

# Multi-analyte Quantitation Software



## LabSolutions Insight for Efficient Multi-analyte Data Confirmation and Review

## Multi-analyte Data Review

With LabSolutions Insight software, quantitative results for a complete series of data files can be displayed side-by-side for comparison and QC review. All of the chromatograms for a selected target compound can be displayed simultaneously, making it easy to review the detected peaks and confirm the quantitative results. Color-coded QA/QC flags quickly identify any outliers that require further examination. Results can be displayed in a variety of ways, allowing users to select the view that is best suited for their workflow, and when necessary, peaks can be re-integrated and re-quantified directly from LabSolutions Insight.



• Using the LabSolutions Insight with a GC/MS Database and LC/MS/MS Method Package

When used in conjunction with one of Shimadzu's application-specific GC/MS Databases and LC/MS/MS Method Packages, LabSolutions Insight allows users to process data files, and perform QA/QC data review for all samples in one easy, seamless workflow.



Environmental Pollutant Analysis



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- Smart Pesticides Database
- [LC/MS]
  - Method Package Residual Agrochemicals
  - Method Package Veterinary Drugs

#### [GC/MS]

- Environmental Quick-DB
- Smart Environmental Database

#### [LC/MS]

Method Package Water Safety

- Metabolic Component
- Analysis
- Smart Metabolites Database
  [LC/MS]

[GC/MS]

- Method Package Primary Metabolites
- Method Package Lipid Mediators
- MRM Library Metabolic enzymes in yeast





#### [GC/MS] • Smart Forensic Database

#### [LC/MS]

- Method Package rapid Toxicology
  Screening
- Method Package Forensic Toxicology

### Color-coded QA/QC Flags

In LabSolutions Insight, quantitative results can be compared to established criteria, and any outliers are color-coded for easy identification and further review. Five color-coded criteria levels can be defined, making it easy to determine which data points are outliers, and which specific QC criteria were not met. Any changes made to calibration curves or manual peak integration are immediately reflected in the color-coded flags.

## • Example of Using Flags for Quantitative Review

The example below illustrates how an orange flag was set to identify moldy odor compound concentrations that exceeded a defined cautionary limit of 1.0 ppt (part-per-trillion), and a red flag was used as a warning to identify those which had exceeded 10 ppt. In the figure below, quantitative results are tabulated at the top of the screen, while the bottom of the screen simultaneously displays peak identification and integration. Both views include the color-coded flags.





## Refined Report Output

Data reports can be customized for specific user requirements. All compounds can be included, or a summary report can be created of just the compound that failed to pass the defined QA/QC parameters. The tabulated report can include calculated concentrations, ion ratios, and chromatograms for all sample data files. Quantitative information (such as peak areas or area ratios) can also be output as CSV files for use in multivariate analysis.



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## System Configurations Using Multiple Client Computers

Additional licenses of LabSolutions Insight allow review and confirmation of multiple analytes on client computers via a LAN. Even when multiple instruments are used, analysis administrator can review data obtained from each instrument on a client computer. It can relieve instrument computers from analysis by running post-acquisition analysis in office and improve operation efficiency. Additional licenses are installed as needed so the system can be easily expanded at low cost in the future.



File management on a file server is recommended for systems with more than 5 users.

#### **Applicable Models**

GCMS-QP series and GCMS-TQ series models LCMS-8030,LCMS-8040,LCMS-8050,LCMS-8060

#### **Operating Environment**

OS: Microsoft® Windows® 7 Professional Workstation software: GCMSsolution Ver. 4.30 or later LabSolutions LCMS Ver. 5.80 or later



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