Clinical Application Note

Rapid reporting of targeted and untargeted Drugs of Abuse analyses

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Links 4 LIMS

AqcTools™

Background

Screening for the analysis of drugs of abuse in biological specimens to detect and identify compounds in hospital patients with suspected acute intoxication is usually the role of the clinical toxicology department. With its high level of selectivity and sensitivity liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) provides an attractive solution to the clinical toxicologist for the rapid analyses of large panels of drug (illicit or prescription) compounds using both targeted and untargeted methods.

Challenges

However when reporting results from either method approach, laboratories often face a range of challenges to ensure the review and reporting of results to LIMS/LIS systems is not a tedious and error prone task. Some of these challenges are:

• Merging of results from multiple analysis method runs (of the same samples) which have been used to overcome poor separation or limited by the instrument analysis software.

• Dealing with cut off limits and '<' or '>' values not always supported by the LIMS/LIS system.

• Interpreting results (i.e. Positive/Negative) locally prior to upload, to overcome limitations of the LIMS/LIS system.

• Finding a compromise between reporting results for a very large number of compounds while still providing appropriate and succinct results to clinicians.

• Providing rapid turnaround times as the patients may be in a critical condition or where the hospital has no control over the length of the patient stay.

• Ensuring appropriate consistency in results quality.

• Automatically incorporating IQC/AQC checks.

Links for LIMS software offers a powerful and flexible solution to overcome these challenges to streamline reporting, starting with instrument setup.

Instrument setup

Instrument users can make use of the **Links for LIMS**

Instrument Setup program to fetch and validate specimens that have arrived in the laboratory directly against their LIMS/LIS system. This ensures data integrity, removes transcription and allows the software to automatically build a Sciex Analyst, Sciex OS or Cliquid compatible batch run file. To achieve this **Links for LIMS** conducts host queries to the LIMS/LIS system using user checked specimen barcode IDs, or can fetch all outstanding test requests. This validates the specimen(s) and test code(s) and optionally can extract patient demographic information to help laboratory staff.
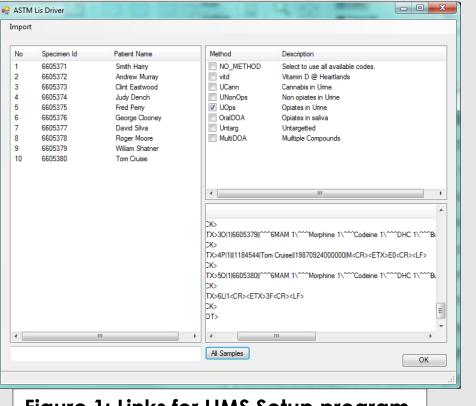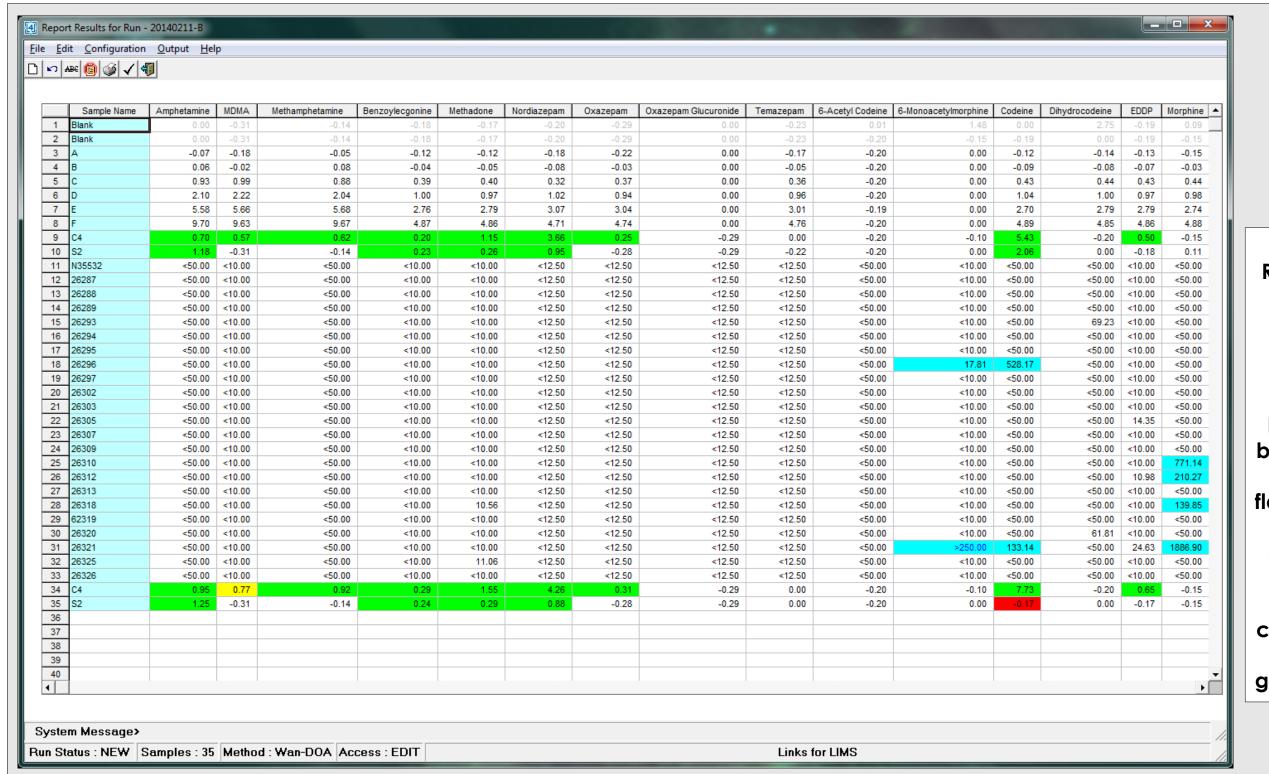

Figure 1: Links for LIMS Setup program

Figure 2: Reviewing results in Links for LIMS prior to LIMS upload. N.B. Results > Cut off limits are highlighted with blue background, LLOQ & ULOQ flags are provided and IQC/AQC quality is colour coded. Also similar compounds types have been grouped together.

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 will automatically synchronize and validate the results with the setup data collected earlier. Any predefined calculations, formatting, rounding, flagging or logic rules relevant to the specific method will also be applied. The display (see Figure 2 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 a method requires ion ratio checks to be made, the relevant calculations and flagging can also be done automatically. However clinicians may not wish to be overloaded with data, especially with results from compounds that are below the cut off or LOQ limits. As a consequence laboratories adopt different strategies to filter and interpret how results are reported. To assist in this process, rather than use third party programs like Excel, **Links for LIMS** can be used to automatically apply those strategies to the results. The outcome can be provided in the display, or sent 'in background' when results are submitted back to LIMS/LIS. To illustrate some of the examples that have been implemented, details are given in the table below.

	LIMS-LIS Order Request	LIMS-LIS Report	Calculations & Logic	Result Examples
1	Single Test code	Single Test code	Standard including rounding and flagging.	27.5
2	Single Test code	Single Test code	Standard plus the positive results > Cut off are concatenated into a single text result where a letter represents a positive compound. All other results are not sent.	ABCDEF. N.B Must be decoded by middleware or LIMS/LIS.
3	Single Test code	Multiple Test Codes – positives only (e.g. Screening)	Standard, plus all compounds with results > Cut off or the normal range, are reported as 'POS' or Abnormal 'A'. The single (Order request) Test code is sent as 'Positive' or 'Negative' to complete the test, and further test codes are automatically added & sent for all positive compounds. All other results are not sent.	P, POS, POSITIVE, A, etc.
4	Single Test code	Multiple Test Codes – positives only with results (e.g. Confirmation)	As above but the compound name is reported where result > cut off.	Cocaine, Temazepam, etc. N.B. May also use generic Test Codes (DOA01, DOA02 etc.) to hold the name.
5	Single Test code	Multiple Test Codes – positives & negatives	Standard plus all components are reported as 'POS' or 'NEG' with or without the results.	27.5 & POS or 0.0 & NEG sent for all compounds.
6	Single Test code	Multiple Test codes matching groups	Positive compounds sorted per group with single or multiple compound names reported.	Cocaine (for cocaine group), Diazepam & Temazepam (for Benzodiazepines group) etc.
7	Suite Test code	Multiple Test Codes – positives only	As 3 above but either the result or the name of the compound name is reported where result > cut off.	Cocaine, Temazepam, or 27.5, 95.0 etc
8	Multiple Test codes	Multiple Test codes	Standard including rounding and flagging.	27.5

Results transmission

Output from **Links for LIMS** software can be sent in many different formats or protocols. In a clinical setting, the ASTM 1394 messaging protocol is preferred as this is compatible with all LIMS/LIS and middleware systems. See below for an example message.

Summary

Links for LIMS software can provide a 'one stop' solution with powerful and configurable functions, to complement a Sciex LC-MS/MS based Drugs of Abuse workflow. Allowing 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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