

AnalyzerPro[®]

Universal MS Data Processing Software



Turning complexity into opportunity; see what others don't see and build a competitive advantage

SpectralWorks



Introducing AnalyzerPro

AnalyzerPro® is a productivity software application for both low and high resolution LC-MS and GC-MS data with support for multiple vendors' data. This comprehensive post-processing utility provides optimized workflows for sample-to-sample comparison, target component analysis, quantitation and library searching for data generated from any LC-MS and GC-MS platform. Using its proprietary algorithms to detect obscured components that existing software packages are unable to find without additional information, AnalyzerPro is the perfect tool to mine your mass spectrometry data. Additional functionality allows the comparison of multiple samples and data sets using our ProfileAnalyzer™ and MatrixAnalyzer™ processing as well as statistical analysis using principal component analysis and analysis of variance (ANOVA) to determine whether there are any significant differences. By supporting data files from multiple vendors, AnalyzerPro is the only data processing software you need. This reduces the requirement for training on additional software packages, increases efficiency and delivers a consistent approach to data processing and presentation of results regardless of instrument or analytical technique.

AnalyzerPro at a Glance

- Deconvolution of GC-MS & LC-MS data
- Supports all major manufacturer's instruments and legacy instruments
- Targeted and non targeted analysis
- Extraction of closely eluting peaks
- Data alignment
- Quantitation
- Statistical analysis, PCA and ANOVA
- Elemental composition
- Integration with RemoteAnalyzer
- Seamless integration with NIST libraries
- Accurate mass compatible
- Background file subtraction
- Tabular display of results
- Custom reports

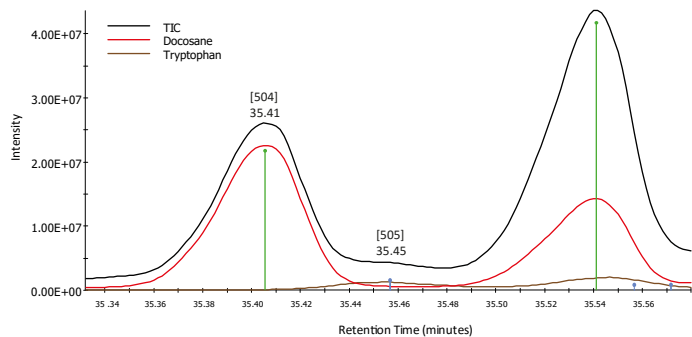
Chromatographic Deconvolution

Data from analytical instruments needs to be processed before it can be analysed and interpreted. The key feature in AnalyzerPro is its ability to chromatographically deconvolute data. Deconvolution is defined as 'reversing the effects of convolution'. For chromatographic data the biggest problem is co-elution of chromatographic peaks as many components will not be completely separated by the column. Using AnalyzerPro we can determine which masses belong to which of the co-eluting peaks. The deconvolution step also allows the creation of target component lists. For comprehensive data analysis, automated library building is available in AnalyzerPro which includes all the components within an entire data set. This differs from a traditional target component list generated from standards in that the components do not need to be identified until later in the analysis. However, the traditional approach is also available in AnalyzerPro.

For example, a metabolomic study was conducted on the kidney tissue of a rat model for polycystic kidney disease. AnalyzerPro processed the data and library searched the found components against an in-house target component library of authentic metabolite standards. Components were also searched against the NIST mass spectral database for tentative identification of the unknowns. Tryptophan, the deconvoluted peak at the retention time 35.45 minutes with a base peak of m/z 202 was only found in the polycystic kidney tissue and not the healthy age-matched and sex-matched control animal kidney tissue. As with many metabolomic studies, there may be several interpretations of this finding which in turn may generate new hypotheses to test.

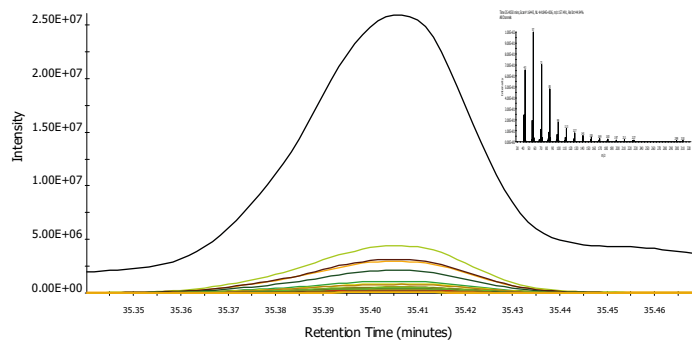
As shown below, AnalyzerPro is able to automatically determine component 505 (tryptophan) in the disease state samples in the presence of high levels of Docosane (a hydrocarbon added for RI calculation).

Kidney 6_6_010[MS], Time 35.4436 mins, Scan# 16466, Intensity 2.69e+007, Relative Intensity 28.25%
All Channels

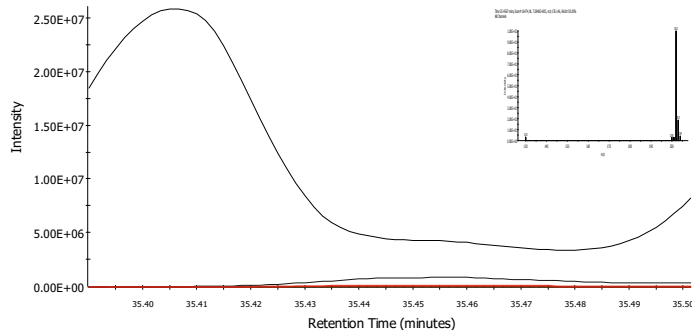


In each case, high quality library searchable spectra were obtained for each component with no prior knowledge of the sample. The following shows the extracted ion chromatograms for each of the masses of the components and their corresponding spectrum.

Kidney 6_6_010[MS], Time 35.3807 mins, Scan# 16428, Intensity 1.70e+007, Relative Intensity 65.39%
All Channels



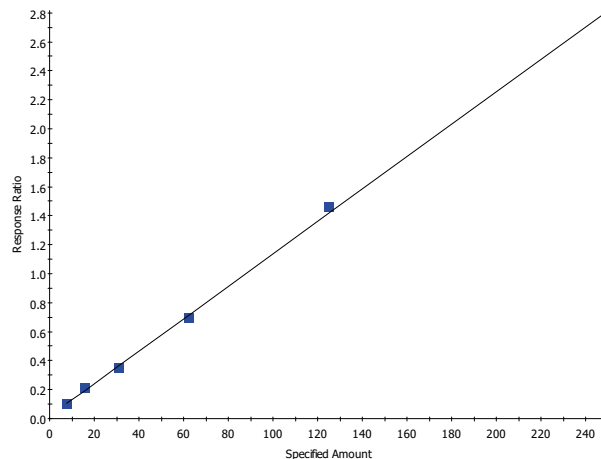
Kidney 6_6_010[MS], Time 35.4607 mins, Scan# 16476, Intensity 1.04e+007, Relative Intensity 40.17%
All Channels



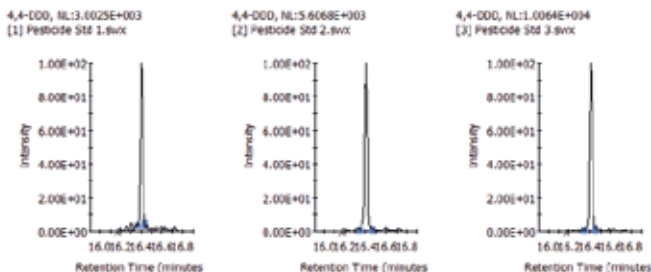
Quantitation

AnalyzerPro is fully compatible with the standard quantitation workflow as well as reporting requirements. The Quan Viewer has been optimized so that large data sets can be reviewed, checked and edited if necessary, in an extremely efficient manner to allow the user to focus on their results. This includes being able to visualize and edit calibration curves.

4,4-DDD, $f(x) = 0.011186x + 0.018508$ $R^2 = 0.9992554558$
RSD%=8.20



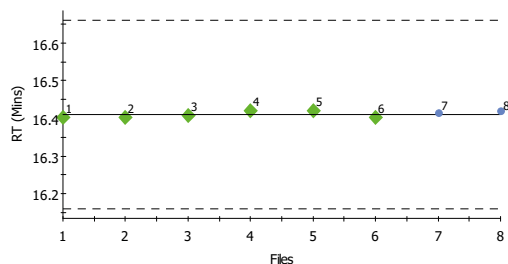
It is possible to scroll through thumbnails of the chromatographic peaks to quickly identify integration results that may require modifying. The selected thumbnail is also displayed in a larger format which allows for easy drag-and-drop editing of a peak's start and end points. The thumbnails can either show the compound, the internal standard or a combination of both. Modified quantitation results are flagged and saved with a time-stamp so that it is always possible to recognize modified results and return to the original results if necessary.



The quality of the calibration data can be assessed with the retention time reproducibility displays in the Quan Viewer for both the compounds and the standards. These displays are color coded so that results can be quickly reviewed by exception.

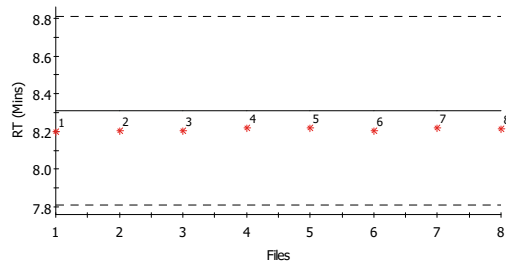
In the example below for the pesticide 4,4-DDD, we are able to quickly determine that the first 6 samples are calibration standards and that they are all within the expected retention time window. Had any of the standards fallen outside the window, a red diamond with have been displayed instead of the green one. The two blue dots representing samples 7 and 8 indicate that these are unknown samples and in both instances contained a measurable amount of the pesticide.

4,4-DDD, Expected RT = 16.4100



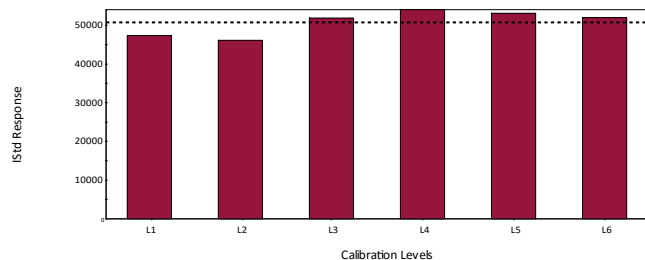
In the case of the internal standards, we can immediately see that the retention times are running slightly earlier than expected but are still within tolerance. The red stars indicate that the responses for all the standards are lower than the user defined response limit.

[IStd] Acenaphthene-d10, Expected RT = 8.310, RSD%=0.08



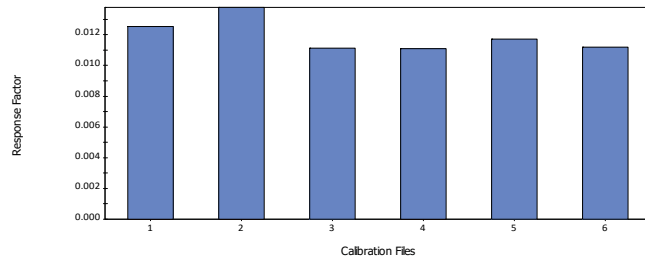
We can visualize the responses for any of the internal standards across all the data set to ensure that the minimum and maximum responses are consistent. The average is represented by the dotted line so that you can effortlessly spot potential problems which can then be further investigated.

Internal Standard Responses for Acenaphthene-d10



It is also possible to review the response factors for each compound, this shows the consistency of the results and is another display to assess the quality of the data.

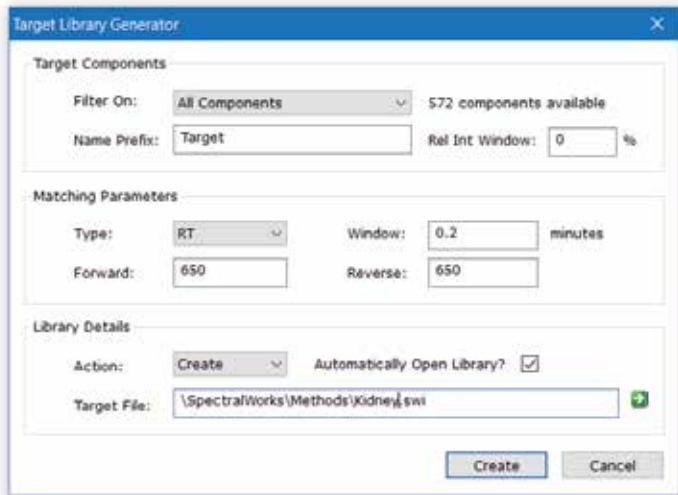
Response Factors for 4,4-DDD, Average Response Factor 0.01191
RSD%=8.20, Not Found=0, Excluded=0



Target Component Analysis

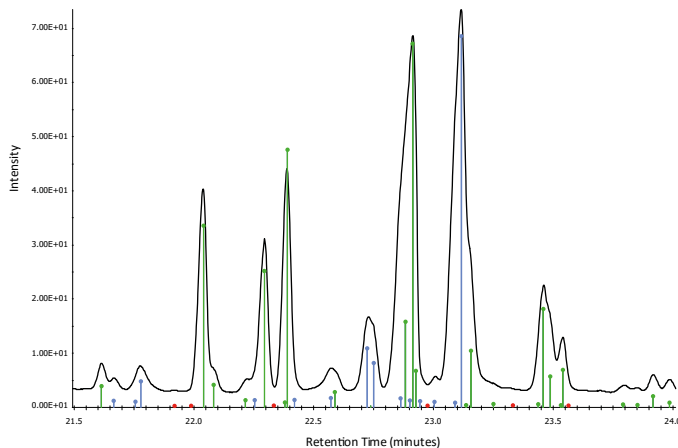
Sample profiling using target component analysis is a useful tool for determining the relative amount of a target substance present in a complex mixture or to search for characteristic components of your samples. It is widely used in application areas such as environmental screening or the forensic determination of drugs of abuse. It is also important to be able to determine non-target components in areas of product adulteration and AnalyzerPro is able to cover these workflows with ease.

AnalyzerPro provides a simple and accurate way to create your target component libraries from the components found in a sample. Retention time or retention index (RI) information as well as spectral, all NIST format library match information and meta data can all be captured for each component. Additional confirmation criteria using specified ion ratios for components can also be set. Target component analysis also captures reliable component abundance information (height and area) for each sample that is processed.

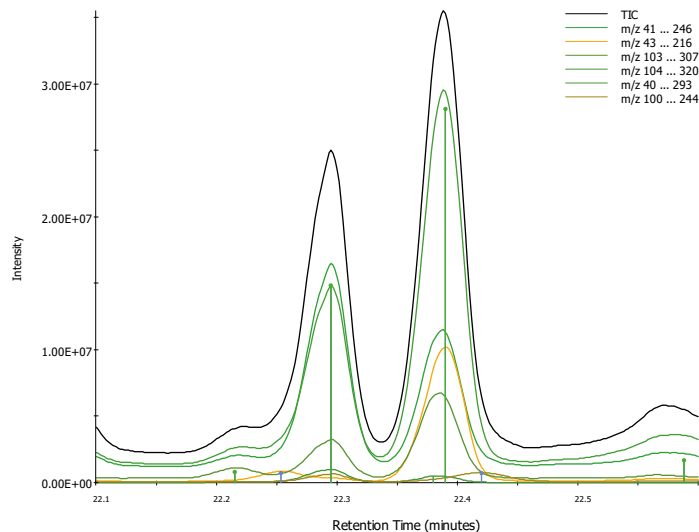


Curation of target component libraries allows additional components to be added (appended) to the library, edited or deleted as required.

In the figure below, found components are shown in green and new non target components in blue. Target components that are not found are indicated by a red marker on the baseline.



Components can be visualized using the component ions, the base peak, selected ions or the sum of the component ions for visual confirmation of the peak deconvolution. This allows you to clearly see the deconvoluted chromatographic components that may be hidden in your data. In the example below, there are six components found over the retention time window. The component chromatograms for each of those components as well as the TIC are shown.



When processing samples, components can be quickly identified and reported as being found, not found or unknown. The unknown components are components that have been found in a sample which were not in the target component library. These components can subsequently be added to your library. When processing a sequence of samples, it is possible to automate this step such that when each new unknown component is detected it is added to the target library. In this way you can build up a comprehensive target library from all of your data files. This 'super' library can then be used for profiling multiple samples using MatrixAnalyzer and its PCA visualization tool.

Export Results for Additional Statistical Analysis

AnalyzerPro is able to quickly and easily export results into csv or Microsoft Excel format so that additional statistical calculations can be performed by complimentary third-party software packages so that you get the very best of your data.

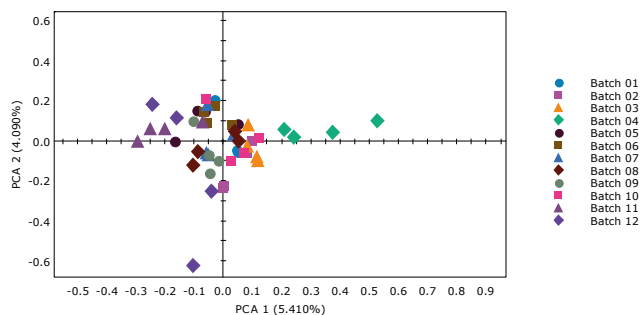
MatrixAnalyzer

MatrixAnalyzer allows you to view the individual target component abundances in each of your processed samples. The data can be normalized to an internal standard component and to sample weight information if required. Results can be reported based on component abundance derived from height or area and from the sum of the component ions, specified component ions or base peak ion depending on specific requirements. The data can be viewed in a number of ways. A standard tabular view includes delta RT/RIs, average values, standard deviation, a component coverage percent and p-values. Further processing and reporting of principal component analysis is also available. MatrixAnalyzer is used extensively in metabolomics but the underlying workflow can be used in many other applications where sample differences are being investigated.

Class information can be incorporated in to your data processing sequence to assist with the interpretation of the PCA results and the component information including abundance can be exported to third party software for further processing. As an example, the PCA report shown below represents 12 derivatization batches for a mixture of metabolite standards. The PCA shows that batch 4 is clearly distinct from the other batches but with a total explained variance of 9.5% for PCs 1 and 2, the batches appear fairly similar.

PCA is used in many applications where differences between samples are being investigated. Additional visualization tools in MatrixAnalyzer allow for comparison of response and retention times for components across all samples and classes further assisting with the interpretation of the overall results.

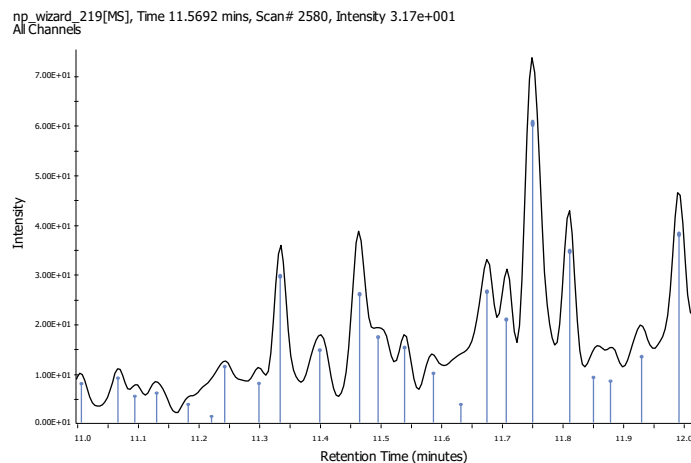
PCA Scores from results with log transformation



ProfileAnalyzer

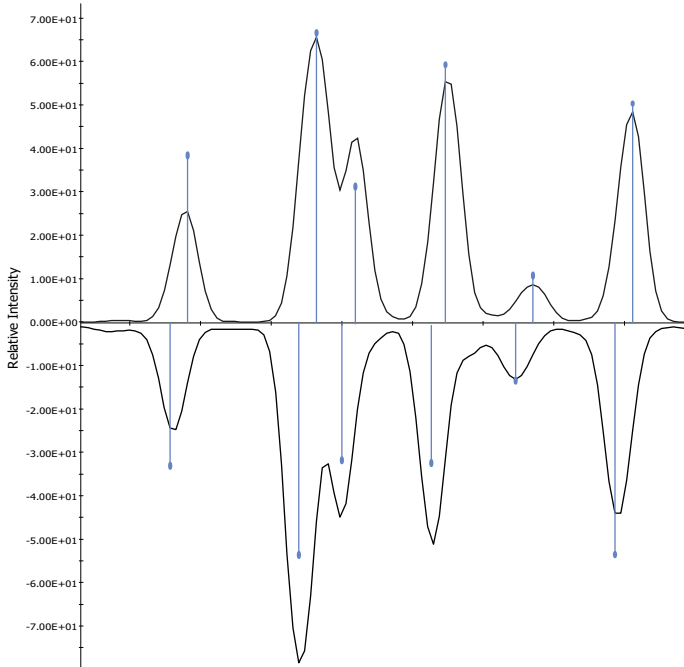
ProfileAnalyzer is an integrated data processing tool within AnalyzerPro which automates chromatographic matching for the analysis and identification of complex mixtures. It can be used in areas from clinical applications such as identifying inherited metabolomic disorders like urinary organic acidurias including phenylketonuria (PKU) to flavour and fragrance analysis where it can be used for product authentication or to detect counterfeit or adulterated products. ProfileAnalyzer turns found components over a chromatographic range into a spectrogram which can be compared objectively against a library of spectrograms to provide an accurate assessment of one sample's similarity to another.

A spectrogram is created by taking the deconvolved components or components based on a targeted library and turning them into a spectrum-like display where the x-axis is either retention time, retention index or in the case of a targeted approach the name of the target component. The y-axis represents either the area or the height of the component. The unknown spectrogram is compared against the best match or a specifically selected spectrogram. A single spectrogram is identical to the typical AnalyzerPro chromatographic display. For example:



After processing, ProfileAnalyzer graphically shows the comparison of the unknown sample against the entries in the spectrogram library which it was searched against. A subsection of a fire debris analysis is shown using a targeted approach.

Spectrogram Display
 Unknown1.swx, NL:1.2435E+009
 gas_gas90_90a.swx, NL:1.1558E+009



In this instance, the top match shows a 73% confidence that our unknown sample matches the profile / spectrogram of Gas 90. This is consistent with findings from an expert assessment of the sample. Below are the top ten results of the unknown compared against the fire debris spectrogram library.

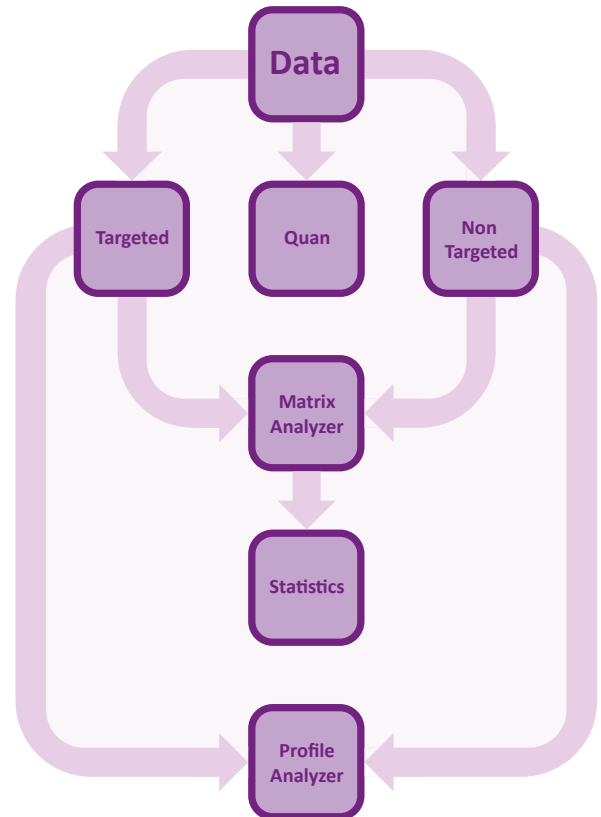
Spectrogram Results from Unknown1.swx

	Spectrogram Library	Confidence %
1	Gasoline, 90% evaporated	73.02
2	Gasoline, 95% evaporated	66.14
3	Gasoline, 80% evaporated	65.79
4	Premium gasoline, 90% evaporated	61.49
5	Premium gasoline, 50% evaporated	60.79
6	Premium gasoline, 75% evaporated	59.18
7	Aromatic - Floquil Dio-Sol Thinner	58.93
8	Mixture: Gasoline, 90% evaporated and kerosene	56.10
9	Aromatic - STA-BIL Fuel Stabilizer	54.83
10	Mixture: Gasoline and diesel fuel	51.14

Bring it All Together

AnalyzerPro is the complete solution for analyzing your complex data files regardless of the instrument it was acquired on or the analytical technique used. From gaining biological insight into your data through to screening pesticides, AnalyzerPro is the perfect software tool for your workflow to ensure quality results are delivered as quickly as possible. Results are presented in a simple and clear manner through its multiple layouts and customized reporting functionality.

AnalyzerPro is also able to interface with our open access software solution for mass spectrometry – RemoteAnalyzer®. RemoteAnalyzer provides a simple and consistent client server web browser interface for sample submission and data review regardless of which vendor supplied the instrument and has recently been expanded to encompass NMR instrumentation as well. Further information regarding RemoteAnalyzer is available in our RemoteAnalyzer open access software brochure.



About SpectralWorks Limited

SpectralWorks Limited is a leading UK based software development company.

We are dedicated to providing innovative solutions targeted for markets within the life sciences industry and have strong working relationships with a number of the major instrument manufacturers. Coupled with our collaborations in academia and industry, we believe we have the right balance between scientific and software development expertise to provide the best scientific solutions for the end user.

Our vision at SpectralWorks is to improve the way software is integrated within the laboratory environment by providing the correct solutions to increase productivity and reduce overheads. We achieve this by maintaining focus on the end user, listening to their requirements and ensuring that they have the right tools to handle their day to day tasks.

In addition to the wide range of mass spectrometry software products, we provide highly respected consultancy services. These services are able to cover the complete software development cycle or specific steps within a project life cycle. These services are frequently utilized by instrument vendors and end users that demand the best for their laboratories.

We are a privately owned company, incorporated in the United Kingdom in January 2004 and are based in Runcorn, United Kingdom. Our offices are located on a 60 acre business park 25 miles from Manchester International Airport and 10 miles from Liverpool's John Lennon Airport.

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Our facilities provide us with access to MS and other instrumentation as well as ensuring that we have the best infrastructure to develop and test software.

As well as direct sales, we have partner resellers. SpectralWorks offers Original Equipment Manufacturers (OEM) the ability to distribute our products and algorithms using their own branding. We also provide custom development for individual companies looking to automate and unify the software used within their laboratories using our extensive industry experience.

Our customer base is varied but predominately based within Australasia, Europe and North America. It encompasses academia, hospitals, government and industry.

Support is available via telephone, email or our web based support site. We always reply to communication as soon as possible and endeavour to reply within 24 hours with a statement of the problem and an estimated date for a solution.

About AnalyzerPro

AnalyzerPro is a data deconvolution software application for LC-MS and GC-MS data. It utilizes proprietary algorithms to detect obscured components that existing software is unable to find without additional information.

For a free 15 day trial licence, visit our website:

<http://www.spectralworks.com>



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