Solution towards a vendor-neutral and secure transfer of data between LIMS and Instruments

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on behalf on an interdisciplinary working group originating from the e-environment community

The Challenge

Improve data security and data integrity in LIMS-to-Instrument integration.

Typical bioanalytical integration scenario:

- Transferring sequence **worklist information** from a LIMS to an LC-MS instrument
- Returning LC-MS **result information** back to a LIMS
- ... to form a secure and compliant closed loop

The journey to improved data security and DI compliance

The challenge reported in EBF White Paper

'Current products still force the bioanalytical laboratories into manual and time-consuming quality-control steps to mitigate the DI risks. With the increased number of citing's during health authority inspections over the last few years, the message is clear: DI issues must be resolved!'

The objective cited in EBF White Paper

Our focus on LC/MS–LIMS interface has many immediate benefits: **primarily reducing the time and effort required to manually perform quality control of data transfer**. The proposal should also be seen as a move away from the current status quo and to showcase that progress can be made relatively simple if and when all agree on a common standard.

White Paper

For reprint orders, please contact: reprints@future-science.com

Improving data integrity in regulated bioanalysis: proposal for a generic data transfer process for LC–MS from the European Bioanalysis Forum

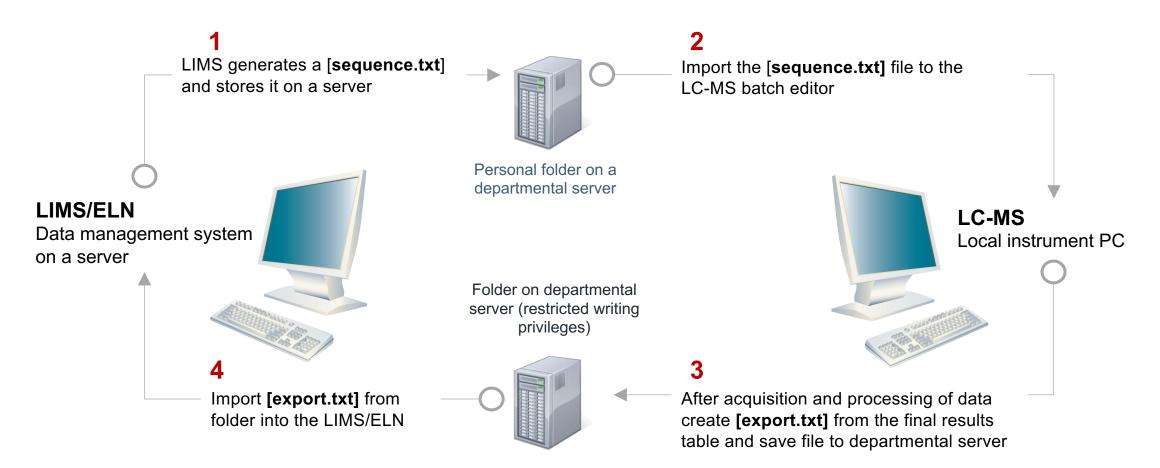
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Bioanalysis (2020) 12(14), 1033-1038

This resulted in a **joint effort of the user and vendor community** to create a vendor-neutral, standards-based solution, as reported in this presentation.

A traditional data transfer cycle

Current data transfer cycles require manual and time-consuming quality-control steps to mitigate the DI risks. Limitations include; ASCII / human readable files, it is a proprietary solution, and it is not secure.



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Key points for a solution

Transferring sequence information from a LIMS to a LC-MS instrument and exporting LC-MS results back to a LIMS.

Mitigate DI risks

Making make data transfer more secure Make it easier to audit

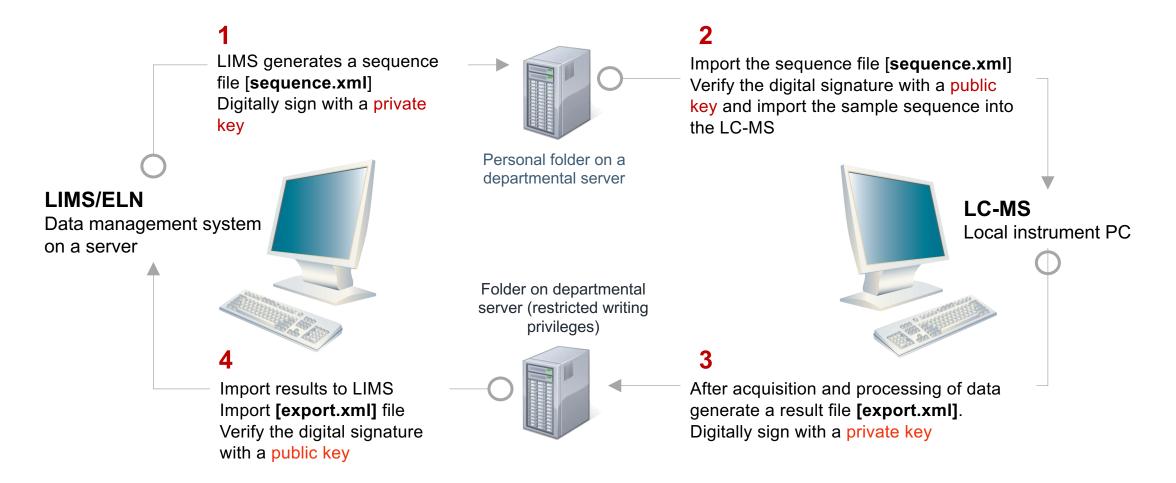
Have a near-zero impact for any user experience The proposed changes for any LC-MS user are near-zero. Sample batches can be loaded from the same folder location and results exported with a single click

Standardized solution for all software / instrument interfaces

No proprietary solution required for specific LIMS-Instrument combinations

A proposed way forward; replacing .txt files with digitally signed .xml files

Advantages include; Ascii / human readable files, it is a standardized solution, and it is a secure The security is based upon a private-public key digital signature pairing



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The technical solution

The key point is to mitigate DI risks by making make data transfer more secure, but it is also important to make it easier to audit and have a near zero impact for any user experience

Standardized Format

Worklist/result information is transferred as a **vendor neutral XML file format** (data model is flexible and scales beyond LC-MS workflows; open to all instrument providers; reuses existing schemas).

- Data model is derived from the AnIML format
- Flexible and scalable beyond LC-MS domain

Standardized Security

Improving security by signing the files with a digital signature using Public / Private key – logic, provided by the World Wide Web Consortium (W3C) Signature Working Group.

- Attributable you can tell who made a signature
- Tamper-evident you can tell if data has changed since signing
- Automated validation before accepting a file, instrument or LIMS can confirm its provenance
- Stored in XML easy to read and write, broad developer experience
- Royalty free logic free libraries for Java, .net, ...

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The proposed model has 2 files; a worklist file and a results file

The core content was identified in the EBF White Paper However, it is important to note that the AnIML file format is scalable, and more fields could be added

LIMS to LC-MS Worklist File

Run/File specific fields

Study/project Run/batch file User good laboratory practices (GLP) Plate barcode File name

Sample specific fields

Sample name/ID Sample barcode/ID Analyte(s)/internal standard(s) name Dilution factor Order number Plate position Sample type Concentration

LC-MS to LIMS Results File

Run/File specific fields

| Study |
|---------------|
| Run |
| Date/time |
| User |
| Plate barcode |
| File name |
| User comments |

Sample specific fields

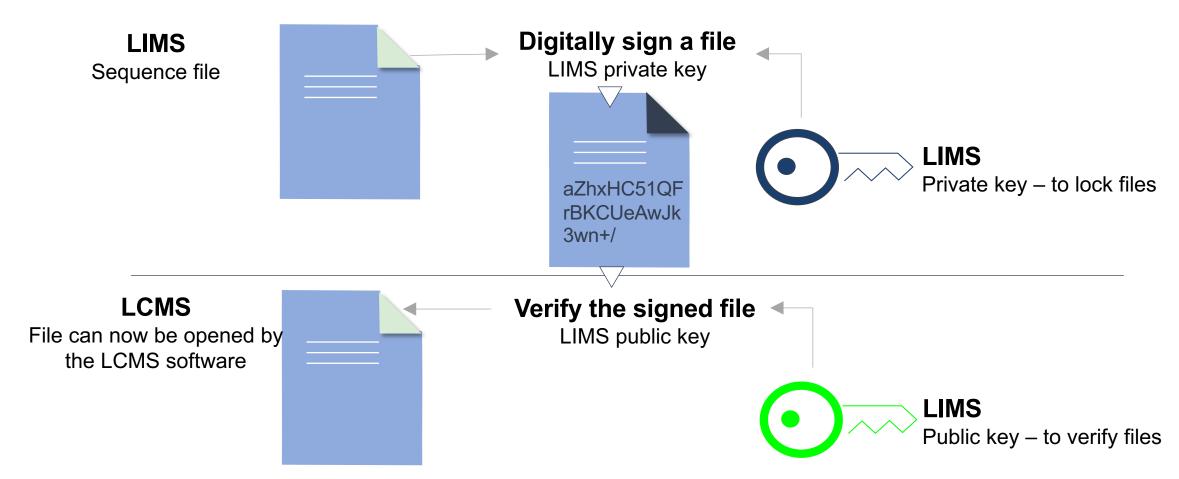
Sample barcode/ID Analyte(s)/internal standard(s) name Analyte raw data (peak area, peak height, ratio, etc.) Analyte(s) concentrations data Dilution factor Plate position

Fields which have been identified in the EBF White Paper Bioanalysis (2020) 12(14), 1033–1038.

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What is a private/public key pairing and a digital signature?

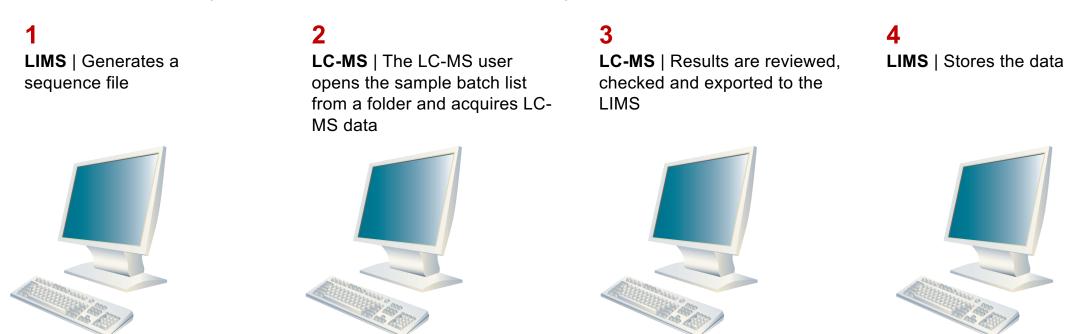
This slide highlights the sequence file data transfer from the LIMS to LCMS (the same technology is used for the return trip back from the LCMS back to the LIMS)



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No change in 'user experience'

A user will be able to open a worklist file, review data and export results, as 'usual'.



Under the hood

LIMS | generates a sequence file, converts it into a digitally signed XML file format with a public key and sent to the 'watcher' folder. **LC-MS** | opens the sequence file and verifies the signature with a public key to make sure it has not been tampered with. A batch file is created to run samples LC-MS | the results are sent to an export file, the results are converted into an XML format and digitally signed with a private key. The file is sent to the LIMS watcher folder. **LIMS** | opens the digitally signed export.xml file with a public key and verifies it has not been tampered-with. Results are then stored into the LIMS.

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Step 1: Export sequence from the LIMS/ELN

Generating a digitally signed [sequence.xml] file

| | ОК | | | |
|---|--|--|---|--|
| SecureDataTransfer ^ Result-Copy Result-Error | Name | ureDataTransfe | | |
| | This PC SecureDataTransfer Result-Copy | Clipboard Organize ✓ ↑ ▶ This PC ▶ Local Disk (C:) ▶ IMfiles ▶ Secure ▶ SecureDataTransfer ∧ Name ▲ ▶ Result-Copy ▶ TestStudy1-Run25(202106) ▶ Result-Import ▲ | Clipboard Organize Net ▼ ↑ ▶ This PC ▶ Local Disk (C:) ▶ IMfiles ▶ SecureDataTransfer ▶ SecureDataTransfer ^ Name ^ ▶ Result-Copy ▶ TestStudy1-Run25(20210622_1044).xml ▶ Result-Import ● | Clipboard Organize New Open Select <li< th=""></li<> |

Step 2: user opens a sample batch file and acquired LC-MS data

Size

The digitally signed sequence.xml file has been verified by the LC-MS software and the content has been converted to a vendor specific sample batch file which can be opened as 'usual' from a specified location.

| - I | _ - L | .IMS | | | | | | | |
|-----------------------|------------------|-------------------|--|--------------|---------------------|---------------------|------|---------------|--------------------------------------|
| File | Home | Shar | e View | | | | | | |
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| | | _ | | | | | | | |

| Name ^ | Date modified | Туре | |
|----------------|------------------|-------------|---|
| 🗹 📙 Batch | 19/05/2021 08:16 | File folder | |
| Export_Results | 19/05/2021 08:17 | File folder | |
| Method | 22/06/2021 09:27 | File folder | |
| Sequence | 19/05/2021 08:16 | File folder | • |
| Template | 19/05/2021 08:20 | File folder | 2 |
| | | | |

LC-MS user

→ ✓ ↑ → This PC → OS (C:) → LIMS

Selects the sample batch file in the 'usual folder location' and opens the sample list in the LC-MS software

Zero change to the user experience

The LC-MS software detects the [**sequence.xml**], verifies the signature and converts the file into the LC-MS sample batch format. The LC-MS user opens the sample batch file in the LC-MS application software.

One example is shown below.

| | | | | | | | | 1 |
|---------|------|-------|------------------|-------------------------------|----------------|-------------------------------|----------------------------|--------------|
| Postrun | Tray | Vial# | Sample Name | Sample ID | Sample Type | Method File | Data File | Data Comment |
| 1 | 1 | 1 | CalibnStd1 | PlasmaCalibnStd_0.9695 pg/mL | 1:Standard:(I) | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level1_ID1.lcd | Study_XH1179 |
| 2 | 1 | 2 | CalibnStd2 | PlasmaCalibnStd_1.939 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level2_ID2.lcd | Study_XH1179 |
| 3 | 1 | 3 | CalibnStd3 | PlasmaCalibnStd_3.879 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level3_ID3.lcd | Study_XH1179 |
| 4 | 1 | 4 | CalibnStd4 | PlasmaCalibnStd_7.08 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level4_ID4.lcd | Study_XH1179 |
| 5 | 1 | 5 | CalibnStd5 | PlasmaCalibnStd_20.14 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level4_ID5.Icd | Study_XH1179 |
| 6 | 1 | 6 | CalibnStd6 | PlasmaCalibnStd_40.28 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level6_ID6.lcd | Study_XH1179 |
| 7 | 1 | 7 | CalibnStd7 | PlasmaCalibnStd_105.922 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level7_ID7.lcd | Study_XH1179 |
| 8 | 1 | 8 | CalibnStd8 | PlasmaCalibnStd_210.352 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level8_ID8.Icd | Study_XH1179 |
| 9 | 1 | 9 | CalibnStd9 | PlasmaCalibnStd_280.469 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level9_ID9.Icd | Study_XH1179 |
| 10 | 1 | 10 | CalibnStd10 | PlasmaCalibnStd_350.586 pg/mL | 1:Standard | LC-MSMS_BioanalysisMethod.lcm | CalibnStd_Level10_ID10.lcd | Study_XH1179 |
| 11 | 1 | 11 | QC checks | AQC | 2:Control | LC-MSMS_BioanalysisMethod.lcm | QC_LevelAQC_ID1.lcd | Study_XH1179 |
| 12 | 1 | 12 | QC checks | LQC | 2:Control | LC-MSMS_BioanalysisMethod.lcm | QC_LevelLQC_ID2.lcd | Study_XH1179 |
| 13 | 1 | 13 | QC checks | MQC | 2:Control | LC-MSMS_BioanalysisMethod.lcm | QC_LevelMQC_ID3.lcd | Study_XH1179 |
| 14 | 1 | 14 | QC checks | HQC | 2:Control | LC-MSMS_BioanalysisMethod.lcm | QC_LevelHQC_ID4.lcd | Study_XH1179 |
| 15 | 1 | 15 | TimePoint_Pre-Do | AccessionCode_IDX1179_ZX1 | 0:Unknown | LC-MSMS_BioanalysisMethod.lcm | SampleID_t0_ID1.Icd | Study_XH1179 |
| 16 | 1 | 16 | TimePoint_0.08h | AccessionCode_IDX1179_ZX2 | 0:Unknown | LC-MSMS_BioanalysisMethod.lcm | SampleID_t0.08_ID2.lcd | Study_XH1179 |
| 17 | 1 | 17 | TimePoint_0.25h | AccessionCode_IDX1179_ZX3 | 0:Unknown | LC-MSMS_BioanalysisMethod.lcm | SampleID_t0.25_ID3.lcd | Study_XH1179 |
| 18 | 1 | 18 | TimePoint_0.50h | AccessionCode_IDX1179_ZX4 | 0:Unknown | LC-MSMS_BioanalysisMethod.lcm | SampleID_t0.50_ID4.lcd | Study_XH1179 |

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Step 3: Export Results (Shimadzu)

Review data and export results

Zero change to the user experience

LC-MS results are reviewed, if changes are made they can be documented in a standard audit trail. In this research application the results are exported to 'EBF LIMS' using a single click.

[Please note, the term EBF LIMS Integration is simply a 'placeholder name' in this research application build]

| | | | Results - Analyte | larger | | | | | |
|--------------------------------|--|------------------|-------------------|--|--------------------|-----------------|---------------|-------|-------|
| | # Name | # | Flag Result | Sample ID | Sample Type | Std. Conc. (pg/ | Conc. (pg/mL) | %Diff | Accur |
| | | | | T | T T | • | T | • | |
| V / | ☐ 1 Analyte Target | ✓ 4 | Report | PlasmaCalibnStd_7.08 pg/mL | Standard | 7.09 | 6.85 | -3.34 | |
| | 2 Internal Standard Target | 5 | Report | PlasmaCalibnStd_20.14 pg/mL | Standard | 20.14 | 20.68 | 2.70 | |
| Open | | √ 6 | Report | PlasmaCalibnStd_40.28 pg/mL | Standard | 40.28 | 40.03 | -0.63 | |
| | | 7 | Report | PlasmaCalibnStd_105.922 pg/mL | Standard | 105.92 | 109.96 | 3.82 | |
| TE3 | | 8 🔽 | Report | PlasmaCalibnStd_210.352 pg/mL | Standard | 210.35 | 223.48 | 6.24 | |
| . 1- | | 9 | Report | PlasmaCalibnStd_280.469 pg/mL | Standard | 280.47 | 290.47 | 3.57 | |
| Load Flags | | 10 | Report | PlasmaCalibnStd_350.586 pg/mL | Standard | 350.59 | 366.84 | 4.64 | |
| | | ☑ 11 | QC Checks OK | AQC | Control | 17.57 | 18.80 | 7.00 | |
| | | ✓ 12 | QC Checks OK | | Control | 5.68 | 5.82 | 2.39 | |
| | | | QC Checks OK | MQC | Control | 176.47 | 188.47 | 6.80 | |
| Export | | ✓ 14 | QC Checks OK | HQC | Control | 291.62 | 316.60 | 8.57 | |
| Results to File | | | Report Report | AccessionCode_IDX1179_ZX1 AccessionCode_IDX1179_ZX2 | Unknown Unknown | | -0.21 7.26 | | |
| | | | Report | AccessionCode_IDX1179_ZX2 AccessionCode_IDX1179_ZX3 | Unknown | | 40.79 | | |
| To EBF LIMS | | | Report | AccessionCode_IDX1179_ZX3 | Unknown | | 40.79 | | |
| | | - 19 | Report | AccessionCode_IDX1179_ZX4 | Unknown | | 46.87 | | |
| Export | the current results to a EBF LIMS compatible | results file. 20 | Report Report | AccessionCode IDX1179 ZX6 | Unknown | | 54.27 | | |
| | | | Report | AccessionCode_IDX1179_ZX7 | Unknown | | 49.38 | | |
| | | | Report | AccessionCode_IDX1179_ZX8 | Unknown | | 47.45 | | |
| | | | Report | AccessionCode_IDX1179_ZX9 | Unknown | | 39.03 | | |
| | | < | | | | | | | |
| | ISTD 506.00>293.00 (+) RT=6.264 | | 12 | Curve Fit: Default (Linear) Weighting: Default (1/A^2) Zero: Default (Not Forced) Mean RF: 5.665278e-003 SD RF: 1.151237e-003 %RSD: 20.320933 | | • | | / | |
| File View Edit Review | %6 | | 0. -0 | | | | | | |

LabSolutions Insight (Reviewer) - (VerifiedSequenceFile_BatchFile230621.lcb - LC-MSMS_BioanalysisMethod.lcm (Read Only)) [Pre-Release]

Export message (Shimadzu)

A simple confirmation

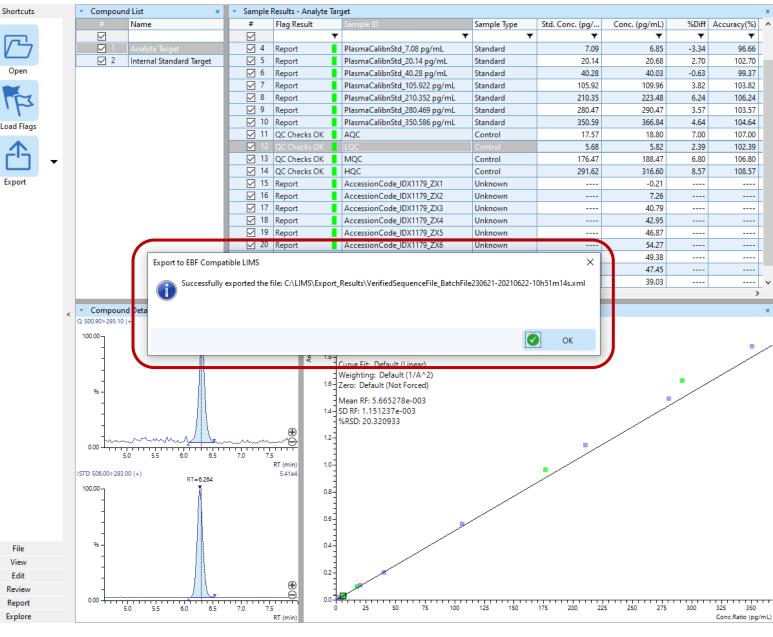
Exporting results to the LIMS

Once the export icon is clicked the results are then automatically processed by the LC-MS software;

- Results are converted into the **[export.xml]** format.

- The **[export.xml]** file is signed with a digital private key and moved to the LIMS watcher folder for verification and upload by the IM.

[Please note, the term EBF LIMS Integration is simply a 'placeholder name' in this research application build]



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Step 3: Export Results (SCIEX)

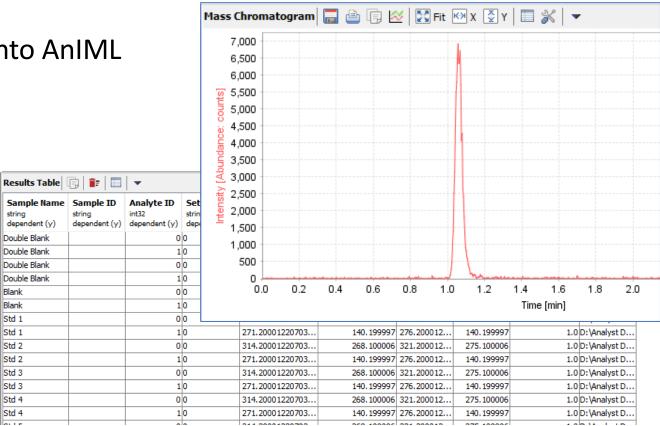
Review data and convert results

A SCIEX application converts Analyst files into AnIML XML result files:

Analyst data files (.wiff): includes sample information, method information, technique information, spectra and chromatograms.

Results table (.rdb): includes the results table, integrated chromatograms and the audit trail for that results table.

Analyst audit trail (.ata, .atd): includes all audit records contained in the original files.



AnIML files converted by SCIEX software provide a complete and accurate representation of the original Analyst[®] data, including result table, chromatograms, method and audit trail.

Signature verification (SCIEX)

Verification of integrity

- A digital signature can be applied to each result file.
- Users can verify signature in a simple dialog
- Tamper evident Users can check the ulletdigital signature status to determine if a file has been modified

| Public key: | Format: X.509 Algorithm: RSA Encoded: MIIBIJANBgkqhkiG9w0BAQ yHk3Qxe04YP2oK3/VTQ+bMnk4q4TQ Wie6JhwiXy+ixGIbNRWFn17Eq0T02 Nj6hhFQz4Lqx3e64TZdBLfv9x4qsK6j SfywVSNpfJZJqWd63QEU+NHUJUvn NfC/9ZVygAkN4GXG+GlbxDvCqcueD6 8fmf3pJaqVGPGBfZZf0KEmrCE9VFIE1 4lYRGORrL89BBfoPjyKGm2+wXPXCg/ | CCYVHvCjtyUyU/ESrWQ1F 2k5JcyhtG2e37Lm3RrF 7WoKbEVwwNSP2nIg1yaT3U JuM8kjwIPRFHNx1jhCnDN kv/I5mgipN9jdOKGuTm | |
|---------------------------------------|--|--|---|
| Signature properties: | userName : john.gibbons timestamp : 2021-01-20T09:57:09 | | |
| Validity period: Valid signature 📀 | Public key: | Format: X.509 Algorithm: RSA Encoded: MIIBIJANBgkqhkiG9w0BAQEFAAC yHk3Qxe04YP2oK3/VTQ+bMnk4q4TQjMhZ8 W1e6JhwiXv+ixGIbNRWFn17EqOT02CRYVH Nj6hhFQz4Lqx3e64TZdBLfv9x4qsK6j2k5JCy SfywV5NpfJ2JqWd63QEU+NHUJUvn7Wokb NFC/92VygAkN4GXG+GlbxDVCqcueD6uM8kj 8fmf3pJaqVGPGBfZZf0KEmrCE9VFIE1kv/Ism 4lYRGORrL89BBfoPjyKGm2+wXPXCg/W2IOj | thArM8NZG2xTmiMC ivCjtyUyU/ESrWQ1F htG2e37Lm3RrF EVwwNSP2nIg1yaT3U wIPRFNNx1jhCnDN gipN9jdOKGuTm |
| | Signature properties: | userName: john.gibbons timestamp: 2021-01-20T09:57:09 | |
| (| Validity period: Invalid signature 🔀 | Start: Fri Sep 27 05:40:24 EDT 2019 End: Sat Sep 26 05:40:24 EDT 2020 EXPIRED | |

Solution towards a vendor-neutral and secure transfer of data between LIMS and Instruments

Step 4: Importing the Results back into the LIMS

The LIMS verifies the signed results file [export.xml], if valid, results are stored into the LIMS system

| 🕆 퉬 🕨 This PC 🕨 Loca | | | | _ | | | | | | | | | |
|---------------------------|---|---|--|---|--|--|---|-----------------|---------|---------|------------|-------------|------------|
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Example

XML file containing analytical results

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 - <ExperimentStepSet>
 - <ExperimentStep Name="Bioanalysis" experimentStepID="e1">
 - + < Method>
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 - + <Parameter Name="ISTD RT" seriesType="Float32" seriesID="s14" dependency="dependent">
 - + <Parameter Name="ISTD Area" seriesType="Float32" seriesID="s15" dependency="dependent">
 - + <Parameter Name="ISTD Height" seriesType="Float32" seriesID="s16" dependency="dependent">
 - </SeriesSet>
 - </Results>
 - </ExperimentStep>
 - </ExperimentStepSet>
 - + <Signatures>
 - </AnIML>

Presented at the 14th EBF Open Symposium

Summary

What are the key advantages in this proposal

Data security is significantly increased

The current data transfer cycle requires manual and time-consuming quality-control steps to mitigate the DI risks. In this proposal, the goal is to negate quality control steps and meet the need of health authorities DI expectations.

The technology is widely adopted and a vendor neutral solution

- The technology is open for all vendors to use and is intended as a generic solution.
- No bespoke interfaces required, reducing implementation and validation cost.
- The key point is that if anyone tampers or changes the sequence or export file the change is recorded. All tampered files are detected.
- Implementations from several key vendors demonstrate the feasibility

It is designed to make a near-zero impact on the current user experience

- The changes are all designed to work 'under the hood'
- In this proposal the fundamental point is the data security is managed by the software and is not exposed to the user.

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How to move this forward as a way to improve data security, helping regulatory audits and creating a standard for moving data between a LIMS and LC-MS

- As with all changes, **we need 'buy-in'** from pharma companies for regulated bioanalysis
- To accelerate this change the quicker the 'buy-in', the quicker a product can be created.
- The 'buy-in' applies to:
 - pharma companies
 - regulators
 - partner consortia (AAPS)
 - more vendors

Going forward....

- Options for a 'Working Group' to consider expanding domain into other assays / techniques
- Future: file-less options

Opportunity to join

• We are looking to create a **group of early adopters** to deploy and refine the approach

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Bioanalysis

Improving data integrity in regulated bioanalysis: proposal for a generic data transfer process for LC–MS from the European Bioanalysis Forum

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