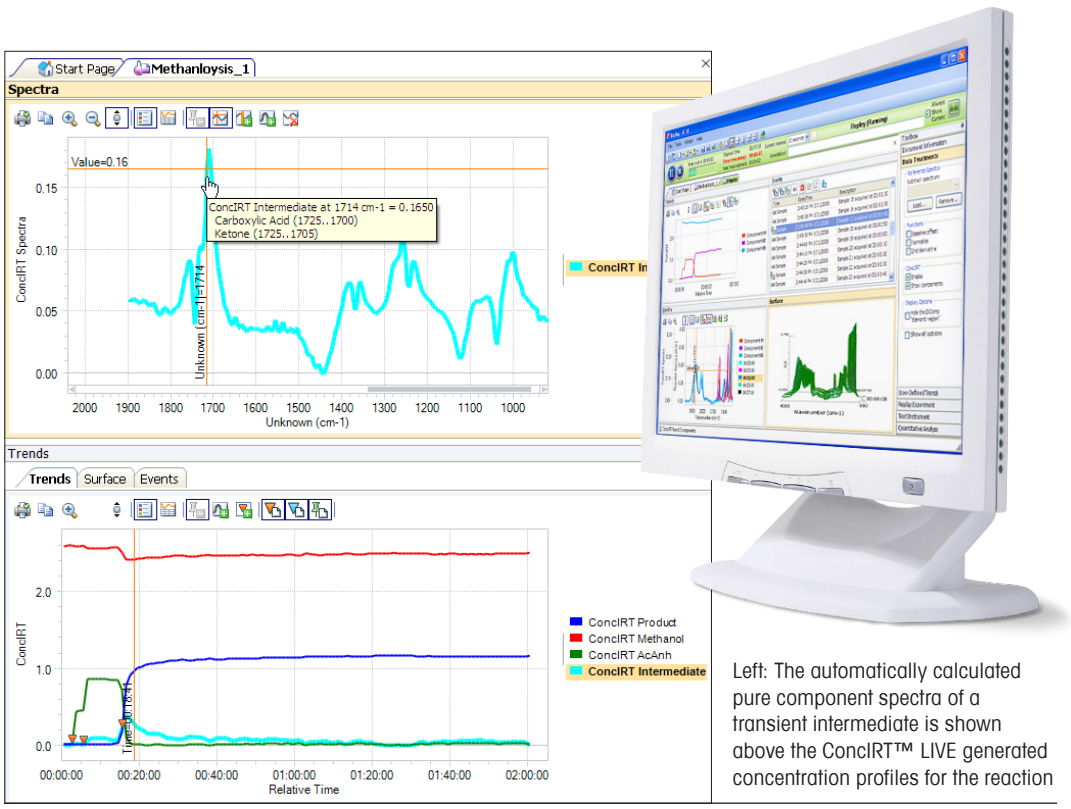
In Situ Spectroscopy

Gain Immediate Reaction Information

with ConcIRT™ LIVE for iC Software

ConcIRT™ LIVE software automatically transforms spectroscopic data into reaction information without the need for any specialized knowledge or data manipulation.

ConcIRT™ provides reaction information, in real time, that allows the scientist to speed the development, and improve the quality, of high-value compounds by characterizing reaction performance through identifying and quantifying key reaction species.



Left: The automatically calculated pure component spectra of a transient intermediate is shown above the ConcIRT™ LIVE generated concentration profiles for the reaction

METTLER TOLEDO

ConcIRT™ LIVE

Built-in Expertise

A combined knowledge base of over 150 years in FTIR-based reaction chemistry has enabled us to develop the advanced ConcIRT™ algorithm which provides the maximum amount of information from each reaction. It generates accurate component profiles and calculated spectra. ConcIRT™ automatically profiles reaction components, in real time, without any user input.

Simply Intelligent

ConcIRT™ LIVE software allows the user to rapidly generate quantitative and qualititative information from dynamically changing spectroscopic data. Typically, the goal of an experiment is to generate concentration profiles (concentration as a function of time) and to identify specific components. ConcIRT™ extracts relevant chemical information without any user interaction or user input required.

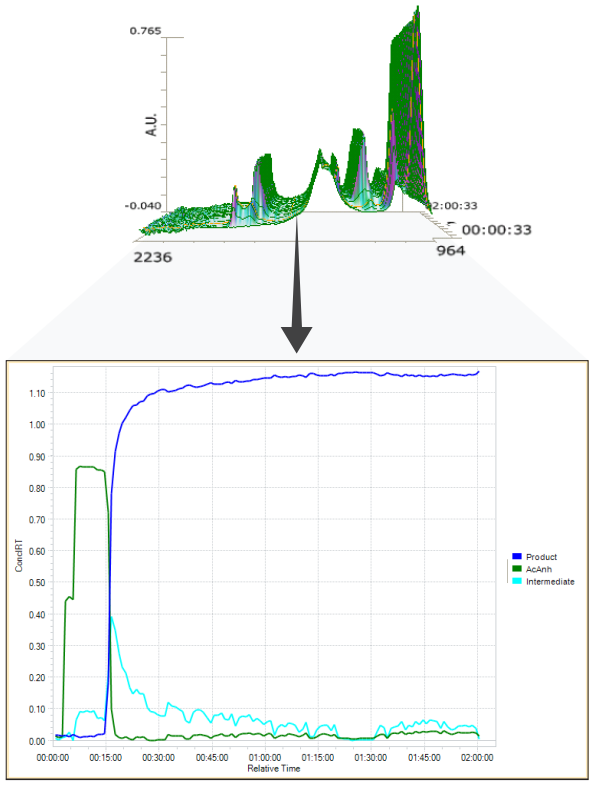
Transforms Data to Information

ConcIRT™ is designed to speed and simplify the understanding of complex chemical reactions and automatically identifies the number of chemical components and their relative concentration profiles. ConcIRT™ separates reaction data into pure component spectra and profiles without the need for any user interaction or specialized expertise.

It searches the reaction data for changes as a function of time, even in the presence of severely overlapping spectral absorptions. Frequencies that change at the same rate are assumed to belong to the same component and are mathematically resolved as a pure component spectrum. The resolved spectrum is then used to calculate the relative concentration profile.

ConcIRT™ generated component spectra can then be compared with pure component reference spectra for additional confirmation. Such processes can help identify unknown intermediates and to determine reaction mechanism or pathways. The relative concentration profiles can be used to study the relative consumption and formation of key reaction species.

ConcIRT™ LIVE is an intuitive application that helps solve complex chemical problems and provides a better understanding of chemical reactions without the need for grab sampling and time consuming reference techniques.



ConcIRT™ LIVE automatically converts *in situ* data into reaction information, providing insight into chemistry without the need of traditional reference techniques.

www.mt.com/iCIR

For more information

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