TECHNISCHE UNIVERSITÄT DRESDEN

CMCB TECHNOLOGY PLATFORM
Center for Molecular and Cellular Bioengineering TU Dresden

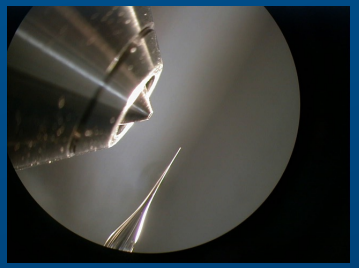
BIOTEC Biotechnology Center TU Dresden

CRTD Center for Regenerative Therapies TU Dresden

B CUBE Center for Molecular Bioengineering TU Dresden

eLabFTW @ a Facility

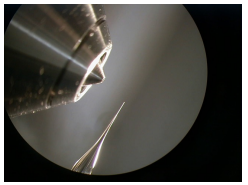
Labbook, Archive & Comm Center



Dr. Marc Gentzel

CMCB - Center for Molecular and Cellular Bioengineering
Core Facility **Mass Spectrometry & Proteomics**

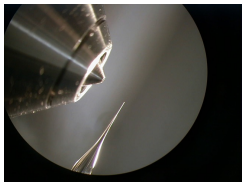
27.05.2024



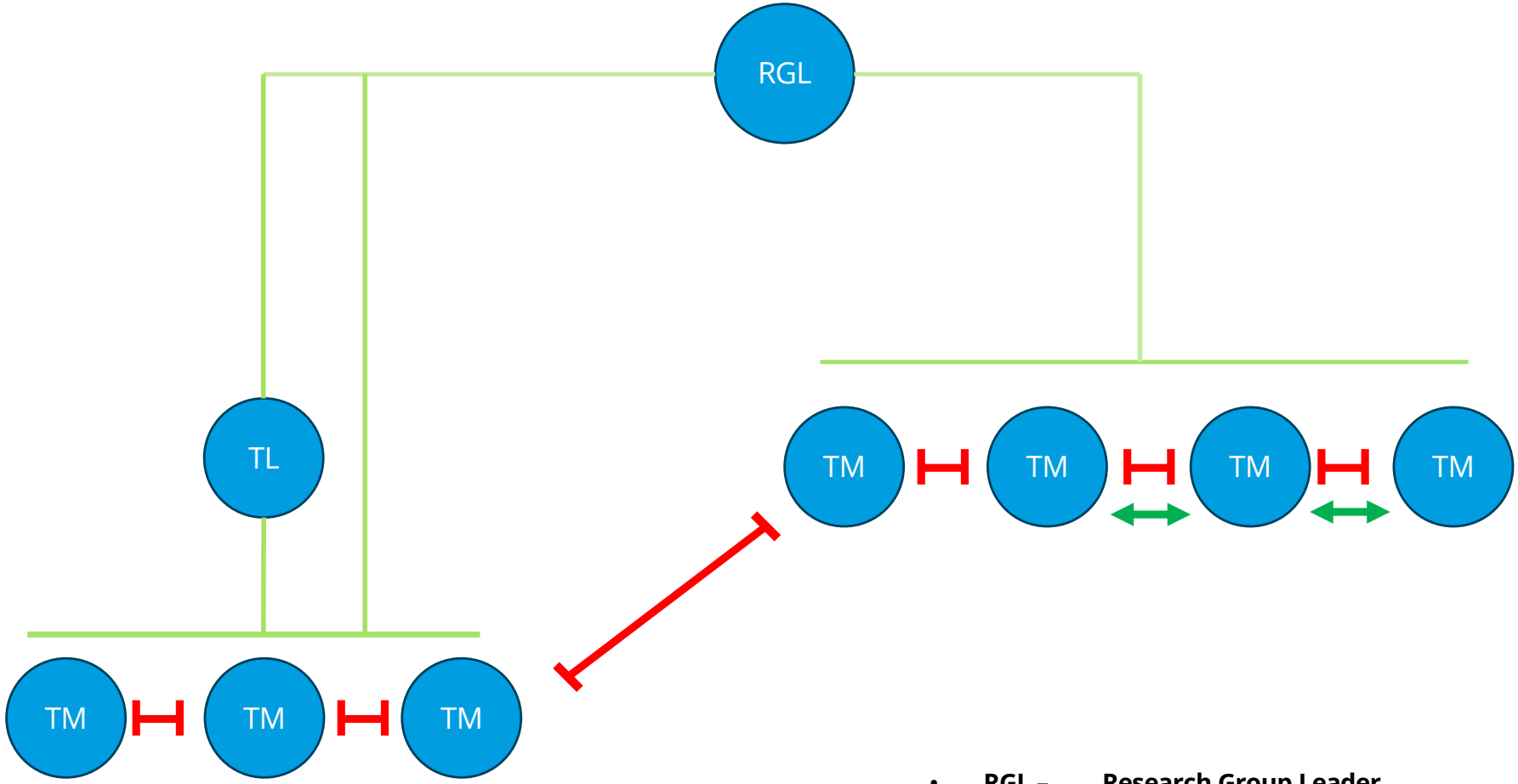
What do we want?

- **Labbook** is for documentation and collection of documents (Facility! – Long Time Scale)
- **Communication Tool** for Lab Work (staff in different buildings)
- it is **not** a replacement for Excel, Affinity, Word, Powerpoint,……,

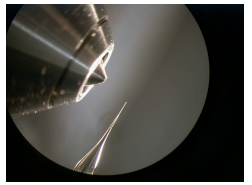
  or any data interpretation software



Classical RG

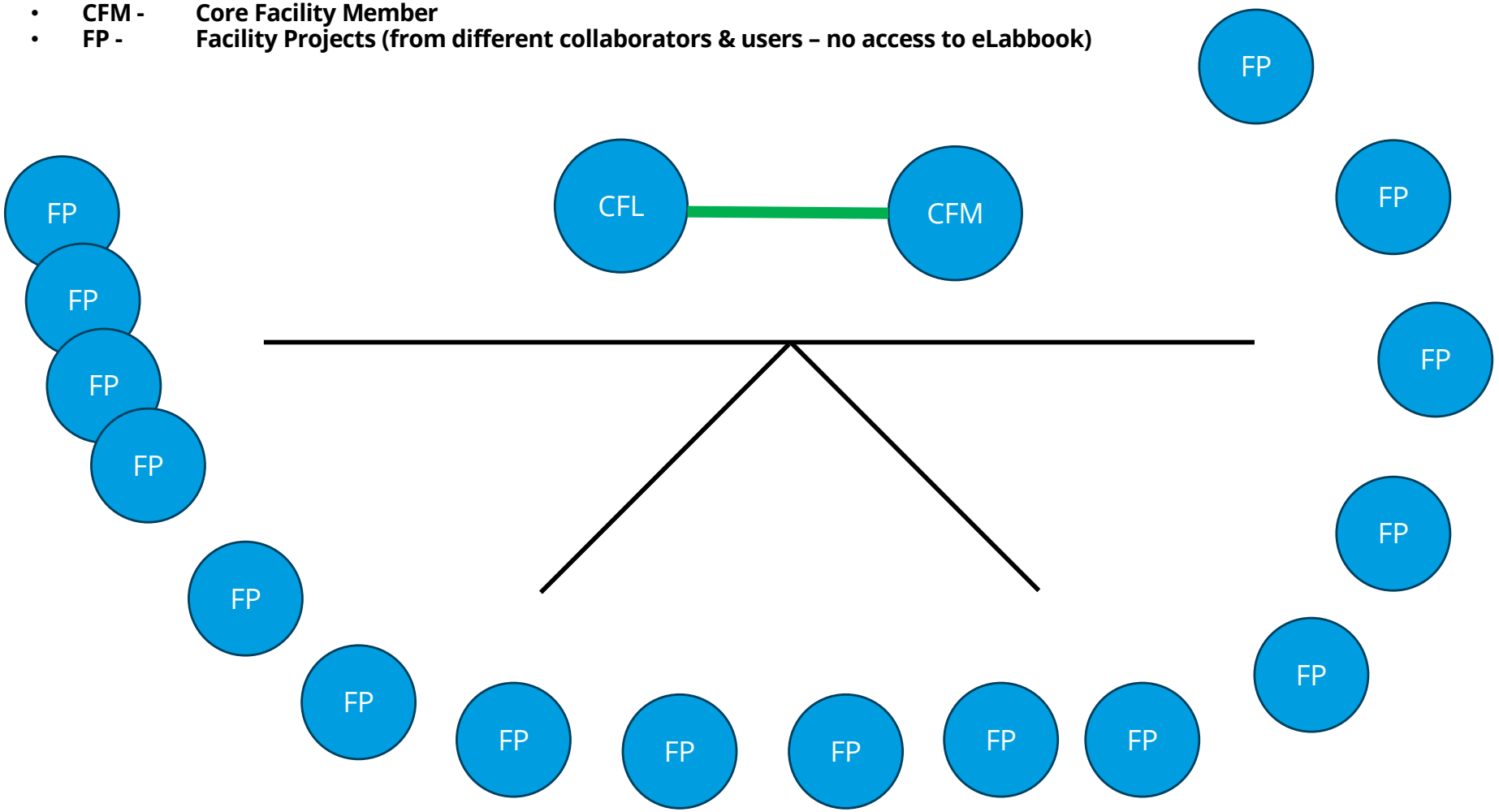


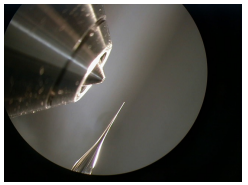
- **RGL – Research Group Leader**
- **TL - Team Leader**
- **TM - Team Member**



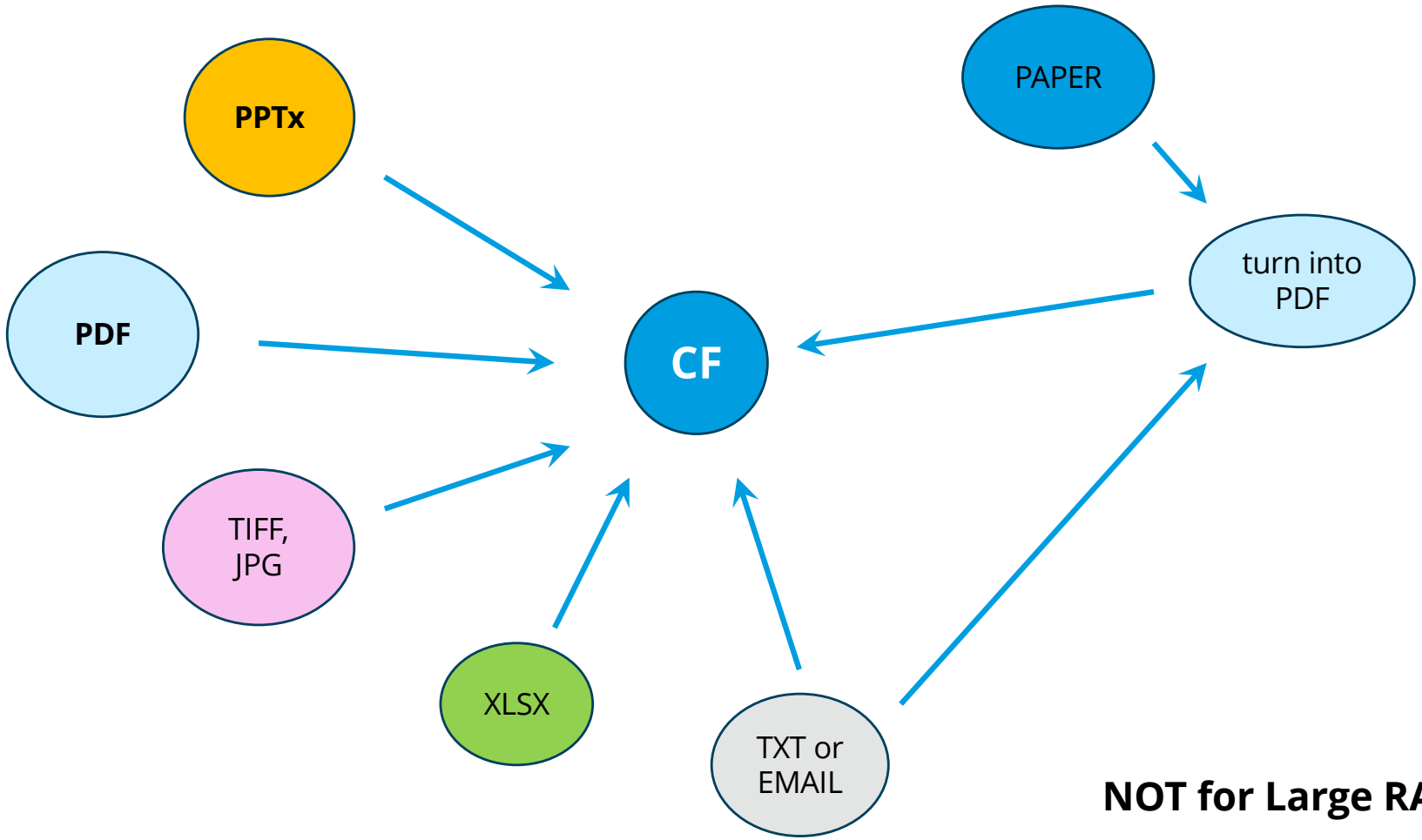
Core Facility

- CFL – Core Facility Leader
- CFM - Core Facility Member
- FP - Facility Projects (from different collaborators & users – no access to eLabbook)

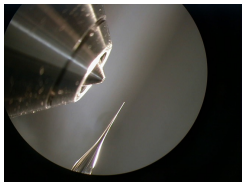




Types of Data submitted to CF



NOT for Large RAW DATA !

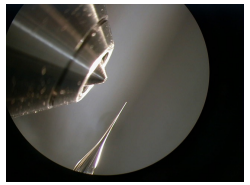


eLabFTW

but

- limited resources for administration
- → effort for labbook should be < 5%

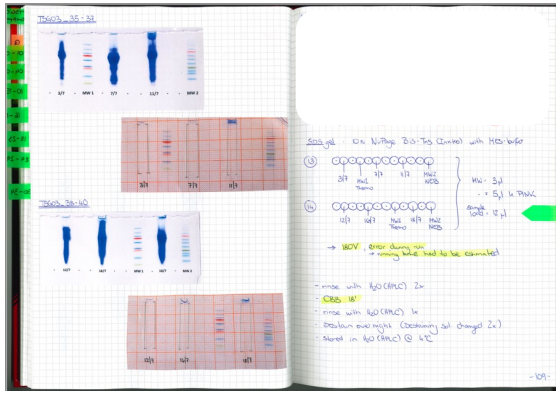
Date	Title	Next step	Category	Status	Tags
2024-05-27	In-Gel Digest (STD)	In-Gel Digest	TEST ENTRIES	05_RUNNING (WE	2024 Q2, Gel LC - Protein Bands Quantitative, QE-HF, RG Leader 01
2024-05-03	In-Gel Digest (STD) 02	MS Analysis	TEST ENTRIES	07_RUNNING (MA	2024 Q2, Co-IP, RG Leader 02, Velos Orbi Elite



CF - The Start

Started with eLabFTW in **06/2021**

First Aims:

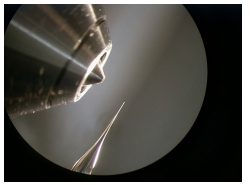


- combine TA Labbook (scanned PDF) with electronic data (and short notes e.g. calculations)
- keeping files together/sorted
- easier finding, communication & time planning

- **NOT** for solving the raw data organization (too big)

- Suitable for **REIMBURSEMENT & Grant Reports** (e.g. DFG91b, SFB, BMBF) calculations

Currently transition to eLabbook only



eLabFTW

Many options to organize, group & tag for search, use of templates

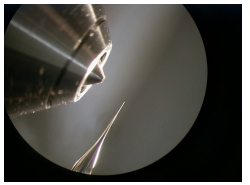
- many varations how to setup → concept for your lab required !
- start with trying on a test setup

  - what are our work flows?
  - what might be a category, resource or status?
  - what is repetetive & suitable for templates?
  - how can analog steps brought to digial (paper-to-PDF)?

eLabbook should accelerate & simplify your work

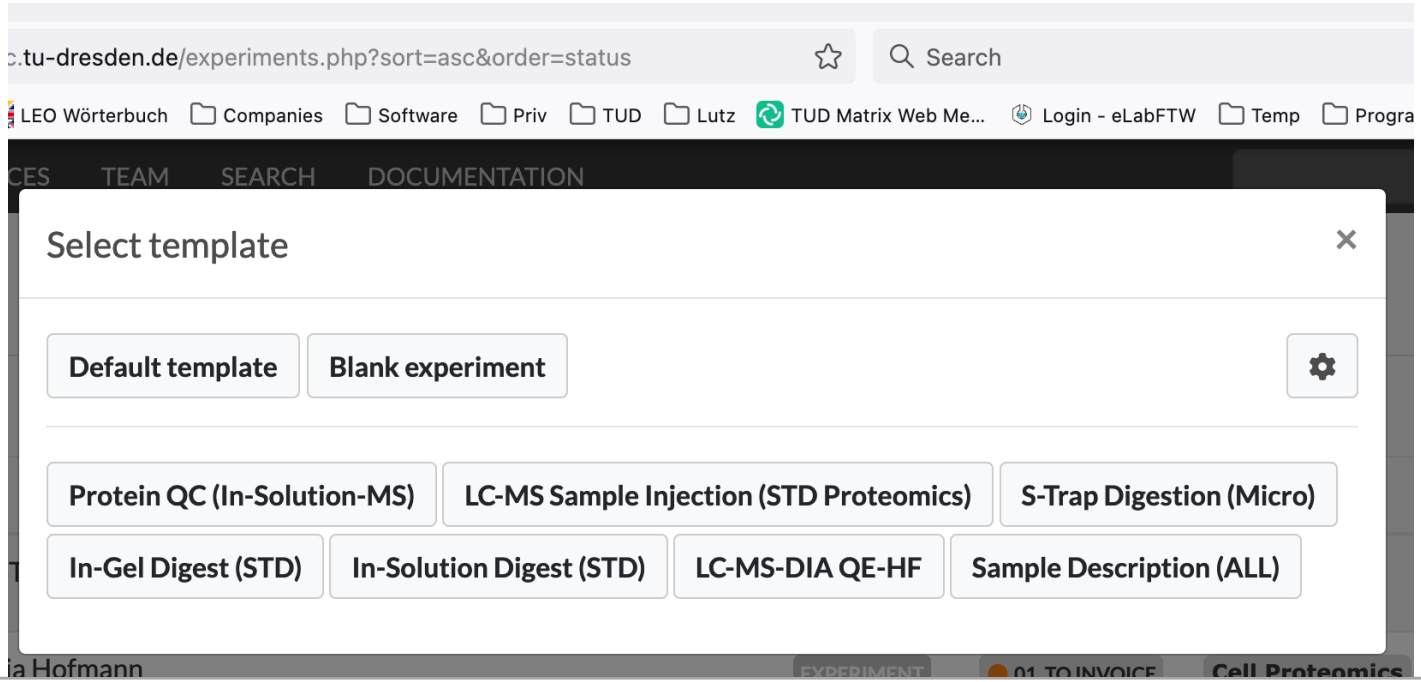
– if not, than something is going wrong, change approach!

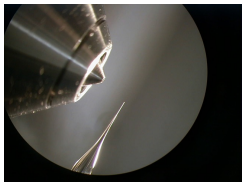
Date	Title	Next step	Category	Status	Tags
2024-05-27	In-Gel Digest (STD)	In-Gel Digest	TEST ENTRIES	05_RUNNING (WE	2024 Q2, Gel LC - Protein Bands Quantitative, QE-HF, RG Leader 01
2024-05-03	In-Gel Digest (STD) 02	MS Analysis	TEST ENTRIES	07_RUNNING (MA	2024 Q2, Co-IP, RG Leader 02, Velos Orbi Elite



eLabFTW

- templates are a key for efficiency !
- easy to adept
- base templates for start, ‘module’ templates to add work steps upon (see next slides)





eLabFTW

File Edit View Insert Format Tools Table

Heading 1 14pt

PROJECT TEAM / Partner:

Submitted on:

AIM:

Experimental Plan:

Lane 01	Lane 02	Lane 03	Lane 04	Lane 05	Lane 06	Lane 07	Lane 08	Lane 09	Lane 10

Here: REPLACE with GEL PICTURE (original without any marks)

Selection of Bands/Areas:

Home - PubMed - N... UniProt Databases LEO Wörterbuch Companies

File Edit View Insert Format Tools Table

Image...
Link... ⌘K
Insert template...
Code sampl
Table
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Special character...
Horizontal line
Page break
Date/time

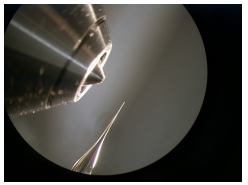
Insert template...

Comments:

Completed on

ADD ANALYSIS

h1 › span



DEMO

Insert template

Templates

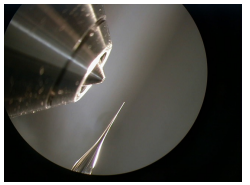
LC-MS Sample Injection (STD Proteomics)

Preview

Sample Recovery & Injection for LC-MS(/MS):

- Sample(s) recovered with 3µl 30% formic acid (FA, Merck) supplemented with 50fmol/µl Peptide RTSTD (Pierce #88320/21)
- diluted with 20µl H_2O (Merck)
- 5µl injected for analysis

Completed:



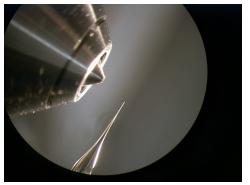
eLabFTW

Experiments Templates

Scope

Filter

Team	Title
Default team	Protein QC (In-Solution-MS)
Default team	LC-MS Sample Injection (STD Proteomics)
Default team	S-Trap Digestion (Micro)
Default team	In-Gel Digest (STD)
Default team	In-Solution Digest (STD)



DEMO

▼ STEPS

- [x] Repeat BCA completed 6 months ago
- [x] S-Trap Digest (7µg) completed 8 months ago
- [x] Mini-Prep Digest (7µg) completed 8 months ago
- [x] LC-MS-DIA completed 7 months ago
- [x] Data Interpretation completed 7 months ago

exact time of check out in details of each step!

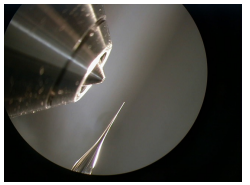
▼ ATTACHED FILES

2023-08-10_Samples-Lysates-for-Marc3.xlsx 12.30 KiB - 2023-09-07 11:55:34

Click to add a comment

20230907_MD_ASMG05-comparison-STrap.pdf 1.44 MiB - 2023-09-07 11:51:51

Click to add a comment



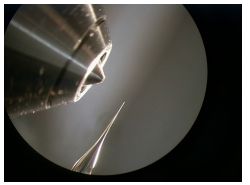
DEMO

Resources

Expand all - Select all

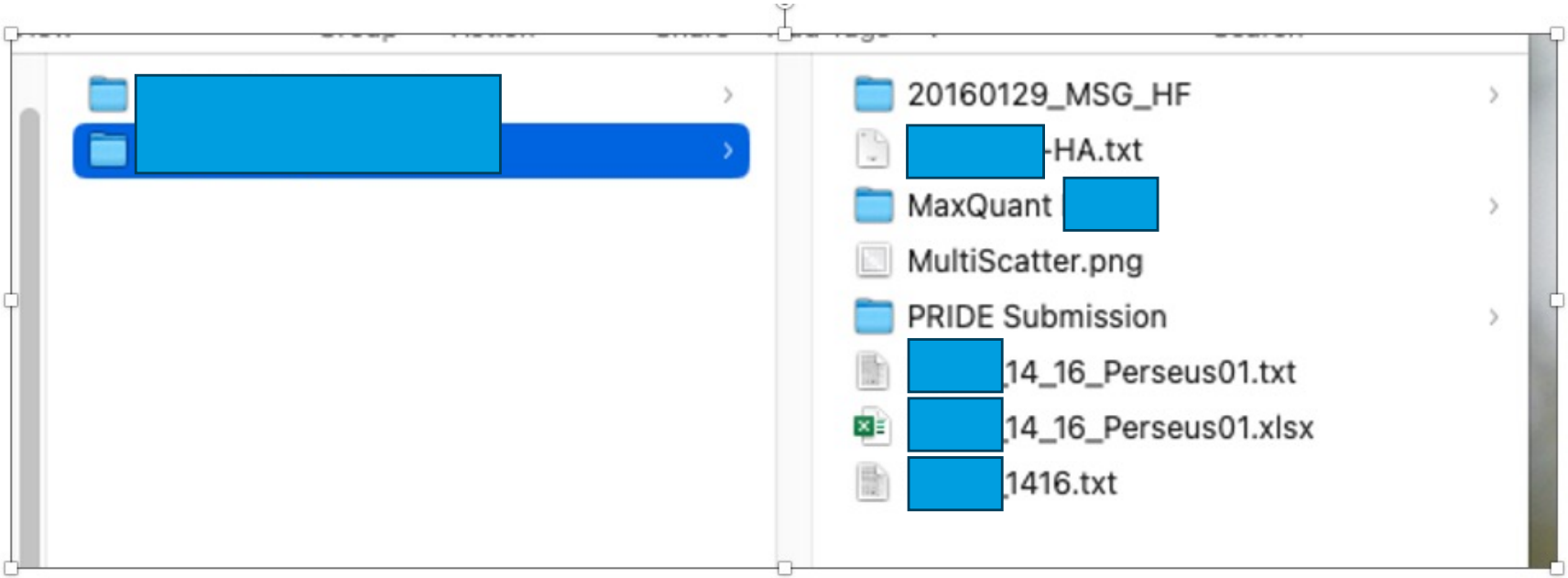
Filter category | Filter status | Filter owner | Filter visibility | 99 | Tags | Show archived

Date	Title	Next step	Category	Status	Tags
2024-04-17	Velos Orbitrap Elite		INSTRUMENTS		
2024-02-28	BCA Assay(s)		MANUFACTURER MA		BCA Assay
2024-02-28	Direct IP Kit (Thermo Pierce #26148) - Direct coupling of AB to beads		MANUFACTURER MA		Co-IP, Crosslinking, Direct IP
2024-03-13	Coomassie Brilliant Blue R250/G250		MATERIALS		SDS Gel Electrophoresis
2024-04-16	Peptide Retention Time Standard (Pierce #88320/21)		MATERIALS		LC_MSMS
2023-03-31	BCA Assay Protocols & Templates		SOP PROTOCOL		BCA Assay

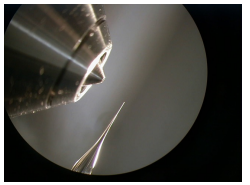


RAW DATA

- organized, structured on file server (raw only & project raw, meta & final data)
- long term storage with backup & protection (by IT CMCB & ZIH)
- also programs are archived



- planning 2015, experiment & analysis 2016, re-analysis & publication 2018



RAW DATA REPOSITORY

PRIDE Archive
PRoteomics IDEntifications Database

Home | Resources | Tools | Help | License | About | Contact

since 2004 (!)

since ~10 years obligatory for publications in many journals

PXD010870

Co-IP (AP-MS) of Connexin-43 - Gap junction protein Connexin-43 is a direct transcriptional regulator of N-cadherin in vivo

Species: Homo sapiens (human);

Project Description: Co-IP Experiment Bait: Cx43-Flag Cell line: Hela Related Publication: Gap Junction protein Connexin-43 is a direct transcriptional regulator of N-cadherin in vivo, Maria Kotini, Elias Barriga, Jonatha...(More)

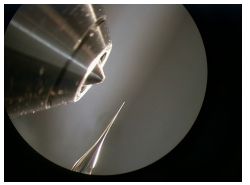
Submitters: Marc Gentzel

Made public: 2018-10-16

Biological

› Matched Items

Name	Type	Size (M)	Download
RM02_MaxQuant_proteinGroups.txt	SEARCH	363925 bit	FTP
RM02_MaxQuant_peptides.txt	SEARCH	1	FTP
MaxQuant_Output.zip	SEARCH	90	FTP
Cx43_Flag.fasta	OTHER	188 bit	FTP
20160129_EK425_RM0216_16fm_RTSTD_120_min_Incl_R060_NCE_25_25ms_T2E4_02.raw	RAW	1377	FTP
20160129_EK425_RM0216_16fm_RTSTD_120_min_Incl_R060_NCE_25_25ms_T2E4_01.raw	RAW	1367	FTP



RAW DATA REPOSITORY

Properties

Organism
Homo sapiens (human)

Organism part
Cell culture

Diseases
Unknown

Modification
monohydroxylated residue

Instrument
Q Exactive

Software
Unknown

Experiment Type
Affinity purification coupled with mass spectrometry proteomics

Quantification
MS1 intensity based label-free quantification method

Dataset reuses
Not available

Number of files
RAW (4), SEARCH (3), PEAK (0), RESULT (0), OTHER (1)

License
Creative Commons Public Domain (CC0)

Title
Co-IP (AP-MS) of Connexin-43 - Gap junction protein Connexin-43 is a direct transcriptional regulator of N-cadherin in vivo

Description
Co-IP Experiment Bait: Cx43-Flag Cell line: Hela Related Publication: Gap Junction protein Connexin-43 is a direct transcriptional regulator of N-cadherin in v
Rauschenberger, Alexandra Schambony, and Roberto Mayor

Sample Processing Protocol
- Co-IP as described in Gentzel, Schille, Rauschenberger, Schambony, MBoC, 2015 *Note: Samples for IP were prepared as mixtures of lysates of transfecte
lysate of untransfected cells; RM0216 90% lysate of untransfected cells, 10% lysate of transfected cells; - acidic elution with 0.1M glycine pH2.5 (approx. 10
overnight with trypsin (Trypsin Gold,PromegaUSA) - followed by digestion with Lys-C (6h)(Roche, Germany) - digest desalted with C-18 reversed phase stage
recovered in 3 microliter 30% formic acid and diluted to 23 microliter with water - 5 microliter injected for LC-MS/MS analysis - LC: Eksigent425 2D-Nano-LC
(Materials: Dr. Maisch, Germany, Picofrit 75 micrometer i.d., NewObjective, USA) - Vented Column Setup, Loading flow rate 400nl/min, separation flow rate 2
formic acid - MS: Q-Exactive HF (ThermoScientific, Bremen, Germany) operated in DDA acquisition mode

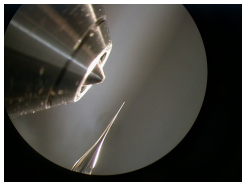
Read less

Data Processing Protocol
- MaxQuant Version 1.6.1.0 including Andromeda search engine - Database Uniprot human 20181215, sequence of Cx43-Flag as cloned,contaminats as pro
Microsoft Excel

Contact
Dr Marc Gentzel, Molecular Analysis - Mass Spectrometry, Center for Molecular and Cellular Bioengineering (CMCB), TU Dresden
Dr Marc Gentzel, Molecular Analysis - Mass Spectrometry Center for Molecular and Cellular Bioengineering (CMCB)TU Dresden Tatzberg 47/49 01307 Dresden Germany (lab head)

Submission Date
27/08/2018

Publication Date
16/10/2018



😉

Thanks to all collaborators,

especially the CMCB IT Team !!

... and last not least ...

Kris Eismann, CF MS & Proteomics