



PACER™ Software

- Targeted Quantitation: Maximum Throughput, minimum effort

High Throughput Targeted Quantitation with Exception Based Review



Bruker's PACER™ software provides extremely fast, accurate quantitative results for high throughput targeted analyses in the routine lab by building on the powerful Bruker GC and LC Triple Quad MS instruments. PACER addresses the real crunch in quantitative data review – peak integration – by using its powerful “Exception Based Review” feature set.

Almost all existing data and quality review systems are focused on the final calculated values (e.g. is a calculated concentration deviating from a pre-determined limit). But this can be too late in the process, as all of those calculated values are based on peak detection and integration, and wrong peaks equals wrong results! PACER looks for problem data (“exceptions”) starting with the chromatographic peak itself, and then all the way through the workflow – a comprehensive, peak-to-paper review!

Intelligent algorithm

At the heart of the PACER exception based review workflow is the unique EMG (Exponentially Modified Gaussian) automated peak integration algorithm.

This intelligent algorithm can identify and correctly integrate the most difficult chromatographic peaks, even at very low signal to noise ratios. PACER eliminates the need for expert (or non-expert) human interaction to judge chromatograms. And because the peak integration is so reliable, the flags produced by user defined quality rules reduce the review process to only those peaks that need attention – *Exception Based Review*.

Save time and use computing power (not more people!) to drive the quantitation workflow.



Feature Rich, Streamlined, ...

PACER focuses on providing a quick and efficient route through the activities of data processing, review, and reporting.

New, modern interface

The PACER interface is designed for simplicity and clarity, presenting information and options at the time you need them.



Exception based review with color-coded flags

In order to facilitate rapid verification of samples, PACER utilizes an optional set of user-defined quality rules which trigger the appearance of flags: colored graphics and letter codes that call attention to areas that may require further investigation. There are two general types of flags: actionable flags (for example, coverage, ion ratio co-elution) and informative flags (for example, ULOQ).

Descriptive text, detailing the nature of the flag is revealed by simply hovering the mouse cursor over the colored flag. Flags can be activated or deactivated as required.

Red flags remind users to check the peak and/or integration performed. Blue flags inform users of issues derived from the found peak area and/or concentration (e.g. a concentration under the Lower Level of Quantitation).

... Results-Driven Workflow

Training peak detection

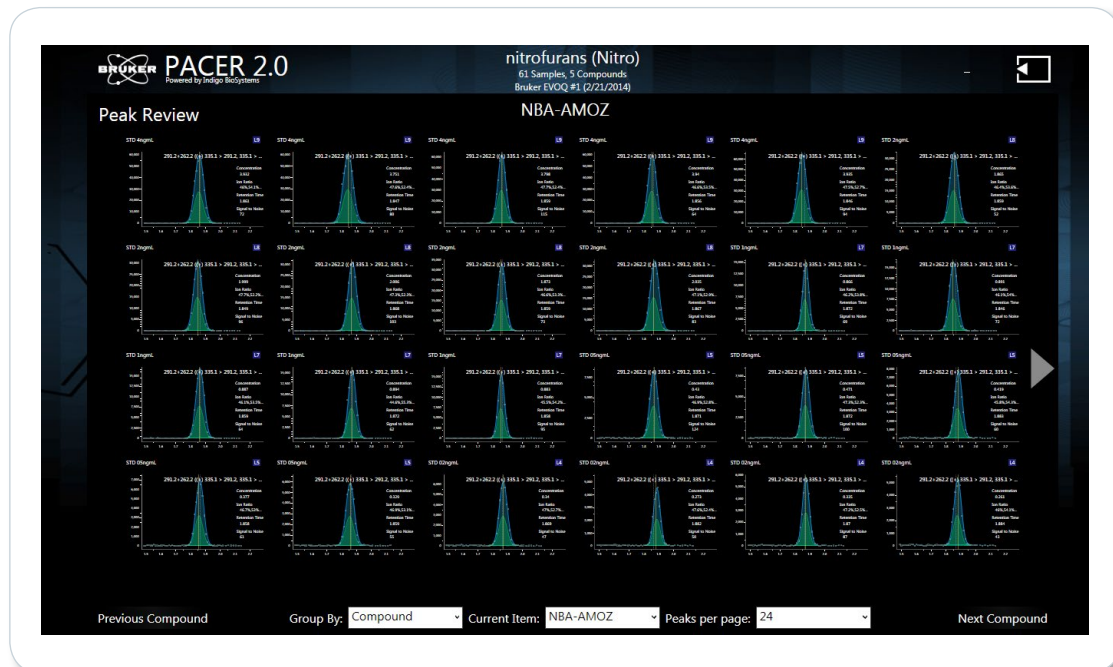
In order to minimize the time needed for detailed peak review, PACER automates a sophisticated set of algorithms based on exponentially-modified Gaussian (EMG) peak detection and integration. These algorithms include a peak modeling technology that can utilize the calibration standards to 'train' and refine the approach used for detecting compounds in highly complex matrices, even when the compounds are present at very low levels.

Batch at a glance

The "Batch at a Glance" feature displays multiple quantifier and qualifier chromatograms on a single screen, providing a quick visual way to identify flags and other significant batch data.

Batch and method locking

To prevent unintentional changes, PACER provides the ability to lock batches and methods. A locked batch or method cannot be processed or modified until it is unlocked.



To generate reports in exactly the format needed in the lab, PACER provides Dash reporting. Dash allows you to customize and print reports in either PDF or CSV format (for import into Microsoft Excel).

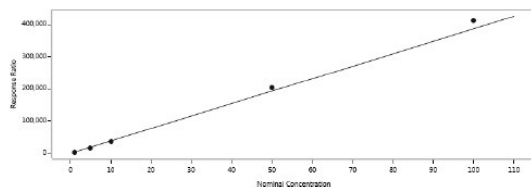
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Recalc List (RCL):	C:\BrukerWS\MSTutorials\TQ\pesticides_test_samples.rcl		
Acquisition Method:	C:\BrukerWS\MSTutorials\TQ\Pesticide_mix_method.mth		
Processing Method:	C:\ProgramData\Bruker\PACER\Methods\Untitled\2014-10-22\@5.38.PM\Untitled		
Instrument ID:	Bruker GC/MS #1	Operator:	
XMS Datafile:	c:\BrukerWS\MSTutorials\TQ\Pesticide_mix_calibration 5ppb.xms		
Sample Name:	M16-5ppb_after	Acq Date/Time:	23-Aug-2011 01:17:56
Vial/ Position:		Injection Volume:	
Sample Type (Level):	Calibration (2)	Dilution:	Mult = 1.000 / Div = 1.000

	As Injected	In Sample	Flags
Conc:	4.596	4.596	

Retention Time:	17.94
Area:	1000620
Height:	655032

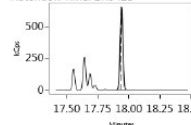
Alpha-cypermethrin
Curve Fit: LINEAR IGNORE 1/X2
Coeff. Det. R²: 0.995
 $y = 3897.29x + -1234.21$



Alpha-cypermethrin

$$(+)\ 163.0 > 127.0$$

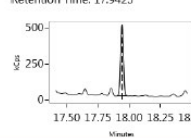
Retention Time: 17.9425



Alpha-cypermethrin Qual: 1

(+) 181.0 > 152.0

Retention Time: 17.9425



In addition to features described above, PACER software includes many other capabilities to improve and enhance the user experience, from tooltips and keyboard shortcuts to advanced copy/paste functionality.

PACER is a compelling and capable software production system for the business of quantitation, building on the powerful Bruker Triple Quad MS instruments.

PACER addresses the real crunch in data review – peak integration – in two critical ways:

- EMG peak detection and integration offers improved performance in seeing the true peak signal buried in the noise, to give you the best chance of not needing to manually review.
- But when necessary, begin your exception based data review process where it needs to begin – not at the calculated value, but at the peak itself. PACER and exception based review streamlines the entire process from sample to report.

The best way to experience PACER is to try it out. Please contact us for a free demonstration!

For research use only. Not for use in diagnostic procedures.



Bruker Daltonik GmbH

Bremen · Germany
Phone +49 (0)421-2205-0
Fax +49 (0)421-2205-103

Bruker Daltonics Inc.

Billerica, MA · USA
Phone +1 (978) 663-3660
Fax +1 (978) 667-5993

ms.sales.bdal@bruker.com - www.bruker.com