

# Data Integrity Workshop Outline

13th EBF Open Symposium

## Proposal for improving data integrity (DI) in regulated bioanalysis (15 minutes)

Increase compliance in today's LC-MS workflows

- **Overview of the current challenges in DI**
- **The proposed way forward in improving compliant data transfers**
- **What's under the hood, the technology behind the proposed way forward**

Gidion de Boer, Neil Loftus, Burkhard Schaefer

## Open discussion (20-30 minutes)

All EBF delegates are really encouraged to voice their thoughts/concerns/support

## Further discussion time is available from 17:30-18:00h (30 minutes)

All EBF delegates are really encouraged to voice their thoughts/concerns/support

# Data Integrity Workshop

13th EBF Open Symposium

## E-Environment; towards a vendor neutral bi-directional data transfer process

Gidion de Boer, Neil Loftus, Burkhard Schaefer (on behalf of the working group)

### Following the EBF 2019 workshop the White Paper was published in Bioanalysis

White Paper

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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

Cecilia Arfvidsson<sup>1</sup>, David Van Bedaf<sup>2</sup>, Susanne Globig<sup>3</sup>, Magnus Knutsson<sup>4</sup>, Mark Lewis<sup>5</sup>, Stuart McDougall<sup>6</sup>, Marco Michi<sup>7</sup> & Philip Timmerman<sup>\*,8</sup>

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The White Paper was published online 22 July 2020 and highlighted the need to increase compliance related to data integrity (DI) in today's LC-MS workflows  
**(Bioanalysis (2020) 12(14), 1033–1038)**

## Headlines from the White Paper

The challenge is clear; improve data security and DI compliance in transferring sequence information from a LIMS to a LC-MS instrument and exporting results back to a LIMS.

### **The challenge reported in the White Paper**

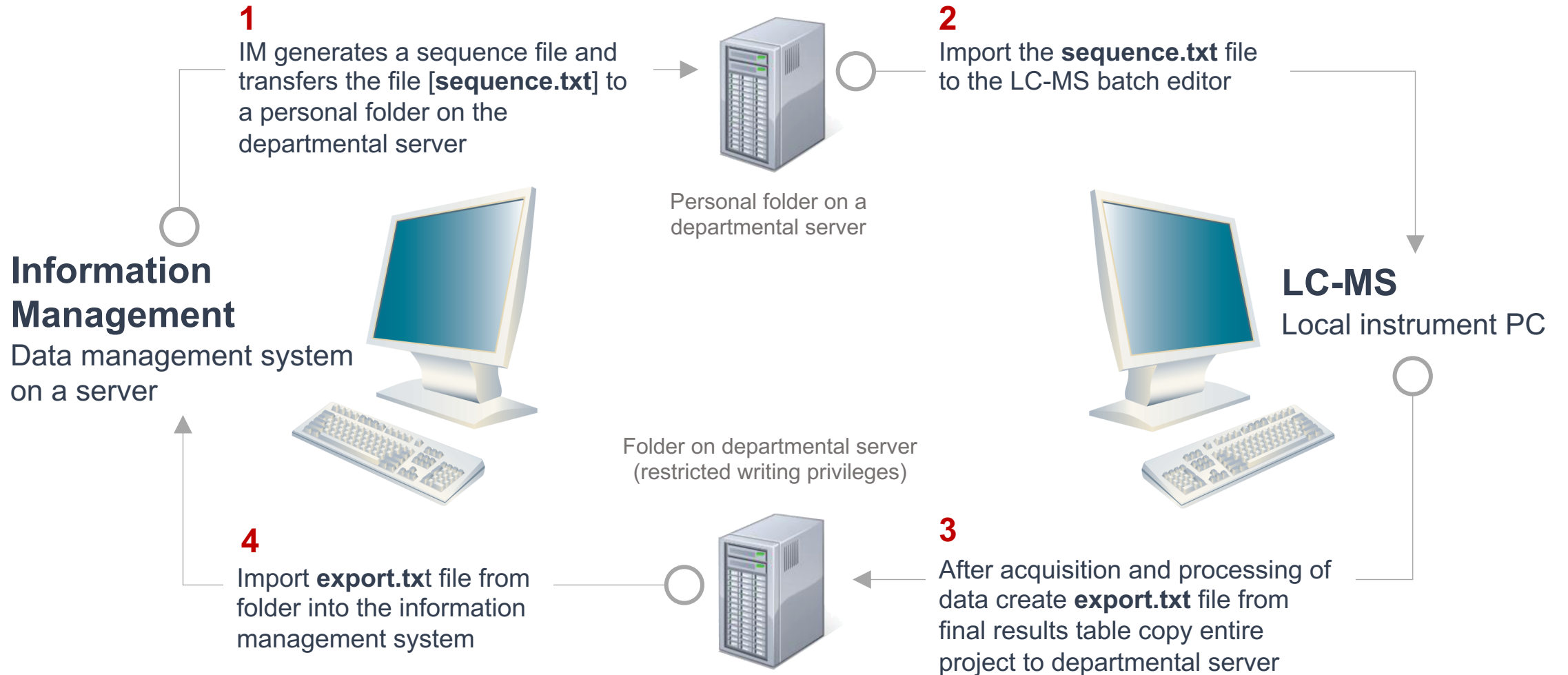
‘Current products still force the bioanalytical laboratories into manual and time-consuming quality-control steps to mitigate the DI risks. With the increased number of citing’s during health authority inspections over the last few years, the message is clear: DI issues must be resolved!’

### **The objective cited in the White Paper**

Our focus on LC–MS–IM 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.

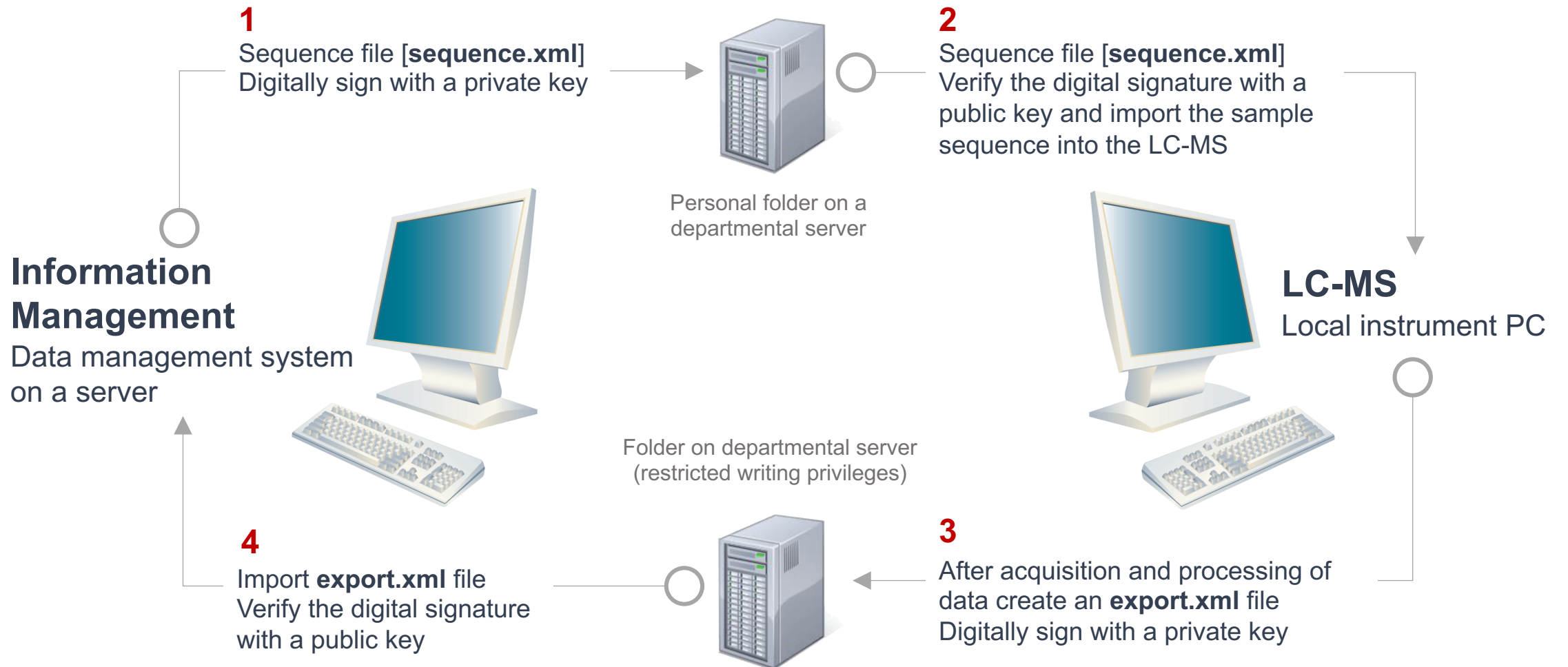
# A common data transfer cycle

Current data transfer cycles require manual and time-consuming quality-control steps to mitigate the DI risks



# A proposed way forward

Replacing .txt files with digitally signed .xml files



## 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

**Proposal:** 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)

### Improving data security by signing an XML file with digital signatures

'Provided by World Wide Web Consortium (W3C) Signature Working Group

<https://www.w3.org/Signature/>

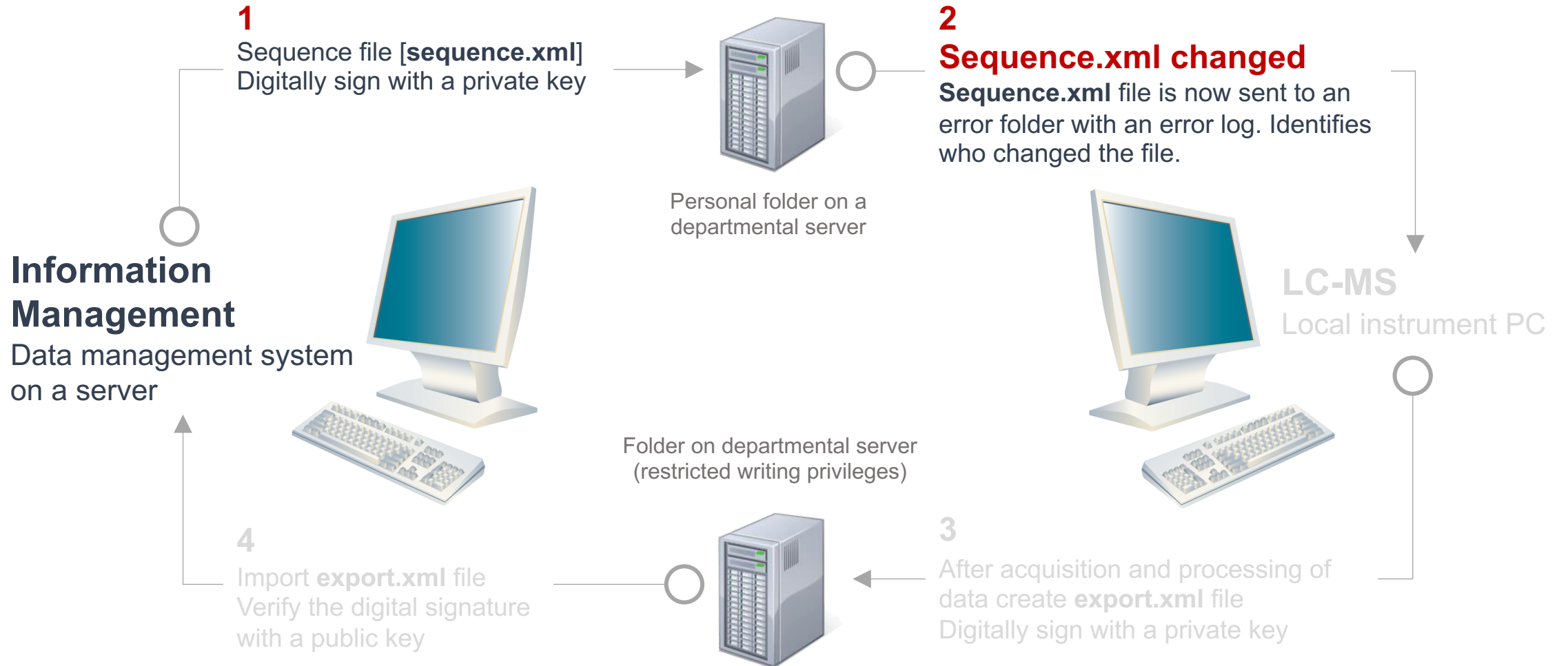
<https://www.w3.org/TR/xmlsig-core2/>

#### W3C XML DSIG Characteristics

- Attributable – you can tell who made a signature
- Tamper-evident – you can tell if data has changed since signing
- Multi-signature support – multiple people and/or systems can sign a data set (approval workflows)
- Automated validation – before accepting a file, instrument or LIMS can confirm its provenance
- Integrates with enterprise PKI – some organizations already have certificate management infrastructures
- Stored in XML – easy to read and write, broad developer experience
- Royalty free, widely implemented – free libraries for Java, .Net, ...

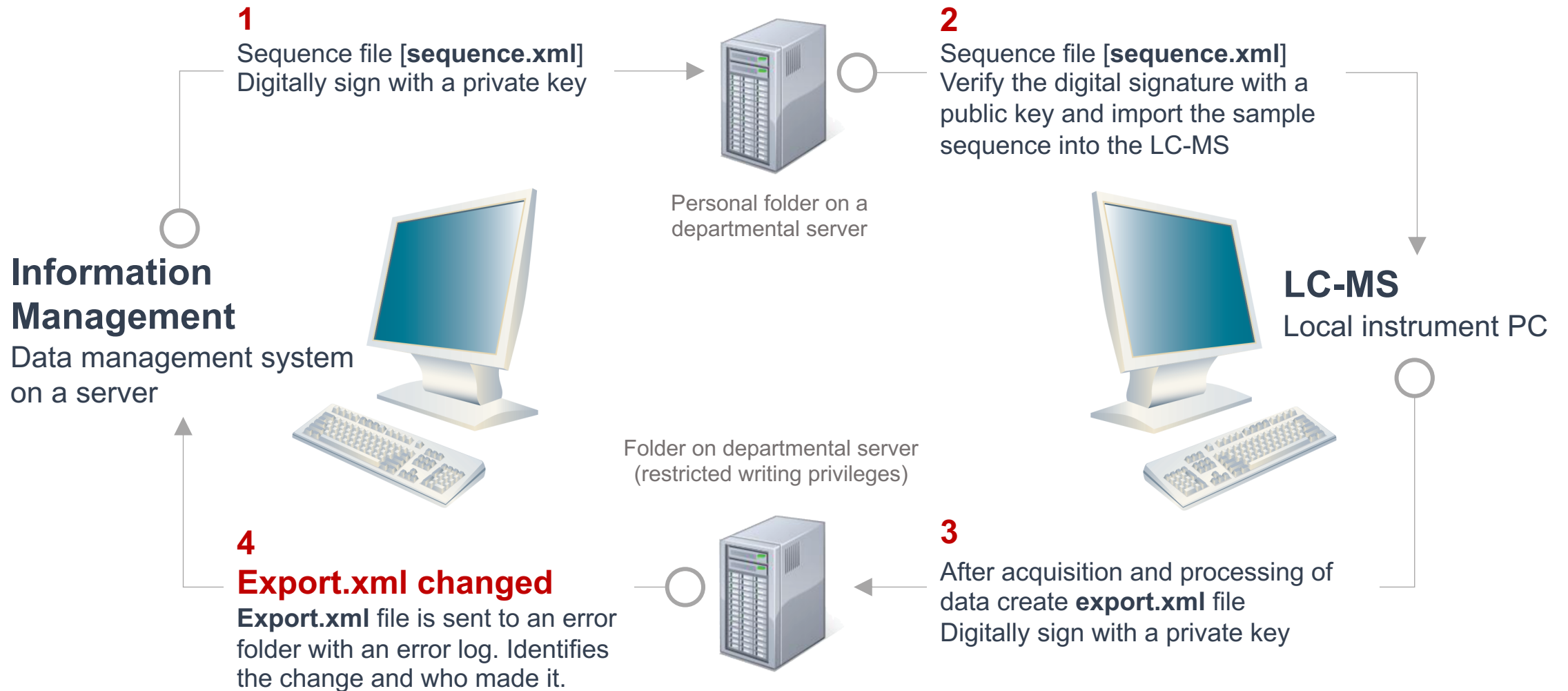
# What happens if a sequence file has been changed or modified?

The digital signature technology checks if the file has been tampered-with (changed/modified/edited)



# What happens if an export file has been changed or modified?

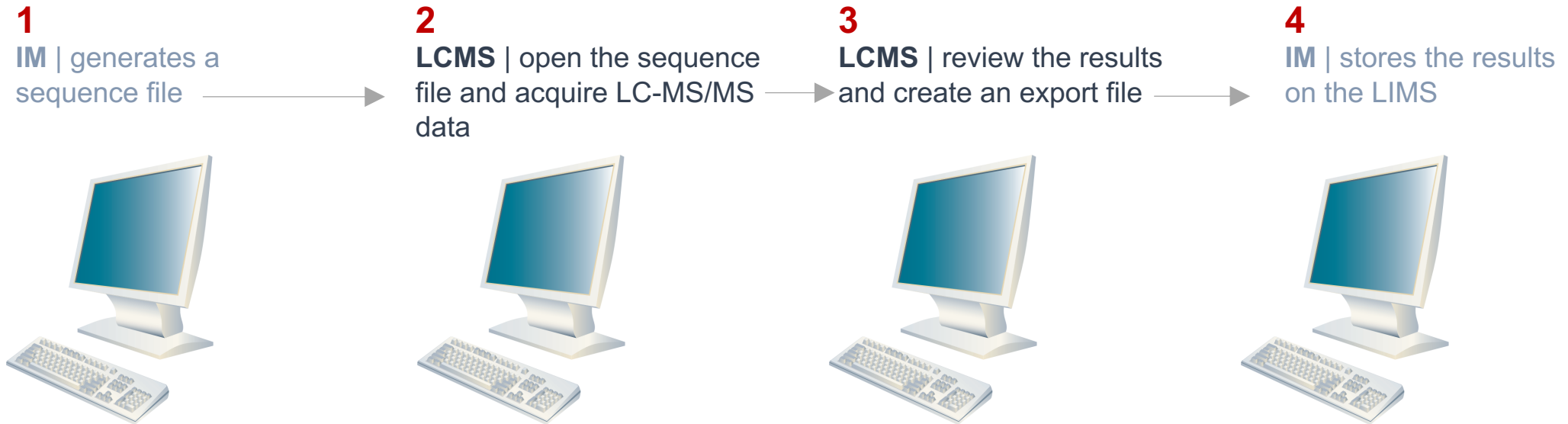
The digital signature technology also checks if an export file has been tampered-with (changed, modified or edited)





# The 'user experience'

A user will be able to open a sequence file, review data and export results



## Under the hood

**IM** | generates a sequence file, converts it into a digitally signed XML file format with a public key and sent to the 'watcher' folder.

**LCMS** | 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

**LCMS** | 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.

**IM** | the LIMS system 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.

## What is happening now; the current position?

Following the EBF initiative a proposed way forward has been suggested to mitigate DI risks  
The result is a vendor-neutral prototype for a secure data transfer using a minimum data set and W3C XML DSIG

### EBF achievements in DI

- Following EBF 2019, software developer meetings involving instrument providers to find a working solution
- White Paper published in July 2020 highlighting the need to accelerate generic/vendor-neutral solutions for secure data transfer tools
- Prototype framework agreed with a proposed XML file format
- W3C XML DSIG considered to be a working vehicle that meets the needs of secure data transfer
  - A digitally signed XML file can identify whether a file has been changed ('tampered with') and who made the change.
  - This technology is designed for LC-MS workflows and should be a near zero change for users.
- Prototype solutions are now being implemented/considered
- Potential expansion
  - additional vendors are welcome
  - support for additional measurement techniques and assays
  - investigate file-less technology

## 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.

### **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.

# Acknowledgements

EBF White Paper authors

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White Paper

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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**

Cecilia Arfvidsson<sup>1</sup>, David Van Bedaf<sup>2</sup>, Susanne Globig<sup>3</sup>, Magnus Knutsson<sup>4</sup>, Mark Lewis<sup>5</sup>,  
Stuart McDougall<sup>6</sup>, Marco Michi<sup>7</sup> & Philip Timmerman<sup>\*.8</sup>

# Acknowledgements

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## Call to action

- **We need your feedback**
  - Is this useful?
  - Would you like to try this?
- **Early adopters**

## **Additional slides**

Vendor solutions

EBF agreed minimum data set





# One example of a user experience; exporting results to the LIMS

## Workflow

- **LC-MS/MS to LIMS**
  - Review data and Export to 'EBF LIMS'
  - Export.xml file is generated and digitally signed with a private key
- **LIMS import from LC-MS/MS**
  - The export.xml file is verified with a public key and the results stored on the LIMS.

The screenshot displays the LabSolutions Insight software interface. At the top, the title bar reads "LabSolutions Insight (Reviewer) - (EBFDataIntegrityProject\_DataPack\_Lcb - ProcessingFile\_TargetAnalysis\_EBF\_DataPack.lcm) [Pre-Release]".

The main window is divided into several panes:

- Compound List:** A table with columns for #, Flags, Flag ID, and Name. It lists "Analyte Target" and "Internal Standard Target".
- Sample Results - Analyte Target:** A large table with columns: #, Data Filename, Sample ID, Sample Type, Found RT, Area, ISTD Area, and Area Ratio. It contains 17 rows of data for various standards and controls.
- Compound Details - CalibrnStd\_Level8\_ID8 - Analyte Target:** A chromatogram showing a single sharp peak at RT=6.291. The x-axis is RT (min) from 4.6 to 7.8, and the y-axis is %.
- Calibration - Analyte Target:** A calibration curve plot with the equation  $y = 0.005129574x + 0.002061001$ ,  $R^2 = 0.9870888$ , and  $R = 0.9935219$ . The x-axis is Conc.Ratio (pg/mL) from 0 to 350, and the y-axis is Area Ratio from 0.00 to 1.75. Data points are shown as red squares and green diamonds.

A red box highlights the "Export" menu in the bottom-left pane, with the "To EBF LIMS" option selected. A tooltip below the menu reads: "Export the current results to a EBF LIMS compatible results file."

# Export message (one example)

LabSolutions Insight (Reviewer) - (EBFDataIntegrityProject\_DataPack\_iproc - ProcessingFile\_TargetAnalysis\_EBF\_DataPack.lcm) [Pre-Release]

Compound List			Sample Results - Analyte Target									
#	Flags	Flag ID	Name	#	Data Filename	Sample ID	Sample Type	Found RT	Area	ISTD Area	Area Ratio	
<input checked="" type="checkbox"/>			Analyte Target	<input checked="" type="checkbox"/>	1	CalibnStd_Level1_ID1	PlasmaCalibnStd_0.9695 pg/mL	Standard	6.274	2965	342510	0.009
<input checked="" type="checkbox"/>			Internal Standard Target	<input checked="" type="checkbox"/>	2	CalibnStd_Level2_ID2	PlasmaCalibnStd_1.939 pg/mL	Standard	6.271	3682	357705	0.010
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	3	CalibnStd_Level3_ID3	PlasmaCalibnStd_3.879 pg/mL	Standard	6.276	7346	367746	0.020
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	4	CalibnStd_Level4_ID4	PlasmaCalibnStd_7.08 pg/mL	Standard	6.284	13865	372766	0.037
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	5	CalibnStd_Level4_ID5	PlasmaCalibnStd_20.14 pg/mL	Standard	6.277	42738	395141	0.108
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	6	CalibnStd_Level6_ID6	PlasmaCalibnStd_40.28 pg/mL	Standard	6.288	85327	411453	0.207
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	7	CalibnStd_Level7_ID7	PlasmaCalibnStd_105.922 pg/mL	Standard	6.292	223834	395380	0.566
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	8	CalibnStd_Level8_ID8	PlasmaCalibnStd_210.352 pg/mL	Standard	6.291	448086	390180	1.148
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	9	CalibnStd_Level9_ID9	PlasmaCalibnStd_280.469 pg/mL	Standard	6.298	584830	391968	1.492
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	10	CalibnStd_Level10_ID10	PlasmaCalibnStd_350.586 pg/mL	Standard	6.299	665343	353199	1.884
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	11	QC_LevelAQC_ID1	AQC	Control	6.316	31901	323859	0.099
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	12	QC_LevelLQC_ID2	LQC	Control	6.305	12223	383073	0.032
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	13	QC_LevelMQC_ID3	MQC	Control	6.316	295687	305200	0.969
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	14	QC_LevelHQC_ID4	HQC	Control	6.314	449187	276243	1.626
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	15	SampleID_t0_ID1	AccessionCode_IDX1179_ZX1	Unknown	6.315	393	397162	0.001
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	16	SampleID_t0.08_ID2	AccessionCode_IDX1179_ZX2	Unknown	6.308	16419	417893	0.039
<input checked="" type="checkbox"/>				<input checked="" type="checkbox"/>	17	SampleID_t0.25_ID3	AccessionCode_IDX1179_ZX3	Unknown	6.306	92431	437400	0.211

Export to EBF Compatible LIMS

Successfully exported the file: C:\Users\loftusn\Documents\ApplicationData\LCMSMS\_TripleQuad\LCMSMS\_DI\_EBF\_DataPack\EBFDataIntegrityProject\_DataPack\_-20201103-15h51m17s.xml

```
<?xml version="1.0"?>
- <AnIML>
  + <SampleSet>
  - <ExperimentStepSet>
    - <ExperimentStep Name="Bioanalysis" experimentStepID="e1">
      + <Method>
      - <Results Name="Analytical Result">
        - <SeriesSet Name="Results Table" length="48">
          + <Parameter Name="Sample Name" seriesType="String" seriesID="s1" dependency="dependent">
          + <Parameter Name="Analyte Name" seriesType="String" seriesID="s2" dependency="dependent">
          + <Parameter Name="Concentration" seriesType="Float32" seriesID="s3" dependency="dependent">
          + <Parameter Name="RT" seriesType="Float32" seriesID="s4" dependency="dependent">
          + <Parameter Name="Area" seriesType="Float32" seriesID="s5" dependency="dependent">
          + <Parameter Name="Area %" seriesType="Float32" seriesID="s6" dependency="dependent">
          + <Parameter Name="Height" seriesType="Float32" seriesID="s7" dependency="dependent">
          + <Parameter Name="Height %" seriesType="Float32" seriesID="s8" dependency="dependent">
          + <Parameter Name="Concentration Ratio" seriesType="Float32" seriesID="s9" dependency="dependent">
          + <Parameter Name="Area Ratio" seriesType="Float32" seriesID="s10" dependency="dependent">
          + <Parameter Name="Height Ratio" seriesType="Float32" seriesID="s11" dependency="dependent">
          + <Parameter Name="Internal Standard Name" seriesType="String" seriesID="s12" dependency="dependent">
          + <Parameter Name="ISTD Concentration" seriesType="Float32" seriesID="s13" dependency="dependent">
          + <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>
```

# Vendor-neutral visualization at BSSN Software

Shimadzu results in  
BSSN Software viewer

Seahorse Scientific Workbench

test1-20201103-12h34m02s working copy

Name: Bioanalysis ID: e1

Analytical Result Methode Proben Quelle Verlauf

Sample Name	Analyte Name	Concentration	RT	Area	Area %	Height	Height %	Concentration Ratio	Area Ratio	Height Ratio	Internal Standard Name	ISTD Concentration	ISTD RT	ISTD Area
abhängig (y)	abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	abhängig (y)	float32 abhängig (y)	float32 abhängig (y)	float32 abhängig (y)
SteroidsMix	Aldosterone	0,154242	0,905	18131,00...	0,000000	3820,000...	0,000000	0,154242	0,000000	0,000000	C13-Testosterone IS...	3,0	2,150	28864
SteroidsMix	11-deoxyc...	0,340649	1,394	13168,00...	0,202410	2790,000...	0,167136	0,340649	0,202410	0,167136	11-deoxycortisol-D...	1,0	1,380	6505
SteroidsMix	11-deoxyc...	0,258105	1,926	27245,00...	0,418793	6770,000...	0,405559	0,258105	0,418793	0,405559	11-deoxycortisol-D...	1,0	1,380	6505
SteroidsMix	11-deoxyc...	1,000000	1,380	65056,00...	1,000000	16693,00...	1,000000							
SteroidsMix	DHEA-D5 L...	2,000000	2,079	739170,0...	1,000000	181835,0...	1,000000							
SteroidsMix	Cortisol	0,246484	1,023	8909,000...	0,136944	2323,000...	0,139160	0,246484	0,136944	0,139160	11-deoxycortisol-D...	1,0	1,380	6505
SteroidsMix	Progesterone	0,197219	3,074	43483,00...	0,668393	12142,00...	0,727371	0,197219	0,668393	0,727371	11-deoxycortisol-D...	1,0	1,380	6505
SteroidsMix	Cortisone	0,180218	0,929	26413,00...	0,406004	7110,000...	0,425927	0,180218	0,406004	0,425927	11-deoxycortisol-D...	1,0	1,380	6505
SteroidsMix	DHT	2,475873	2,730	1235,000...	0,004279	216,0000...	0,003079	0,825291	0,004279	0,003079	C13-Testosterone IS...	3,0	2,150	28864
SteroidsMix	C13-Testo...	3,000000	2,150	288640,0...	1,000000	70148,00...	1,000000							
SteroidsMix	DHEA-S	0,470319	0,463	9781,000...	0,013232	2505,000...	0,013776	0,235160	0,013232	0,013776	DHEA-D5 ISTD	2,0	2,079	73917
SteroidsMix	Estrone NEG	0,210489	1,578	8655,000...	0,133039	1905,000...	0,114120	0,210489	0,133039	0,114120	11-deoxycortisol-D...	1,0	1,380	6505
SteroidsMix	Test3	0,112293	1,770	16071,00...	0,000000	3513,000...	0,000000	0,112293	0,000000	0,000000	C13-Testosterone IS...	1,0	2,148	29690
SteroidsMix	Aldosterone	0,123203	0,905	15524,00...	0,000000	2306,000...	0,000000	0,123203	0,000000	0,000000	C13-Testosterone IS...	1,0	2,148	29690
SteroidsMix	11-deoxyc...	0,266944	1,391	7031,000...	0,120051	1397,000...	0,089357	0,266944	0,120051	0,089357	11-deoxycortisol-D...	1,0	1,379	5856
SteroidsMix	11-deoxyc...	1,000000	1,379	58567,00...	1,000000	15634,00...	1,000000							
SteroidsMix	DHEA-D5 L...	1,000000	2,077	797798,0...	1,000000	197574,0...	1,000000							
SteroidsMix	Progesterone	0,138455	3,072	25946,00...	0,443014	6577,000...	0,420686	0,138455	0,443014	0,420686	11-deoxycortisol-D...	1,0	1,379	5856
SteroidsMix	Cortisone	0,082680	0,931	20163,00...	0,344272	5523,000...	0,353269	0,082680	0,344272	0,353269	11-deoxycortisol-D...	1,0	1,379	5856
SteroidsMix	C13-Testo...	1,000000	2,148	296905,0...	1,000000	72643,00...	1,000000							
SteroidsMix	17b-estradi...	-0,041936	1,500	1288,000...	0,021992	307,0000...	0,019637	-0,041936	0,021992	0,019637	11-deoxycortisol-D...	1,0	1,379	5856
SteroidsMix	DHEA-S	0,102250	0,463	4178,000...	0,005237	1336,000...	0,006762	0,102250	0,005237	0,006762	DHEA-D5 ISTD	1,0	2,077	79779
SteroidsMix	Estrone NEG	0,135721	1,578	5297,000...	0,090443	977,0000...	0,062492	0,135721	0,090443	0,062492	11-deoxycortisol-D...	1,0	1,379	5856
SteroidsMix	Test3	128,454559	1,777	1749294...	0,000000	4595792...	0,000000	128,454559	0,000000	0,000000	C13-Testosterone IS...	1,0	2,151	30569
SteroidsMix	Aldosterone	127,215279	0,904	1068994...	0,000000	2518873...	0,000000	127,215279	0,000000	0,000000	C13-Testosterone IS...	1,0	2,151	30569
SteroidsMix	11-deoxyc...	130,540771	1,395	1023956...	145,6905...	2347544...	127,0659...	130,540771	145,6905...	127,0659...	11-deoxycortisol-D...	1,0	1,382	7028
SteroidsMix	DHEA	130,733002	1,577	2718414...	3,738666	719828,0...	3,958840	130,733002	3,738666	3,958840	DHEA-D5 ISTD	1,0	2,081	72710
SteroidsMix	11-deoxyc...	126,721611	1,928	2120518...	301,7114...	5340765...	289,0806...	126,721611	301,7114...	289,0806...	11-deoxycortisol-D...	1,0	1,382	7028
SteroidsMix	11-deoxyc...	1,000000	1,382	70283,00...	1,000000	18475,00...	1,000000							
SteroidsMix	DHEA-D5 L...	1,000000	2,081	727108,0...	1,000000	181828,0...	1,000000							
SteroidsMix	Cortisol	127,706413	1,022	4882930...	69,475266	1397783...	75,658081	127,706413	69,475266	75,658081	11-deoxycortisol-D...	1,0	1,382	7028
SteroidsMix	Progesterone	130,986023	3,075	3530190...	502,2821...	1025774...	555,2230...	130,986023	502,2821...	555,2230...	11-deoxycortisol-D...	1,0	1,382	7028
SteroidsMix	Cortisone	126,698471	0,930	5656351...	80,479645	1572292...	85,103760	126,698471	80,479645	85,103760	11-deoxycortisol-D...	1,0	1,382	7028

Grafik Daten



# The scope of the IM to LC-MS data transfer

A minimum data set as defined in the White Paper

Vendor independent fields to be included in the run/batch/worklist transfer **from the IM system to the LC-MS**

## Run/File specific fields

- Study/project
- Run/batch file
- User GLP
- Plate barcode

## Sample specific fields

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

Vendor independent fields to be included in the run/batch/worklist transfer **from the LC-MS to the IM system**

## Run/File specific fields

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

## Sample specific fields

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