your operations.

Start with current and future applications

Historically, UV/Vis and UV/Vis/NIR instruments have been used for very specific QC applications such as measuring adherence to color standards or evaluating reflective properties of an optical coating. If your lab is expected to continue as a high-volume QC environment, then ease of use, rapid data acquisition, reporting, reproducibility and durability are all important. On the other hand, if there is a research or product design and development aspect to your lab, then flexibility and large sample compartment size might be important features of your UV/Vis instruments.

Also important in these application areas are cell changers to speed and simplify multi-sample measurements.

Regardless of the current and future direction of your lab, ease of use in operation and design of experiment are important as they free you for other, higher-value tasks such as analysis of results. Ideally your software will offer workflow automation based on proven professional practices in UV/Vis and NIR procedures (Figure 1).

Select the right performance criteria

Your application determines the required detection range and resolution. In the middle range of high performance instruments, you should expect UV/Vis coverage from 190 to 900 nm, and if NIR is needed, the range should extend from at least 190 to 3000 nm. PerkinElmer® spectrophotometers handle a very wide range of wavelengths, from 175 nm to 3300 nm.

Other key performance criteria such as stray light and working absorbance range will also help define the instrument that you need. Stray light performance at a variety of wavelengths should be carefully tested by the manufacturer, and test conditions should be clearly stated.

The degree to which the instrument eliminates stray light is an important specification for high-performance UV/Vis spectrophotometers. Stray light is often defined as unwanted

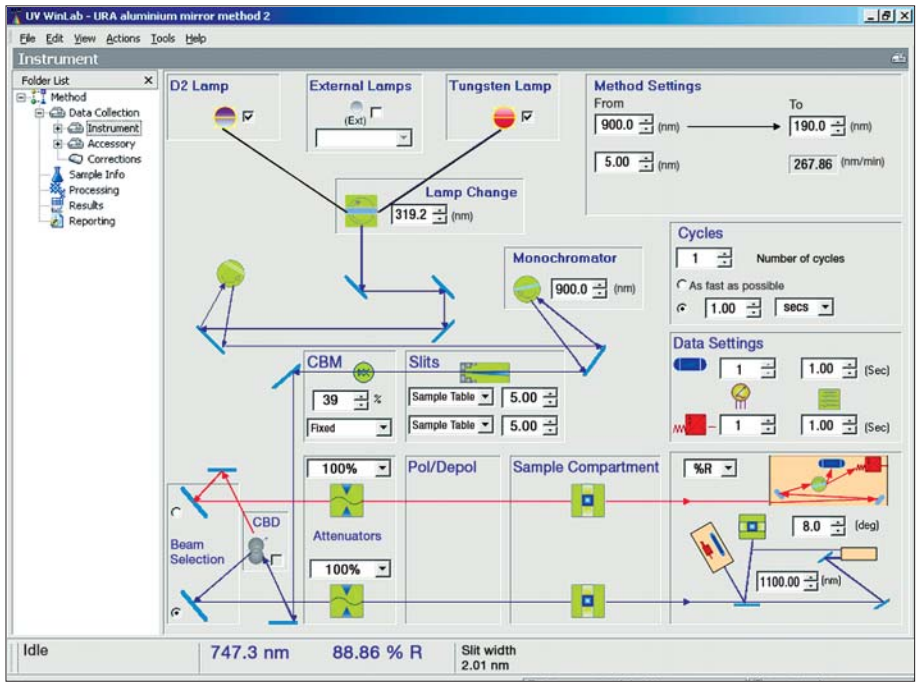

Figure 1. All instrument set-up parameters are easily accessed within UV WinLab software.

radiation that is picked up by the detector and can be from many sources, including leakage from outside the instrument and from interreflections in the optical system. The presence of stray light reduces the accuracy of absorbance measurements and may limit the type of applications that can be performed on the system.

A variety of test methods are available to evaluate stray light levels – for example, ASTM and Pharmacopeia methods. For highly accurate quantitative and qualitative analysis in the UV/Vis region, stray light performance of at least ≤ 0.0007 %T is desirable, and the highest performing UV/Vis and UV/Vis/NIR systems can typically achieve levels of around ≤ 0.00003 %T (measured at 340 and 370 nm). Stray light is controlled by a variety of measures including the use of double monochromators, high-quality diffraction gratings, light-tight optical compartments and optical baffles.

The most sophisticated UV/Vis/NIR systems, such as the PerkinElmer LAMBDA™ 650/850/950 series, contain a host of performance enhancements such as these. In fact, the new LAMBDA series has unmatched stray light performance in this class of instrument.

Absorbance range is another important selection criterion. For most clear liquids, measurement up to 3 A is acceptable. Turbid or concentrated liquids may absorb more light than this, and for optically thick solid samples – for example, glass, semiconductors and similar materials – up to 8 A may be needed. For extremely sensitive and accurate measurements on highly absorbing samples, the instrument should provide sample and reference beam attenuators. Consistent and accurate results are just as important as potential resolution and detection limits. For increased accuracy, the beam chopper common in most UV/Vis instruments should switch between sample and reference beams at 60 Hz to provide good individual blank readings. In order to accomplish this it should be of a four-segment design. This design provides individual blank readings for the sample and reference beams, providing greater accuracy.

A common beam mask in the instrument should allow precise adjustment of beam height to match samples of various dimensions. For those who need to accurately measure birefringent samples, it is essential to have an internal beam depolarizer that corrects for inherent instrument polarization as well as a sample compartment polarizer/depolarizer facility.

Avoid future limitations through sampling flexibility

Large sample compartments free you from many of the constraints imposed by traditional UV/Vis instruments. Even better is a second sample compartment for maximum flexibility in design of experiments and in handling large or awkward samples. It may not be quantified on a spec sheet, but the extra room afforded by large multiple compartments to mount and work without damaging valuable samples or accessories dramatically improves convenience of operation.

Instruments with smaller or a single sample compartment can lead to frustration if you attempt to easily mount polarizers or depolarizers or quickly reconfigure the compartment for a new analysis. Integrating spheres in particular can be a challenging fit in many UV/Vis instruments. Many of them cannot accommodate a large 150 mm sphere or have had to locate the spheres in the main sample compartment. Other instruments cannot be operated in ambient light with the sample lid open for oversize samples.

With flexible sampling compartments and a wide variety of accessories, a broader range of users are able to run different analyses. Yet while flexibility is important, high-precision measurements are essential and any instrument in this class

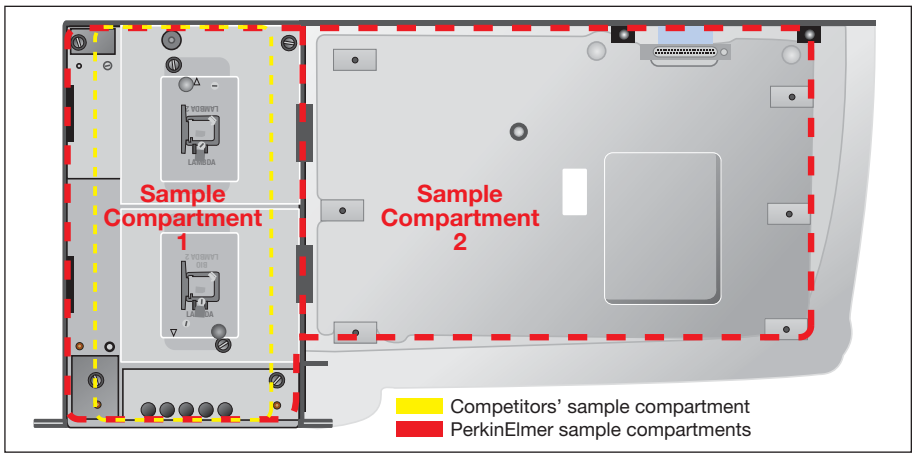

Figure 2. Yellow area shows the size of a typical competitor's sample compartment.

should make it easy to obtain high-precision reflectance measurements. Having a second sampling area in which to accommodate these accessories simplifies operation, as well as provides more room for larger and awkwardly-shaped samples (Figure 2).

Accessories that meet your needs are vital

No doubt you have a clear sense of your analytical needs. Yet you may have struggled in the past with poorly designed or self-made accessories that were difficult to use and compromised consistency. Perhaps detectors in your current system are not interchangeable. Or the system attempts to make do with a single beam attenuator that mounts in the sample compartment and steals space from accessories and experimental designs.

Figure 3. Samples are simply placed on the URA sample platform.

Figure 4. The URA sampling module can be simply interchanged depending on sampling need.

Your new high-performance UV/Vis system should offer a range of ready-made accessories that easily snap in and align themselves. The accessories should also be "smart" and communicate with the system software and other hardware. Modularity is also very helpful so that accessories and system components are easily inserted or swapped with other UV/Vis systems from the same manufacturer.

The latest PerkinElmer UV/Vis systems raise accessory interchangeability to an unprecedented level. Three of the most important are the Universal Reflectance Accessory (URA) (Figure 3), the General Purpose Optical Bench (GPOB) and the range of integrating spheres.

Unique to PerkinElmer, the URA provides high sensitivity, absolute reflectance measurements by automatically and reproducibly changing angles with no adjustments to sample or optics, reducing costs and producing results faster. Multi-angle analyses typically require several accessories and many manual adjustments. With the URA, sampling angles are selected with a mouse click. By using a horizontal sampling plate, the URA also eliminates the inconvenience and damage caused by vertical clamping. The URA is a clearly better way to achieve faster results in UV/Vis/NIR.

Product development, research and even QA/QC sometimes demand highly customized instrument configurations. For these situations, your unique needs are best served by a GPOB. Large and awkwardly shaped samples such as optics, telescopes and beam splitters are easily accommodated through custom optical layouts. The best way to produce a new layout is through magnetic optical mounts. Ideally, the optical bench should just be a single unit that replaces two snap-out sample compartments so that long paths of up to 400 mm can be established, if needed.

Integrating spheres remain one of the most versatile accessories for high precision reflectance and scattered transmittance measurements on virtually any solid or liquid.

A UV/Vis spectrophotometer will ideally accommodate a range of spheres from 60 to 150 mm as well as specialist options. The spheres should include a transmittance

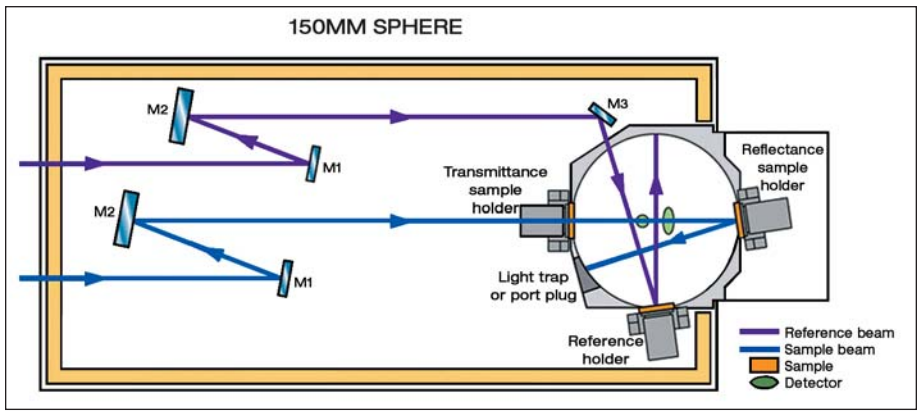

Figure 5. A 150 MM integrating sphere, showing the range of sample holders.

sample holder at the entrance to the sphere to collect all of the light that passes through the sample. A typical high-performance instrument should comfortably hold a 150 mm sphere with a reflectance sample holder mounted opposite the entrance, but to achieve this the instrument will require a large sample compartment. Large reflectance samples that will not fit inside any instrument will require the integrating sphere to have an additional external port that should be easily accessible.

Expect higher productivity and ease of use

Investing in a sophisticated UV/Vis instrument can yield impressive gains in operator efficiency as the instrument automates previously tedious tasks. Manual installation and alignment of accessories, for instance, can be time consuming and if not done properly compromises results and reduces the accuracy and reproducibility. Taking this into account, it is possible to quantify the time saved for other tasks as a result of simplified instrument operation.

Being able to easily swap out sampling modules and relying on the instrument to self-align are tremendous time savers. For absolute specular reflectance measurements, using software to set angles is another time saver. With the URA, an operator can have the instrument automatically run through almost unlimited precise angle changes. Other instruments that require manual angle changes risk damage to samples.

If you calculate the total amount of time saved for each operation, you could save at least one hour per day, and typically many more when using the URA. Clearly this additional time could be used to increase throughput, add work on another instrument, develop new methods – or free you to write reports.

By integrating flexible sampling options, professional user-friendly software, self-aligning accessories, automated measurements, accuracy and reproducibility, the result is a good measure of ease of use.

Insist on software designed to follow best practices

Emulating proper laboratory workflow has become essential for instrument software. Guiding method development, operation, reporting and analysis can be dramatically simplified with the right software that follows a consistently logical sequence and helps to ensure good laboratory practice. Instrument setup, which can be difficult in many systems, should be simply and clearly laid out on-screen with parameters that are easy to adjust. For instance, accessory parameters should be accessible in a diagram of the complete optical system and able to be changed simply by typing in a new value. All settings should be stored in methods for easy access for routine tasks.

Other software tools such as secure databases, method locking, audit trails, and electronic signatures are required in regulated environments and helpful in most labs. Also beneficial for all labs are functions such as intelligent querying and trending.

Quality maintenance and service – often overlooked, but essential

Even a complex instrument should be designed for convenient ongoing maintenance and to minimize unexpected service. Something as simple as replacing a deuterium light source should be a task any operator can handle in a minute. As with any technology investment, however, your UV/Vis instrument should be covered by a service plan that fits your volume of work. Moreover, the instrument maker should have deep expertise in UV/Vis and UV/Vis/NIR application support to address problems you may have in method development, operation and troubleshooting.

To be effective, a service engineer should know the service history of your instrument and the methods you are running. But before a service visit may be necessary, you should have telephone access to an expert who can address your questions on the spot to avoid downtime. PerkinElmer OneSource℠ Laboratory Services are available in more than 125 countries through more than 1,000 factory-trained service professionals.

Other services that your instrument vendor should ideally provide include validation, education and training, and consulting that can increase your uptime and productivity.

Selecting the right system for your lab

As you evaluate the current crop of UV/Vis and UV/Vis/NIR instruments, be sure to rate each system according to the criteria described above and summarized for your convenience below. With this guide, you should be able to choose a system that dependably meets your present and future needs.

If the new PerkinElmer LAMBDA 650, 850 or 950 UV/Vis and UV/Vis/NIR spectrophotometers are on your considered list, please contact your local PerkinElmer representative for more information, phone 1-866-250-6070 ext. 800 or visit *www.perkinelmer.com/lambda*.

Table 1. Decision making assistant. Use this grid to evaluate systems in key areas highlighted in this white paper.

	System A	System B	System C
UV/Vis detection range 190-900 nm			
Far-UV capability to 175 nm			
NIR detection range to 3300 nm			
Double holographic grating monochromators			
Stray light performance typically ≤ 0.00002 %T at 340 nm (ASTM method)			
Dual sample compartments			
Four-segment beam chopper providing individual blank measurements for sample and reference beams			
Quick-change modular second sampling area			
150 mm integrating sphere			
Fully automated accessory for absolute and relative specular reflectance measurements			
Automated depolarizer option to correct for inherent instrument polarization			
Sample compartment polarizer/depolarizer option (must work in combination with automated depolarizer)			
Automated sample and reference beam attenuators for accurate measurements on high absorbance samples			
Photometric Range up to 8 A			

PerkinElmer Life and Analytical Sciences
710 Bridgeport Avenue
Shelton, CT 06484-4794 USA
Phone: (800) 762-4000 or
(+1) 203-925-4602
www.perkinelmer.com

PerkinElmer®
precisely.

For a complete listing of our global offices, visit www.perkinelmer.com/lasoffices

006991_08