

Forensic Application Note

Rapid reporting of targeted and untargeted Drugs of Abuse analyses

CSols

laboratory systems integration

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Links **4** LIMS



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Background

With its high selectivity and sensitivity, liquid chromatography tandem mass spectrometry (LC-MS/MS) has become the tool of choice for the analysis of illicit drugs in forensic laboratories. Whether the analysis is for criminal proceedings like drug driving, sports doping, custody cases, workplace or abuse/rehabilitation monitoring, the ability to offer both screening and confirmatory methods in targeted and untargeted approaches provides the accurate, flexible and robust detection of any compound. Methods also work reliably in a wide range of matrices including oral fluids, urine, serum, blood and hair, extending the scope of LC-MS/MS to many different applications.

Challenges

Whatever the method or matrix though, forensic laboratories face a range of challenges to ensure the review and reporting of results, and their subsequent transfer of reportable results to their Case Management or LIMS system, is not a tedious and error prone task. Aside from the sheer volume of data, some of these challenges are:

- Ensuring the consistency of the instrument run sequence, for example to ensure that calibration and control samples (AQC's) are placed and named correctly according to laboratory SOPs.
- Also ensuring that sample placement is reliable, especially where samples are run in duplicate (i.e. A & B sample).
- Merging of results from multiple analysis method runs (of the same samples) where multiple methods have been used to overcome issues with inadequate separation or a limitation of the instrument analysis software.
- Dealing with cut off limits and limits of detection (LODs) for each compound.
- Applying tools to accurately monitor the rigour of the run.
- Quickly interpreting results (i.e. Positive/Negative) locally, filtering samples for confirmatory testing.
- Offering flexible reporting for large number of compounds.
- Automating IQC/AQC checks and Uncertainty of Measurements statistics.
- Being able to produce data files or a communications mechanism to easily move data between the instrument and a Case Management or LIMS system, with full auditing and no loss of data integrity.

In order to overcome these challenges the CSols **Links for LIMS** and **AqcTools** software offer powerful and flexible solutions to streamline reporting, starting with instrument setup.

Instrument setup

Instrument users can make use of the **Links for LIMS Instrument Setup** program to interact directly with LIMS using for example, worklists to build Sciex Analyst, Sciex OS or Cliquid compatible batch runs ready for immediate use by the instrument. Predefined templates can enforce placement of all sample types, automatically duplicate samples, and uniquely name batch and file names for full data integrity. See Figure 2 for example run.

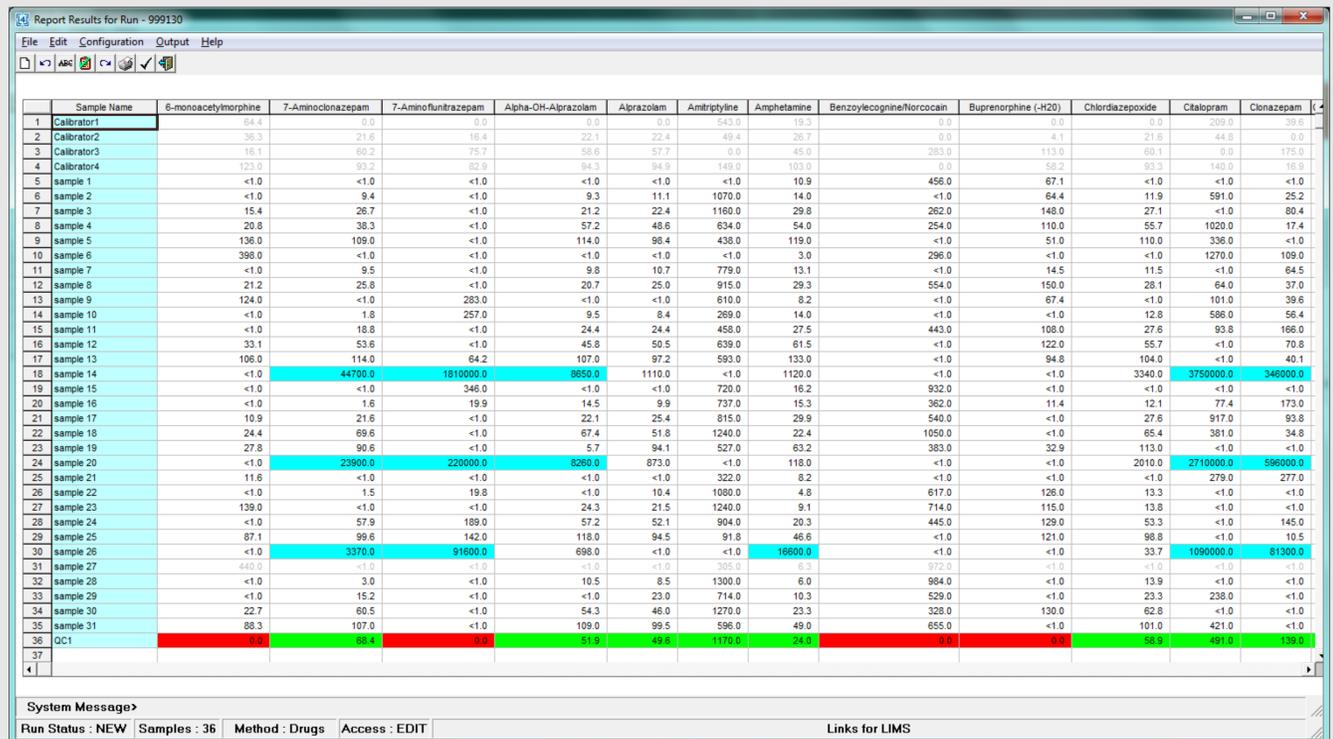


Figure 1: Reviewing results in Links for LIMS prior to LIMS upload after loading LC-MS/MS results. N.B. Results > Cut off limits are highlighted with blue background, LLOQ & ULOQ flags are provided and IQC/AQC quality is colour coded.

Results loading and reviewing

Once a batch run is completed all results can be read directly by the **Links for LIMS Report Results** software module. This first automatically synchronizes and validate the results file with the setup data collected earlier. It will then automatically apply any calculations, formatting, rounding, flagging or logic rules relevant to the specific method. The display (see Figure 1 above) is fully configurable allowing results, derived results and demographic information to be displayed if required. Where large numbers of compounds or samples are analysed the display scrolls accordingly. If the SOP requires further validation of results, using for example ion ratios, retention times, internal standard recoveries, or other measures, the relevant calculations and flagging can also be done automatically rather than having to rely on third party applications like Excel. For screening methods, predefined 'cut off' limit values can be used to automatically identify 'positives' and only these are reported. **Links for LIMS** will also create a new batch run of positive samples ready to allow the confirmatory run to quickly run on a second instrument without the need for further manual administration.

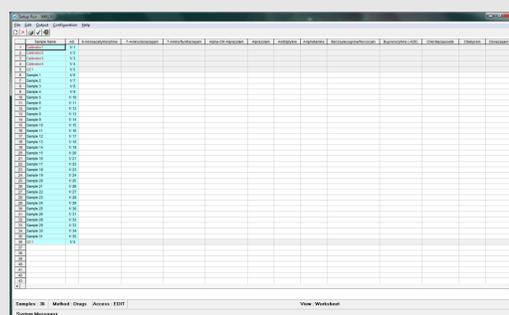


Figure 2: Links for LIMS setup run ready for transfer to the instrument



AQC & Unknown Results checking & transmission

Links for LIMS will automatically flag AQC results that lie outside 2SD or 3SD (Standard deviations) of the mean for each AQC sample (Westgard rules). For more comprehensive AQC charting, exceptions and trend checking all AQC results can be transferred to the CSols **AqcTools** software (See chart – Figure 2). Unknown results can be sent in many different electronic formats or protocols to suit the Case Management or LIMS system. Full auditing of the transfer is used and data integrity can be enforced using encryption.

Summary

Links for LIMS software can provide a 'one stop' solution with powerful and configurable functions, to complement a Sciex LC-MS/MS based Forensic Drugs of Abuse workflow. This will allow the instrument to be used to its' maximum capacity, often saving several hours of manual or Excel based interpretation per run. In addition the software eliminates data transcription from both instrument setup and results transfer steps, and prevents between 3% & 5% transcription errors.

Further Information

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