

# Spectroscopy Focus

## A ZERO FOOTPRINT OPEN ACCESS SYSTEM FOR UNIFIED OPERATION, DATA PRESENTATION AND USER TRAINING

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*Advances in high throughput techniques, chemistries and analyses, have revolutionised the research landscape. The use of automated systems underpins the majority of mass spectrometry approaches. This has been adopted in the Pharmaceutical industry, through all the 'Omics' but it has yet to be fully accepted within some of the chemistry communities. In many cases the high throughput approach means that the vast majority of users are not specifically trained mass spectrometrists. They don't need to be, but the sample submission, data acquisition and data presentation now demands a user friendly, robust client interface – the so called open access software. This allows mass spectrometry to be fully utilised as a research tool in wider application fields that have their own specialists. They still require a thorough understanding of mass spectrometry but they no longer need to have the day to day hands on capabilities.*

**A FAMILIAR WEB STYLE USER INTERFACE IS USED IRRESPECTIVE OF THE UNDERLYING HOST INSTRUMENT**

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All of the major MS companies have their own versions of these systems. Here, at the School of Chemistry, University of Southampton we housed the first academic open access (OA) API system which was installed for the research school in 1995. This was followed by OA EI and CI GC-MS as well as an additional OA API system in 2000, the latter used by both undergraduate and post-graduate chemists. These systems readily afford routine sample analyses for 15-20,000 samples per year with the benefit to our chemistry community of fast sample turnaround. This in turn aids increased productivity, scope and quality of their research.

Key to providing any high throughput open access service is the ease of accessibility for the end user as well as the ease of administration and training for the primary analyst. Whilst the introduction of open access dramatically reduced the analysts' time required for data acquisition, historically we had three different open access software options from two different vendors which meant that significant time was taken up training the individual users. We have more than 150 postgraduate and undergraduate students that require access to each system. The annual influx of students therefore creates a requirement for training. Coupled with the multiple systems in use, the training load is exacerbated. A further call on our time is the need to provide electronic copies of data for publications and presentations.

A simple but expensive option would be for research groups have their own copies of each data processing software package. However, this would be prohibitively expensive and would also have required a regular training regime and would do nothing to reduce the requirement for users to be familiar with multiple data processing systems. Another approach is the use of proprietary software packages, available on a PC within the MS facility, for access to e-data but this again erodes analysts' time in training, re-training due to lack of use and users often wasting their time on unnecessary reprocessing of data.

### DEPLOYMENT

To address these issues and further enhance the administration of OA systems a vendor independent, web-based open access interface, RemoteAnalyser, has been developed in conjunction with SpectralWorks. This offers a one-stop-shop option for sample submission across multiple platforms, provides uniform e-data output and enhances data security by immediately archiving a clone of the raw data files on a remote server. The only requirement for the user is access to a web-browser enabled computer, e.g. Internet Explorer, Netscape etc. There is no additional software licence cost to the user. Figure 1 shows a schematic representation of the deployment possibilities of RemoteAnalyser.

The data processing, file storage and web server can be configured to run on a single server or a number of servers depending on specific requirements and level of throughput. Currently we have two GC/MS systems and one LC/MS system configured on one server and each system can be accessed by users on campus and external remote clients via the internet. As the service expands, it will possible to add additional servers as required.

### USABILITY

For on-site users, as well as external clients, there is only a requirement to become familiar with a single software system for sample submission and data analysis and presentation. Figure 2 shows the RemoteAnalyser sample submission page for a typical user. Users can be configured to have specific permissions and access to specific instruments or methods as required.

A familiar web style user interface is used irrespective of the underlying host instrument. In this way, users are presented with a consistent look and feel to sample submission and interaction with the service. Users may arrange for multiple injections from a single sample vial if required. Simple point and click menus allow for sample submission and reviewing of results of completed sample analyses as well as editing of user settings.

Sample submission can be either instrument or method centric. In the former, the chemist is able to select the specific instrument that they want to run their sample(s) on. In the latter, they select the method they want to run and the system will direct them to the most relevant instrument based on technique and availability.

This can be configured on a per user basis. Authorised users can register samples for analysis from anywhere if they have the relevant permission and is currently in operation with an external institution.

One-off training sessions can now be undertaken in a lecture theatre or even via a live web-link for off-site users, dramatically reducing MS department staff time dedicated to user training. With a single system there is also a reduced requirement for re-training due to infrequent use of one or the other systems. Authorised users are also able to remotely view their results.

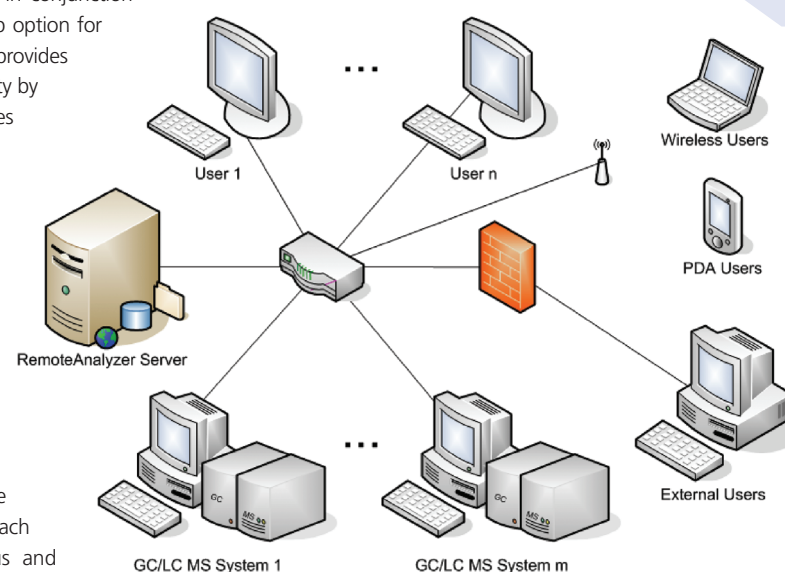


Figure 1. Deployment possibilities for RemoteAnalyser.

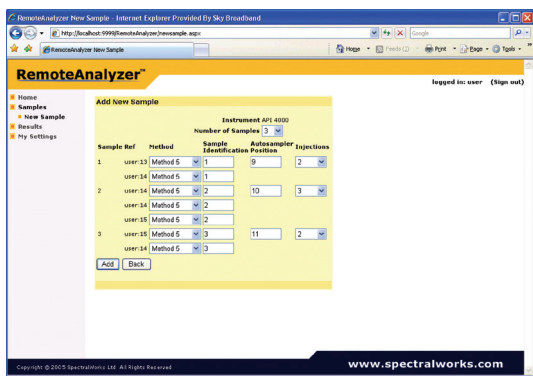


Figure 2. RemoteAnalyser User Sample Login

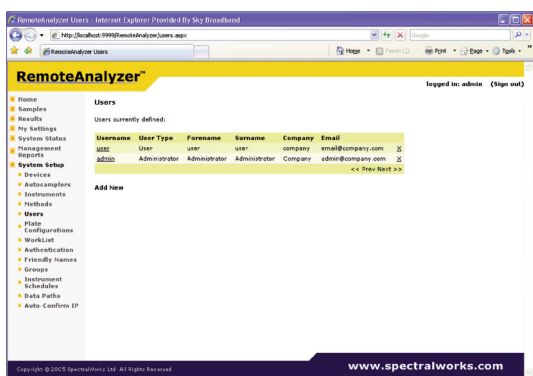


Figure 3. RemoteAnalyser Administrators Page

### MANAGEMENT SYSTEM SET-UP AND TRACKING

A typical administrator's screen for RemoteAnalyser is shown in Figure 3. From this page a number of options can be selected to give access to user accounts, instrument configuration and method set up etc. RemoteAnalyser works in conjunction with the native instrument software to provide a simple to use top level interface. Reports can be customised to provide management information such as instrument utilisation or user/group activity. Additionally, automated report templates can be created to be printed or emailed, for example, monthly invoices can be generated for each research group based on their usage.

### DATA ACQUISITION AND PROCESSING

Data acquisition is carried out using the native instrument software so the acquired data files are maintained entirely intact and independent from subsequent data processing. Data files are converted into a file format optimised for file size and data processing speed. Processing methods are created by the administrator using the relevant section in 'System Setup' and the secure results are made available on the server or passed to another location as required. Further data processing can be carried out using local copies of AnalyzerPro, where AnalyzerPro fully integrates and communicates with the RemoteAnalyser server. Within AnalyzerPro, additional MS data processing capabilities, including integration with NIST library searching and target compound analysis, are available.

### SUMMARY

The system is currently in use at Southampton School of Chemistry and the benefits outlined above are already being realized.

The mass spectrometrists does not need to compromise choice of open access instrumentation based on functionality of proprietary open access software since RemoteAnalyser is a cross-platform option.

Additional benefits include the ease of system and sample monitoring, enhanced administration benefits such as real-time accounting and tracking of group and individual usage.

Administration of the system is extremely flexible and the administrator can monitor and interact with any sample at any time. The output to the users is posted immediately on the server for ready access at anytime and can be easily transferred to an electronic document or electronic notebook.

RemoteAnalyser is the 21st Century solution to instrument management, data handling and reporting. The cross platform capability of this software means instrument choice due to software related issues is not relevant, i.e. RemoteAnalyser = no compromise.



## VISION Software for UV-Visible Spectrophotometers Unveiled

**Thermo Fisher Scientific** has announced the availability of the latest upgrade to its VISION software package for Thermo Scientific Evolution™ and Helios™ UV-Visible spectrophotometers. Version 4.1 adds unique features to the already advanced VISIONsecurity™, VISIONlife™ and VISIONpro™ software, including the ability to remotely trigger the start of data collection and automatic readings via remote fibre optic probes. The new software provides extended capabilities for a wide range of applications in general QA/QC, materials science and life science markets.

Version 4.1 enables VISIONlife and VISIONpro software to instruct Thermo Scientific UV-Visible spectrophotometers to automatically start collecting kinetics data. This is particularly useful in the life science market where fast reactions need to be studied. The upgrade package enables the interface between the pneumatic drive of a rapid mixing accessory to mix reactants and trigger the spectrophotometer to start collecting the data remotely. When coupled with the Evolution 300, version 4.1 enables 50 data points to be collected in the first 1000 milliseconds of the reaction with a dead time of less than 8 milliseconds.

The new software also features remote fibre optic probe triggering to provide automatic readings remotely from the instrument, thus increasing time efficiency and providing greater sample throughput. This feature is of interest to researchers whose target vessel is located a short distance (<10 meters) away from the spectrophotometer. For example, a remote fibre optic probe could be used inside a drybox or controlled atmosphere environment.

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## New Spectrographs Added to a Growing Range Of Spectroscopy Solutions

**Andor Technology** will launch two new spectrographs at Laser 2007 and will also announce details of 3rd party agreements with two new specialist spectrograph manufacturers, Headwall Photonics and Specim.

The Shamrock SR-500 and SR-750 spectrographs are welcome additions to Andor's Shamrock family, offering ultimate resolution for more detail and clarity across a wide range of applications including Raman and fluorescence. Features include direct and responsive control of the spectrograph and camera through Andor Solis (s) software allowing the user to control wavelength and calibration, grating selection, shutter control and filter selection as well as a "step and glue" facility to seamlessly join spectra together.

The Shamrock SR-500 has an aperture of f/6.5, reciprocal dispersion of 1.7nm/mm, and a wavelength resolution of 0.05nm. The SR-750 has an aperture of f/9.8, reciprocal dispersion of 1.1nm/mm and a wavelength resolution of 0.03nm. Both offer a mechanical scan range of 0 to 1200nm, wavelength accuracy of ±0.2nm and a focal plane size of 28x14mm.

Adding to the growing range of spectroscopy solutions Dr. Colin Coates, Andor's Market Development Manager, explains "Combined with Andor's range of high performance detectors and associated accessories we are now able to offer our customers pre-aligned and calibrated data collection solutions for spectroscopy. Since our inception almost 20 years ago Andor has spent time consolidating our range of detectors, spectrographs and accessories to give our customers world beating data collection solutions to fit every application".

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