

Willkommen  
Welcome  
Bienvenue

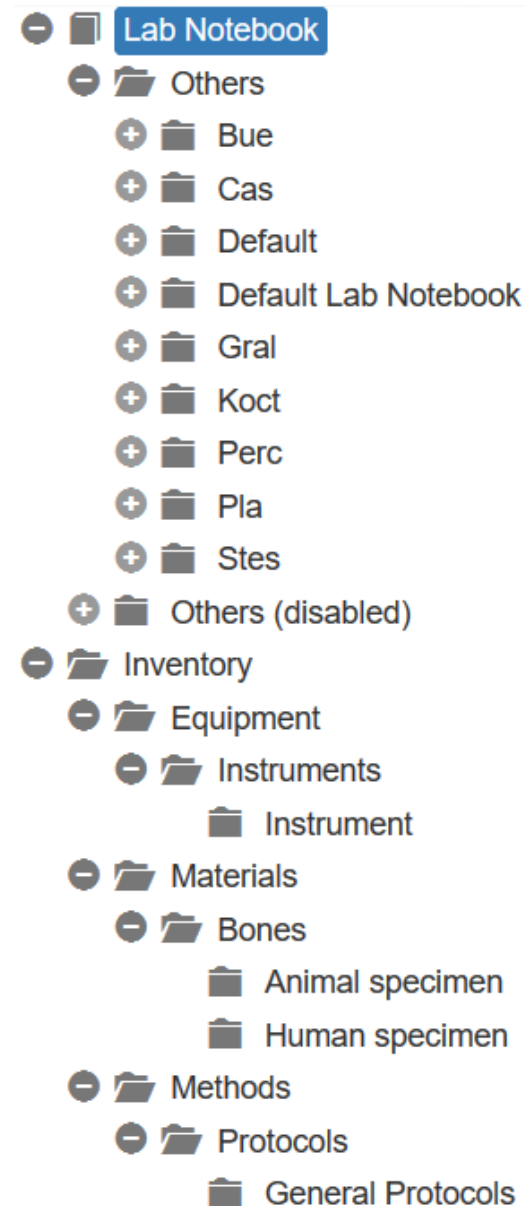


# OpenBIS Pilot Lab 206

Jakob Schwiedrzik

# Overview

- 7 active users
- Databases
  - Materials
  - Instruments
  - Protocols
- Organized by users
- Projects are created by the group head and shared with the respective Postdocs/students
- Main activities
  - ELN
  - Data repository
  - Script subversion
  - Sharing information



# Materials database

Object Browser

Global Search

Collection: Animal specimen  
[/MATERIALS/BONES/ANIMAL\\_SPECIMEN](#)

Operations

Filter	Table AND	Global OR	Options	Columns				
	Storage	Body part	Freezing date	Responsible person	Source	Species	Specimen ID	Operations
<input type="checkbox"/>		Femur	2018-09-27 13:48:30 +0200	Tatiana Kochetkova	Butcher	cow	Bov_01	Operations
<input type="checkbox"/>	<a href="#">206_BIOFREEZER_L435_01</a> [ NoRow , NoCol ] NoBox - NoPos	Femur	2018-09-27 13:48:30 +0200	Tatiana Kochetkova	Butcher	cow	Bov_01_A	Operations
<input type="checkbox"/>		Femur	2018-12-14 00:00:00 +0100	Tatiana Kochetkova	Butcher	cow	Bov_01_B	Operations
<input type="checkbox"/>		Femur	2018-12-14 12:48:30 +0100	Tatiana Kochetkova	Butcher	cow	Bov_01_B1	Operations
<input type="checkbox"/>		Femur	2018-12-14 12:47:30 +0100	Tatiana Kochetkova	Butcher	cow	Bov_01_B2	Operations
<input type="checkbox"/>		Femur	2018-12-14 12:46:30 +0100	Tatiana Kochetkova	Butcher	cow	Bov_01_B3	Operations
<input type="checkbox"/>		Femur	2018-12-14 12:45:30 +0100	Tatiana Kochetkova	Butcher	cow	Bov_01_B4	Operations

# Instrument database

Object Browser

Erste Schritte

Global Search

Collection: Instrument

/EQUIPMENT/INSTRUMENTS/INSTRUMENTS\_EXP\_1

+ Operations

<input type="checkbox"/>	S1	INSTRUMENT	Philips XL30 ESEM	Philips	Gerhard Buerki		Operations
<input type="checkbox"/>	S2	INSTRUMENT	REM Mikromechanik	Zeiss	Gerhard Buerki		Operations
<input type="checkbox"/>	S3	INSTRUMENT	FIB Lyra	Tescan	Gerhard Buerki		Operations
<input type="checkbox"/>	S4	INSTRUMENT	FIB Vela	Tescan	Gerhard Buerki		Operations
<input type="checkbox"/>	S5	INSTRUMENT	Bioindenter		Jakob Schwiedrzik		Operations
<input type="checkbox"/>	S6	INSTRUMENT	AFM RAMAN NT-MDT	NT-MDT	Tatiana Kochetkova	U105a	Operations
<input type="checkbox"/>	S7	INSTRUMENT	Hysitron Ubi Nanoindenter	Hysitron	Jakob Schwiedrzik		Operations
<input type="checkbox"/>	S8	INSTRUMENT	Hitachi S4800	Hitachi	Gerhard Buerki	U104	Operations
<input type="checkbox"/>	S9	INSTRUMENT	Alemnis indenter version 2	Alemnis	Jakob Schwiedrzik		Operations
<input type="checkbox"/>	S10	INSTRUMENT	Desktop SEM indenter HYSEMMEC	Hitachi/Alemnis	Jakob Schwiedrzik	6A/B	Operations

# Protocol database

Object Browser

Erste Schritte

Global Search

Collection: General Protocols  
[/METHODS/PROTOCOLS/GENERAL\\_PROTOCOLS](#)

Operations

Filter	Identifier	Code	Type	Name	Operations
<input type="checkbox"/>	<a href="#">/METHODS/PROTOCOLS/GEN4</a>	GEN4	GENERAL_PROTOCOL	Use of OpenBIS	Operations
<input type="checkbox"/>	<a href="#">/METHODS/PROTOCOLS/GEN5</a>	GEN5	GENERAL_PROTOCOL	Sample preparation bone microanalysis	Operations
<input type="checkbox"/>	<a href="#">/METHODS/PROTOCOLS/GEN6</a>	GEN6	GENERAL_PROTOCOL	Polarized Raman Dübendorf	Operations
<input type="checkbox"/>	<a href="#">/METHODS/PROTOCOLS/GEN7</a>	GEN7	GENERAL_PROTOCOL	FIB bone micropillars	Operations
<input type="checkbox"/>	<a href="#">/METHODS/PROTOCOLS/GEN8</a>	GEN8	GENERAL_PROTOCOL	Bloindenter	Operations
<input type="checkbox"/>	<a href="#">/METHODS/PROTOCOLS/GEN9</a>	GEN9	GENERAL_PROTOCOL	Raman Thun	Operations

1 - 6 of 6 items 10 Per Page Page 1 of 1

Lab Notebook

- Others
  - Bue
  - Cas
  - Default
  - Default Lab Notebook
  - Gral
  - Koct
  - Perc
  - Pla
  - Stes
- Others (disabled)
- Inventory
  - Equipment
    - Instruments
      - Instrument
  - Materials
    - Bones
      - Animal specimen
      - Human specimen
  - Methods
    - Protocols
      - General Protocols
- Stock
  - Stock Catalog
  - Stock Orders

# Example protocol

## Object: Polarized Raman Dübendorf

[/METHODS/PROTOCOLS/GENERAL\\_PROTOCOLS/GEN6](#)




### ▼ General info

**Name:**

Polarized Raman Dübendorf

### ▼ Children

<div>Filter <input type="text"/>  <span>AND</span> <span>OR</span> <span>Options ▼</span> <span>Columns ▼</span></div>				
Identifier	Code	Type	Name	Modification Date
<a href="#">/KOCT/FEMHALS/EXP1</a>	<a href="#">EXP1</a>	EXPERIMENTAL_STEP	<a href="#">Raman Pol Bovine 16012019</a>	2020-01-24 11:16:58
<a href="#">/KOCT/FEMHALS/EXP1_1</a>	<a href="#">EXP1_1</a>	EXPERIMENTAL_STEP	<a href="#">Raman Pol Bovine 03062019</a>	2020-01-06 08:48:23
<a href="#">/KOCT/FEMHALS/EXP2</a>	<a href="#">EXP2</a>	EXPERIMENTAL_STEP	<a href="#">Raman Pol MTLT 27032019</a>	2020-01-24 11:18:19
<div>1 - 3 of 3 items <span>10 ▼</span> Per Page <span>◀</span> Page <span>1</span> <span>▼</span> of 1 <span>▶</span></div>				

# Example protocol

**For what:**

Non-destructive qualitative analysis of material composition and molecular anisotropy.

**Materials:**

Confocal Raman microscope (alpha300R, WITec, Ulm, Germany) equipped with a piezo-scanner

Objectives: 10x (0.25 NA), 50x (0.80 NA), 100x

**Time requirement:**

~ integration time \* number of spectra

For average polarized spectra acquisition at one spot: 7 min for 180°, 15 min for 370° with 10° polarization step.

**Procedure:****Software (Project FIVE):**

Scanning table – 700g; CCD#2. For table positioning – positioning tab, for spectra acquisition – oscilloscope tab.

Polarizer motors controller: STSv1.0 (or latest running version), Ray line (785 nm), set position to 0 + check motors position visually.

**Calibration:**

Calibration on Si reference with 100x objective at chosen grating (300gr/mm works well). Raman spectra calibration parameters:

***PRS Si calibration***

<b>laser power</b>	40 mW
<b>Integration time</b>	0.1 s
<b>Grating</b>	150 g/mm   300 g/mm
<b>Center <math>\lambda</math></b>	969   1500

# Example protocol

## Measurements:

Samples are mounted to the sample chamber (max 4 at once, better to have the same sample height). Before any spectra acquisition on each sample – overview image with 10x objective is done (Image stitching → sample positioning, geometry → center at current position,  $X=Y \sim 5000$ ). Then change the objective and take another smaller overview of the ROI (listen position → once,  $X=Y \sim 500$ ). For spectra acquisition: switch off the light & optical microscope, oscilloscope → start, find Z with the best Raman spectra. Then enter sample name (ex. *B8-ost1\_785nm\_50xSD\_30mW\_PoloutAll*), set accumulation to 1. For single spectra acquisition use the WITec soft, for multiple polarized spectra – use the Labview soft (STSV1.0), enter the sample name there and manually check polarizer motor position before collecting the new set of spectra.

Typical Polarized Raman parameters for spectra acquisition on bone are shown below:

### *PRS on bone setup parameters*

<b>Laser <math>\lambda</math></b>	785
<b>Laser power</b>	30 mW
<b>Objective</b>	50x 0.80 NA
<b>Integration time</b>	30 s
<b>Grid</b>	300 gr/mm
<b>Center <math>\lambda</math></b>	1500
<b>Polarizer angles range</b>	0 – 180 / 0 - 370
<b>Polarizer angle step</b>	10

## Data manipulation (CCR):

Highlight spectra in the list → drag → CCR+Smooth → OK → values: 4 & 9



# Example protocol

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**Data extraction:**

Export file → Use data obj name → no number before, spectral units: rel 1/cm

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**▼ References**

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**References:**

Mandair, G. S., & Morris, M. D. (2015). Contributions of Raman spectroscopy to the understanding of bone strength. *BoneKEy Reports*, 4(August 2014), 1–8. <https://doi.org/10.1038/bonekey.2014.115>

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**▼ Identification Info****Type:**

GENERAL\_PROTOCOL

**Collection:**

/METHODS/PROTOCOLS/GENERAL\_PROTOCOLS

**Code:**

GEN6

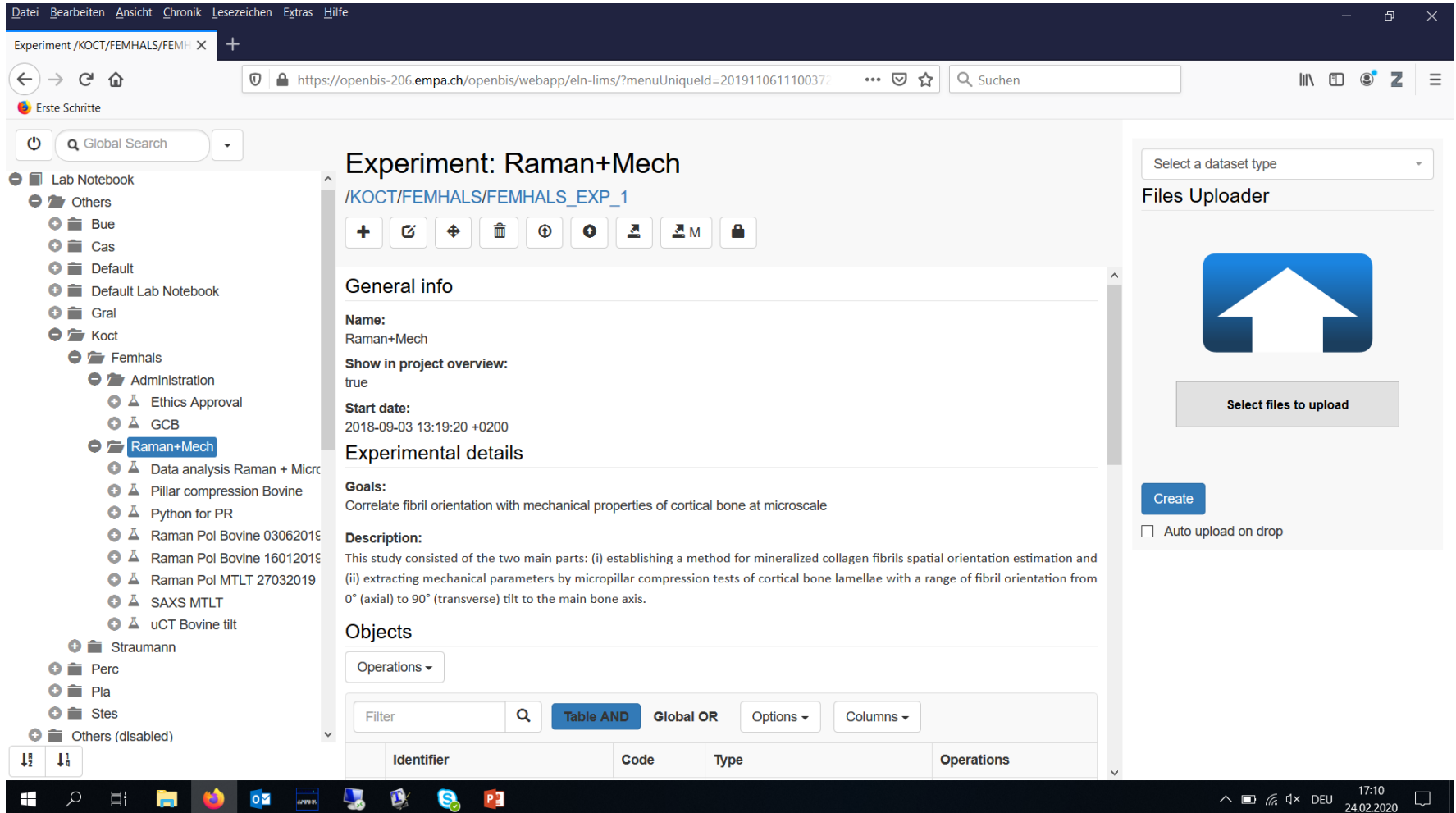
**Registrator:**

sjj

**Registration Date:**

2019-11-06 10:51:57

# ELN and project structure example



The screenshot displays the Empa ELN (Electronic Laboratory Notebook) interface. The top navigation bar includes menu items: Datei, Bearbeiten, Ansicht, Chronik, Lesezeichen, Extras, and Hilfe. The browser address bar shows the URL: <https://openbis-206.empa.ch/openbis/webapp/eln-lims/?menuUniquelId=201911061110037/>.

The main content area is titled "Experiment: Raman+Mech" with the identifier `/KOCT/FEMHALS/FEMHALS_EXP_1`. It features a toolbar with icons for adding, editing, deleting, and other actions. The "General info" section includes the name "Raman+Mech", a checkbox for "Show in project overview" (checked), and the "Start date" (2018-09-03 13:19:20 +0200). The "Experimental details" section contains "Goals" (Correlate fibril orientation with mechanical properties of cortical bone at microscale) and a "Description" (This study consisted of the two main parts: (i) establishing a method for mineralized collagen fibrils spatial orientation estimation and (ii) extracting mechanical parameters by micropillar compression tests of cortical bone lamellae with a range of fibril orientation from 0° (axial) to 90° (transverse) tilt to the main bone axis).

The left sidebar shows a hierarchical tree structure of the project, including folders like "Lab Notebook", "Others", "Bue", "Cas", "Default", "Default Lab Notebook", "Gral", "Koct", "Femhals", "Administration", "Ethics Approval", "GCB", "Raman+Mech", "Data analysis Raman + Micro", "Pillar compression Bovine", "Python for PR", "Raman Pol Bovine 03062019", "Raman Pol Bovine 16012019", "Raman Pol MTLT 27032019", "SAXS MTLT", "uCT Bovine tilt", "Straumann", "Perc", "Pla", "Stes", and "Others (disabled)".

The right sidebar contains a "Files Uploader" section with a "Select a dataset type" dropdown, a large blue upload icon, a "Select files to upload" button, a "Create" button, and a checkbox for "Auto upload on drop".

The bottom of the interface shows a table with columns: Identifier, Code, Type, and Operations. The table is currently empty, with a "Filter" input and "Table AND Global OR" buttons above it.

# Summary

- ELN is currently actively used by 7 users
- Since most instruments are connected to PCs with internet access, the ELN can be used on site
- Using the general experimental step templates is feasible
- Later on, we plan to develop specific templates for certain types of measurements
- Chosen structure:
  - User based
  - Projects created by group head/project responsible and shared with collaborators
  - Admin information is stored as first experiment in every project
  - Experimental campaigns are grouped into logical subprojects
- Combination of ELN with data repository and material/instrument database allows to keep track of projects and is especially attractive for archiving