



OGI-IT (L)IMS

an overview



IMS-Information Management System

- **Information** is stored in databases (DB) - we use document oriented DB so that the DB Model (collections of documents) can match as close as possible the real world document model. This is in contrast to a relational model where the real world model is decomposed in a more complex relational one (many tables and relations)
- Information is transformed (sorted, queried, aggregated) so that **Management** decisions can be made
- A web based front end (web app), generated by the data model description (schema), enables the use on different computer **Systems** like desktops, tablets or even smartphones



LIMS - Laboratory IMS

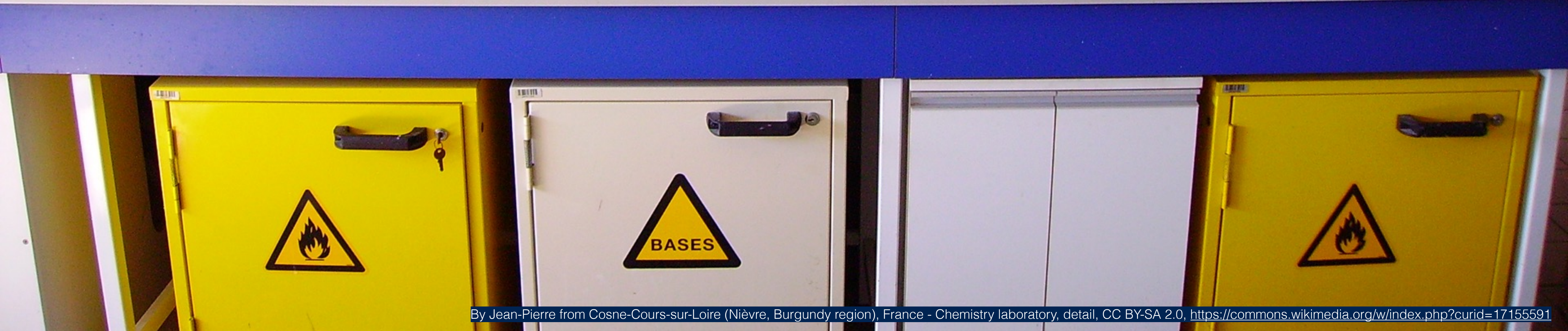
first IMS implementation was for a chemical analytical **Laboratory**
some lab documents (collections) are:

- Studies (Studien)
- Samples (Studienproben)
- Operating Procedures (Laborvorschriften)
- Batches (Laborarbeiten)
- Equipment (Laborgeräte)
- External Materials (externe Materialien) i.e. chemicals, pure substances, matrices, etc.



Laboratory ?







Zählzylinder
Plastikgefäße
Stapel/Strapfen

MCH-Walzen
Messzylinder

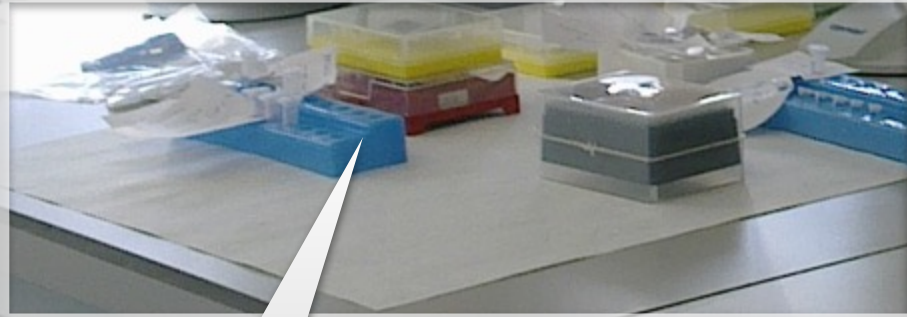




Equipment
(Laborgeräte)



External Materials
(externe Materialien)



Derived Products
(Laborprodukte)



Samples
(Studienproben)









working on a „Batch“

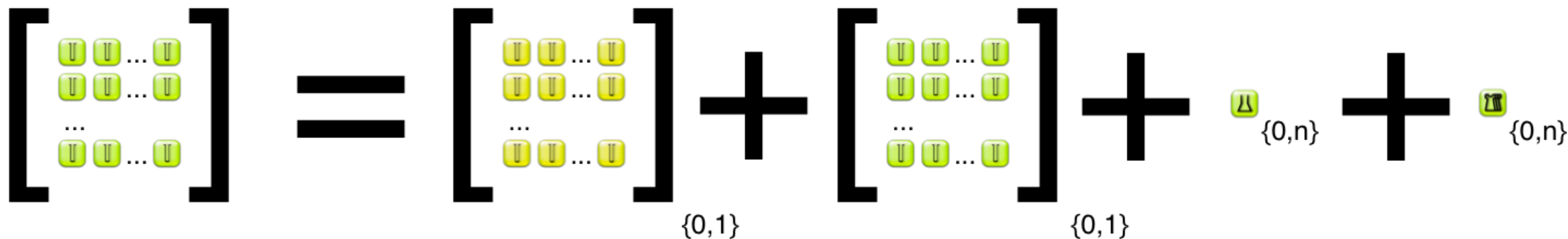
derived products (Laborprodukte) = samples (Studienproben) +
derived products (Laborprodukte) +
equipment (Laborgeräte) +
external material (externe Materialien)



Legend (Legende)

-  Batches (Laborarbeiten)
-  Samples (Studienproben)
-  Equipment (Laborgeräte)
i.e. pipettes, scales, HPLC, etc.
-  External materials (externe Materialien)
i.e. chemicals, pure substances, matrices, etc.
-  Derived products (Laborprodukte)
i.e. injection samples, standards, etc.

 a batch is the execution of a SOP (standard operating procedure)





LIMS features 1/2

- Standard Operating Procedures (SOP) are phrased step by step using generic placeholders for the equipment, probes and chemicals used
- Derived products of the execution of such a SOP, have calculated properties based on generic formulas defined in the SOP
- Laboratory work like sample preparation, standards production etc. can be predefined by SOPs (Laborvorschriften, Laboraufträge)
- and the execution documented (Laborarbeit)
- derived products (injection samples, standards, etc.) from laboratory work are then generated into the LIMS having all the needed properties (concentration, dilution, etc.) by the touch of a button



LIMS features 2/2

special lab hardware connected to the LIMS

- a Companion App to the SCIEX Analyst Software for LC/MS/MS (Liquid chromatography–mass spectrometry/ mass spectrometry) equipment
- template based network label printer (brother)
- optical barcode-scanner (1D, 2D) with optical feedback (cognex)



Visual Feedback

- image-based barcode reading
- get visual feedback when scanning

OGI-IT LIMS v.0.6.3

Studienproben

- 1B2

Studie	Name	Status	Tags	Lagerort
xxx	1A1	OK	Timo1	TK 26
				TK 26
				TK 26
				TK 22
				TK 26
				TK 26
				TK 26
				TK 26
				TK 26
				TK 27
				TK 26
				TK 26
				TK 22


Kontext

Benutzer

Standard-Scanner2
Standard-Scanner3

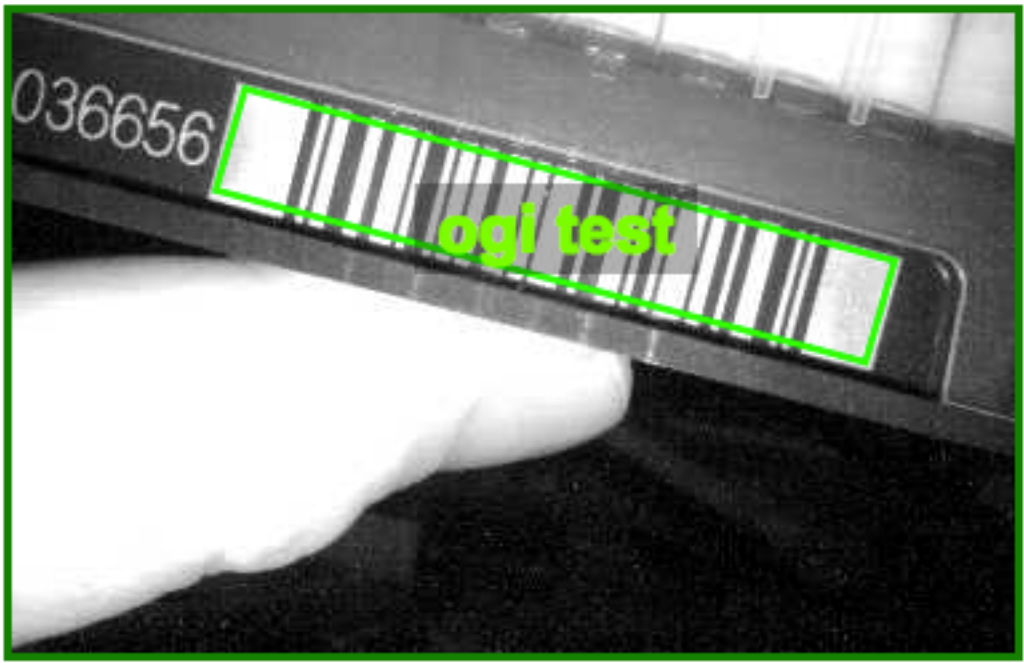
50036656
FC13780848
FC13780848
FC13780836
FC13780812
FC13780823
FC13780836
FC13780848
FC13780848
FC13780824
FC13780836
50036656
50036656

Löschen



Laborprodukte: QK1

Löschen



Laborgeraete: ogi test

Name: 1B2
UUID: 21ada87c-ff4d-43be-b851-39493e770e42
Studie: xxx
Status: OK

Importarbeit: [details](#)

Name bei Zuweisung: bla bla Studienproben import job
Sammlung Name: Importarbeiten

aktueller Lagerort: [details](#)

Name bei Zuweisung: TK 26
Sammlung Name: Laborgeraete

Lagerung

VorgangsUUID	Datum	Benutzer	Lagerort
a75744b9-10cf-40e0-8517-5422115d8f89	22.1.2015, 13:04:38	ogi	details

Name bei Zuweisung: TK 26
Sammlung Name: Laborgeraete

Temperatur Report

Auswertungsdatum: 2015-01-26T17:41:47.343Z

relevante Lagerort Temperatur: [details](#) relevante Lagerort Temperatur - Name: [details](#) TK 26 2015

Löschen

036656

Laborgeraete: ogi test

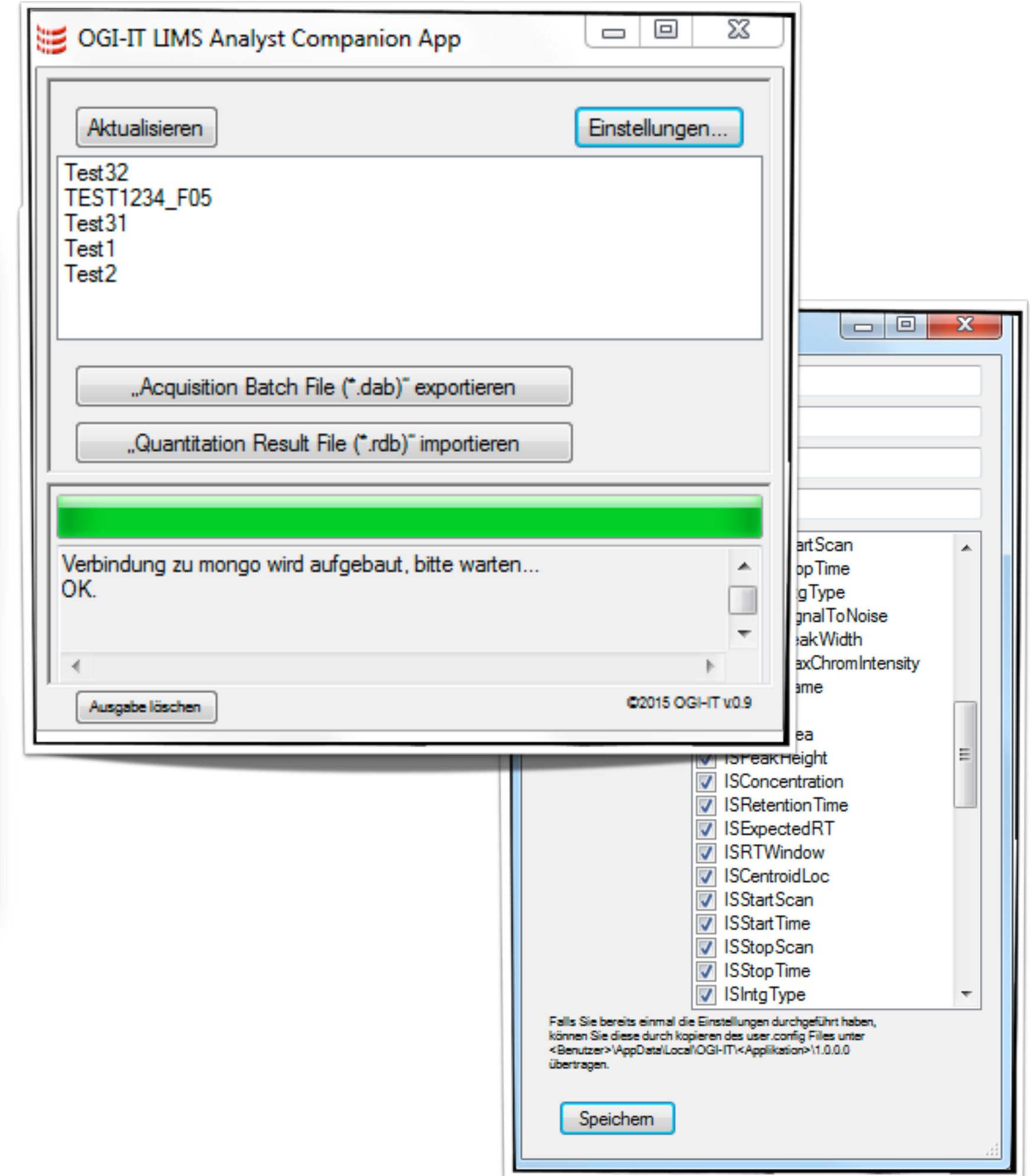
ctrl+s in Such...
ctrl+d in Such...
ctrl (cmd) un...
selektieren od...
Derzeit sollte...
sein.

Aktionen / Re...
Links / Hilfe



Analyst Companion App

The OGI-IT LIMS Companion App is started inside of the SCIEX Analyst Software, a widely used LC/MS/MS (Liquid chromatography–mass spectrometry/ mass spectrometry) instrument control software. It allows both import of „Acquisition Batches“ from the LIMS and export of „Quantitation Results“ back into the LIMS.





IMS features 1/2

- documents are grouped into collections based on their type (schema)
- documents in collections may have different types (schemas) when document requirements change over time
- role based document access (user may have multiple roles assigned)
- every collections may have different actions defined, which also depend on the users role and document content
- sign action - used to advance the state of a document in the document workflow, show document changes during this workflow and based on the role and content of the document
- after first signing, deleted documents are moved into the „archived documents“ collection



IMS features 2/2

- document import (csv, json) based on import jobs (documented import)
- document export (json)
- reporting (web, pdf, csv)



(L)IMS web app

roles, collections, queries, documents



OGI-IT LIMS v2

localhost:3101

ogi (all) Studien Alle

1 - 12 / 12

<input type="checkbox"/>	Name	Beschreibung		
<input type="checkbox"/>	Teststudie2	NaCL in Wasser		
<input type="checkbox"/>	Teststudie	NaCl in H2O		
<input type="checkbox"/>	Just_a_Test_Study	Hallo		
<input type="checkbox"/>	Name_bitte_ändern		Val GLP	final
<input type="checkbox"/>	Test2	Test2 B	Val GMP	final
<input type="checkbox"/>	TEST	mexalen in pipi		short
<input type="checkbox"/>	Lena		Study GLP	
<input type="checkbox"/>	xxx	Teststudie da meine Studienproben zur Studie mit Namen "xxx" passen		
<input type="checkbox"/>	Name		Study GLP	
<input type="checkbox"/>	Studie Neu 1		Val GMP	audited
<input type="checkbox"/>	NAME PATCH TEST	bla bla bla		signed
<input type="checkbox"/>	Test der NEUEN U			signed

+ Hinzufügen

Login

- login
- selecting different roles changes the available collections
- search capabilities
- column formatting capabilities
- actions
- „scrolling“ thru the result set of documents



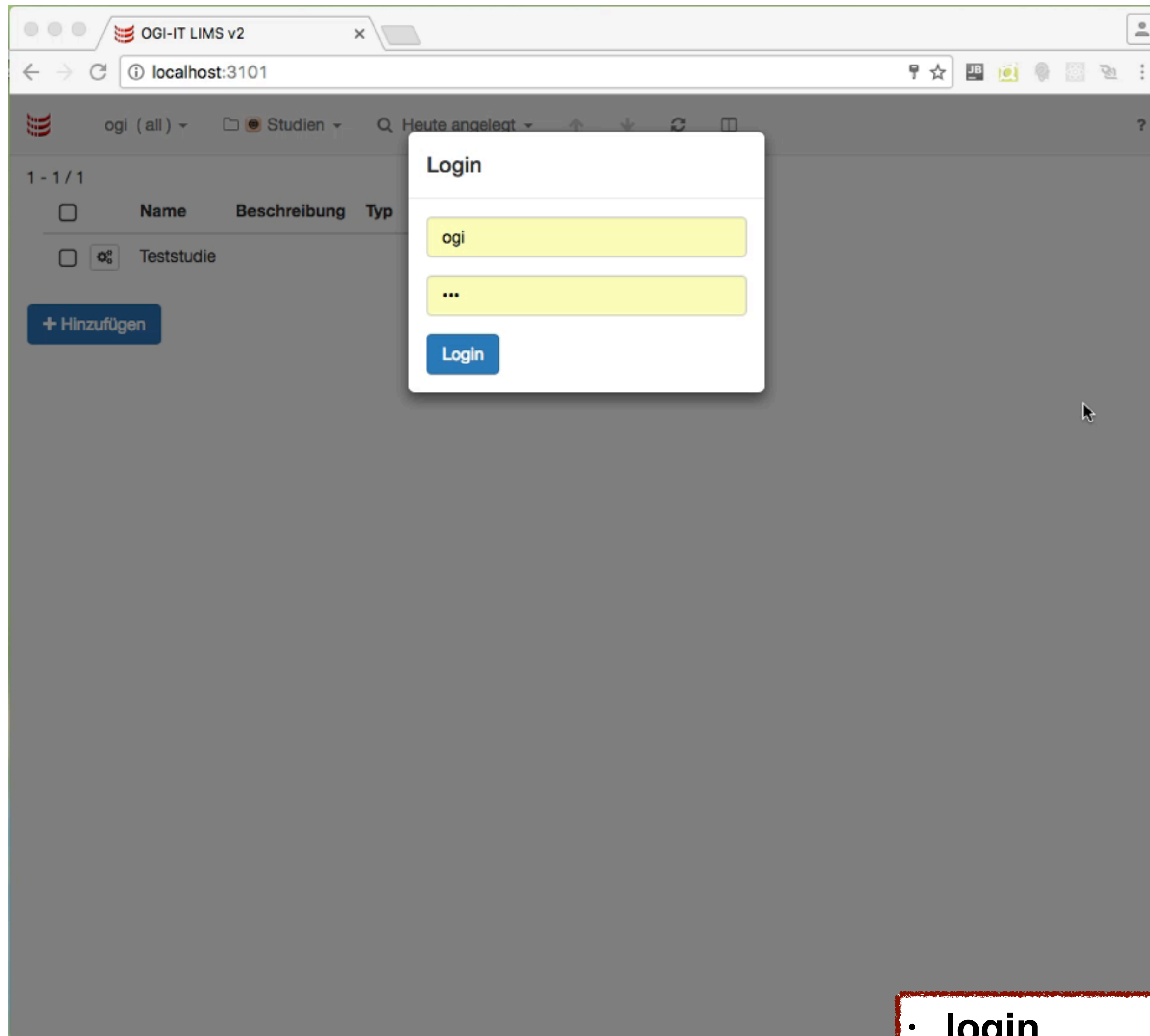
Technologies

- mongodb - document oriented nosql database
- JSON Schema - definition and verification of documents structure, including definition of visual representation
- nodejs - event-driven, asynchronous, cross-platform, runtime environment, programmed mainly in javascript and optimized for real-time web applications
- react, redux, sagas - front end framework for web applications



example of a document

Study (Studie)



- login
- add new study
- enter data into a („complex“) document
- view document



document „workflow“

sign (unterschreiben)



OGI-IT LIMS v2

localhost:3101

ogi (all) Studien Heute angelegt

1 - 2 / 2

<input type="checkbox"/>	Name	Beschreibung	Typ	Zustand
<input type="checkbox"/>	Teststudie	NaCl in H2O	Study GMP	
<input type="checkbox"/>	Teststudie2	NaCL in Wasser	Val GLP	audited

+ Hinzufügen

- start: not signed document
- sign to „committed“
- change document
- see changes since last sign
- after change sign is invalid
- sign to audited with password



References

documents with references to other documents
or populating some fields with data from another document („cloning“)



OGI-IT LIMS v2
localhost:3101
ogi (all) Laborvorschriften Q Alle

1 - 20 / 20

<input type="checkbox"/>	Name	Typ	Zustand
<input type="checkbox"/>	Löschen_4	Sonstige	
<input type="checkbox"/>	Löschen5	Kontrollprobe	
<input type="checkbox"/>	Löschen3	Sonstige	
<input type="checkbox"/>	Name_bitte_ändernJAJA	Sonstige	
<input type="checkbox"/>	TEST_STD81814_SR_neueFormeln_1	Standard	
<input type="checkbox"/>	LVTest_mitMark	Sonstige	
<input type="checkbox"/>	LV mit measured	Sonstige	
<input type="checkbox"/>	Standards herstellen mit Formeln	Standard	
<input type="checkbox"/>	Test aus Laborarbeit	Sonstige	
<input type="checkbox"/>	Clone Test	Sonstige	
<input type="checkbox"/>	Formeltest	Sonstige	
<input type="checkbox"/>	TODO add error for this case	Sonstige	
<input type="checkbox"/>	Verdünnung mit Formel	Verdünnung	
<input type="checkbox"/>	Ogi's spezial Rezept für Palatschinken	Lösung	
<input type="checkbox"/>	Live 1	Sonstige	signed
<input type="checkbox"/>	Markdown Test	Sonstige	
<input type="checkbox"/>	Konst Test	Sonstige	withdrawn
<input type="checkbox"/>	Was komplizierteres	Sonstige	
<input type="checkbox"/>	4 Standards erstellen	Sonstige	
<input type="checkbox"/>	5ml Aliquot erstellen	Sonstige	

+ Hinzufügen

- new document „Laborvorschrift“
- clone from „Laborarbeit“
- save
- view generated instructions „Anweisungen (Ansicht)“
- view references to other documents under „Abhängigkeiten“



Reporting



WI4m
A5

OGI-IT LIMS v2 x OGI-IT LIMS v2 x

localhost:3101

ogi (all) Report-Jobs Alle

1 - 24 / 24

<input type="checkbox"/>	Name	Zustand	<input type="checkbox"/>	Name	Zustand
<input type="checkbox"/>	Test_StdAbw_2	start	<input type="checkbox"/>	Sequenz_Test	end
<input type="checkbox"/>	Test_Standardabweichung	end	<input type="checkbox"/>	absurd_kleines_format_B10	end
<input type="checkbox"/>	Test_Probenverzeichnis	end	<input type="checkbox"/>	Temperatur_ingeschraenkt	end
<input type="checkbox"/>	Test_runCommand	end	<input type="checkbox"/>	TestCSV	end
<input type="checkbox"/>	Test_Studienbericht	end	<input type="checkbox"/>	Laborarbeiten_schema_test	end
<input type="checkbox"/>	Laborarbeiten_Design_Test	end	<input type="checkbox"/>	Report_mit_Reinhard	end
<input type="checkbox"/>	Studienproben_table_test	end	<input type="checkbox"/>	TestmitBarbara1	end
<input type="checkbox"/>	Studienproben_csv_test	end	<input type="checkbox"/>	Studienproben_jsonStyle	end
<input type="checkbox"/>	Studienproben_normal_test	end	<input type="checkbox"/>	TReport_lang	end
<input type="checkbox"/>	Temperatur_mit_Problem	end	<input type="checkbox"/>	TemperaturReport	end
<input type="checkbox"/>	Sequence_Test_csv	end	<input type="checkbox"/>	Test_csv_1_2SECTIONS_not_working	end
<input type="checkbox"/>	Sequence_Test_basic	end	<input type="checkbox"/>	TestReport-1	end

+ Hinzufügen

- new report (standard deviation)
- choose template
- choose study
- wait that pdf is generated
- view (HTML) preview
- view pdf with TOC, header and footer



Batches

(Laborarbeit)



OGI-IT LIMS v2

localhost:3101

ogi (all) Laborarbeiten Heute angelegt

0 --1 / 0

+ Hinzufügen

- preparation of a batch:
- create a new batch
- clone the operation procedure from a SOP (Laborvorschrift)
- set the name and suffix of the batch
- save the batch, so that the definition can be checked and results regenerated
- change one of the proposed pipettes
- sign the batch (committed)
- execution of a batch
- execute each step (in this example only one step)



OGI-IT LIMS v2

localhost:3101/detail/Laborarbeiten/5769680f8a2c0dced0bcbf97

1 / 25 @ Alle 1 - 25 / 41

Kompakt Anweisungen (Definition) Anweisungen (Ansicht) Abhängigkeiten zu berechnende Eigenschaften Resultat (Vorschau) Unterschriften Alles

Name: Neue_Laborarbeit
Suffix: S

zugrundeliegender Laborauftrag (kann nach Zuweisung beliebig verändert werden) zu bearbeitende Proben Typ Vorschau Arbeitsschritte

details

Name bei Zuweisung	Auftrag für Standards mit Formeln
Sammlung Name	Laborauftraege

Bitte beschreiben Sie Welche Proben in den Laborarbeiten zu bearbeiten sind.
Standard

Anweisungsschritt	Durchführungsdatum	Zeitmarke	n
Stelle V1A her, indem 50 ul Konzentrat mit 20 ml 20_vH_MeOH verdünnt werden. Es darf nur eine Matrix HuPK 03650 verwendet werden!	22.6.2016, 11:38:04		

Standard	Volumen [µL]	Std/V	Matrixvol [mL]
Std0	0	-	2
Std1	50	Std4	0.95
Std2	150	Std4	1.35
Std3	54	Std7	0.9585
Std4	80	Std8	0.92
Std5	180	Std8	0.82
Std6	30	Std9	0.97
Std7	60	Std9	0.94
Std8	100	Std9	0.9
Std9	20	V1A	1.98

Dokumentiere die verwendeten Pipetten:
EP16-20var
EP17-100var
EP20-200var
EP14-1000var
EP33

execution plan step 1

Laborarbeit durchführen

Abbrechen

• generate resulting products (Laborprodukte)



OGI-IT LIMS v2

localhost:3101/detail/Laborarbeiten/5769680f8a2c0dced0bcbf97

2 / 25 @ Alle 1 - 25 / 42

Kompakt Anweisungen (Definition) Anweisungen (Ansicht) Abhängigkeiten zu berechnende Eigenschaften Resultat (Vorschau) Unterschriften Alles

Name Neue_Laborarbeit
Suffix S
zugrundeliegender Laborauftrag (kann nach Zuweisung beliebig verändert werden) zu bearbeitende Proben Typ
Vorschau Arbeitsschritte

details

Name bei Zuweisung	Auftrag für Standards mit Formeln
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Standard

Anweisungsschritt	Durchführungsdatum	Zeitmarke	n
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Standard	Volumen [µL]	Std/V	Matrixvol [mL]
Std0	0	-	2
Std1	50	Std4	0.95
Std2	150	Std4	1.35
Std3	54	Std7	0.9585
Std4	80	Std8	0.92
Std5	180	Std8	0.82
Std6	30	Std9	0.97
Std7	60	Std9	0.94
Std8	100	Std9	0.9
Std9	20	V1A	1.98

Dokumentiere die verwendeten Pipetten:
EP16-20var
EP17-100var
EP20-200var
EP14-1000var
EP33

execution plan step 1

Laborarbeit durchführen

Abbrechen

- set state of resulting products (Laborprodukte) to OK
- put one and then all of the resulting products into a storage (freezer)



Thank you