

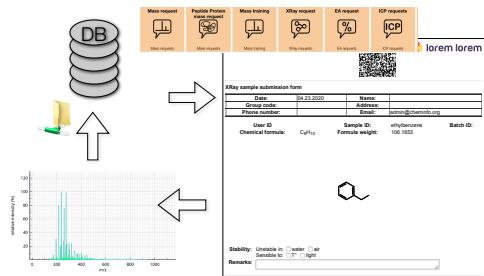
**eln.epfl.ch (www.c6h6.org)**  
Scientific data management in the browser

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## Importing analytical results

## Traceability and analytical results



**Manual submission to [eln.epfl.ch](http://eln.epfl.ch)**

- **On bruker spectrometer (TopSpin)**
    - **save** - ask for productCode and batchCode
    - **autosave** - experimental name: **LP1001\_f1**
  - **On infrared, ms, ...**
    - need to create specific workflow
    - save to a special directory with name like "**patiny\_LP1001\_f1.jdx**"
      - or **397b762d1c39\_LP123\_F1.jdx**"
    - copy / paste to a specific webpage

## Traceability and analytical results



## List of connected instruments

File	Last modified	Name
...	2 min ago	SGC1 - 1 - injection chemist-subunit procedure - Instruments -
New		
My Drive		
Shared with me		
Recent		
Wanted		
Starred		
Search Google Drive		
View settings		

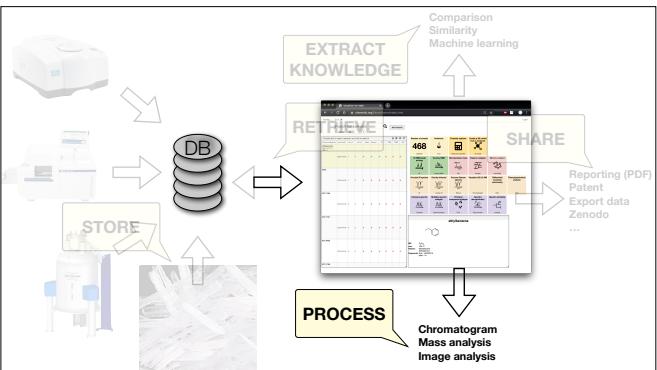
## Automatic submission to cheminfo - IconNmr

Code\_Batch

## Image analysis

Bit depth, mask, ROI, resolution  
Hull, MBR, Ferret min, Ferret max, Compactness

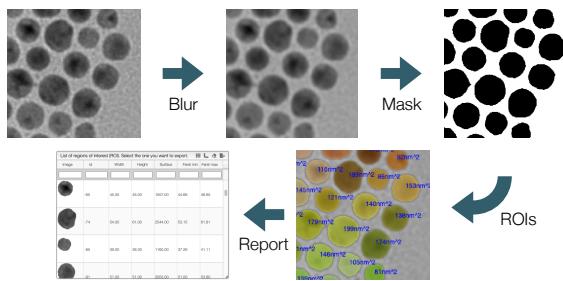
2



## Image formats

	TIFF	GIF	JPEG	PNG
Bits per channel	8, 16, 32	256 indexed colors	8	8, 16
Alpha		1 bit		8 or 16 bits
Compression	yes / no may be destructive	yes (non destructive)	yes (destructive)	yes (non destructive)

## Image analysis of regions of interest (ROI)

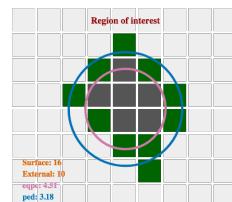


## General ROI information

- Surface (number of pixels)
- External (pixels that has external border)

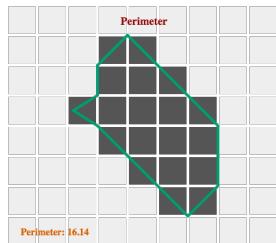
$$D_{EQPC} = 2\sqrt{\frac{\text{Surface}}{\pi}}$$

$$D_{PBD} = \frac{\text{External}}{\pi}$$



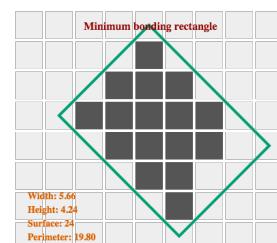
## Perimeter

- All external pixel SIDES
- 2 external sides:  $- (2\sqrt{2})$
- 3 external sides:  $- 2 * (2\sqrt{2})$



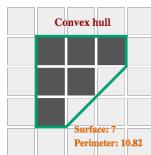
## Minimum bonding rectangle (MBR)

- Smallest rectangle containing all the pixels



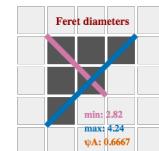
## Convex hull

- Rubber band around all the pixels



## Feret diameters

- Caliper diameters



## Other parameters

$$roundness = \frac{4 \times surface}{\pi \times (feretDiameters . max)^2}$$

$$solidity = \frac{surface}{convexHull . surface}$$

$$sphericity = \frac{2\sqrt{\pi \times surface}}{perimeter}$$

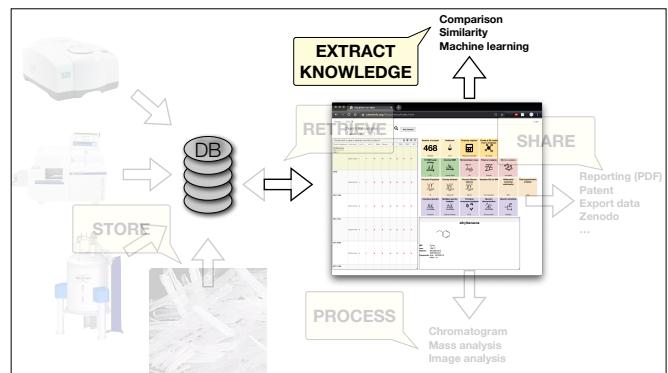
## External links

- [Demo](#)

# Multiple spectra analysis

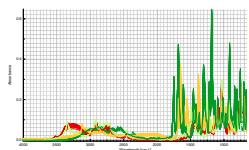
Superimpose hundreds of spectra in one click  
Integration, relative spectra  
Export data for kinetic analysis

# 3



## The goal

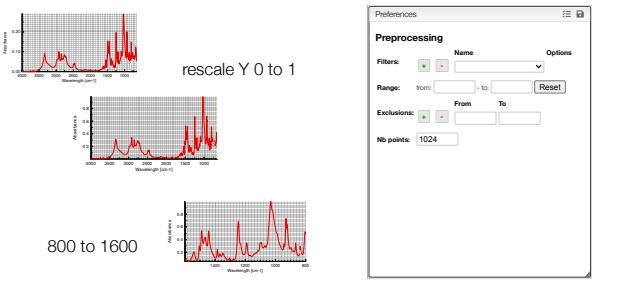
- Compare spectra coming from various instruments
- Superimpose spectra
- Integrate, calculations



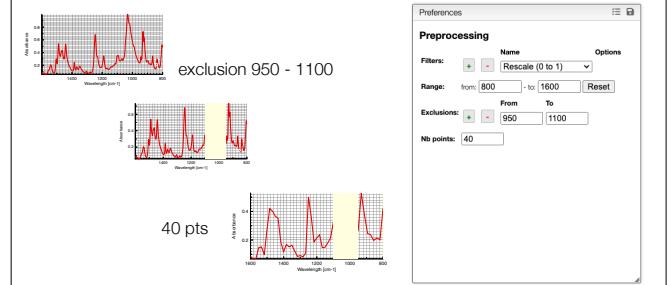
## The problems

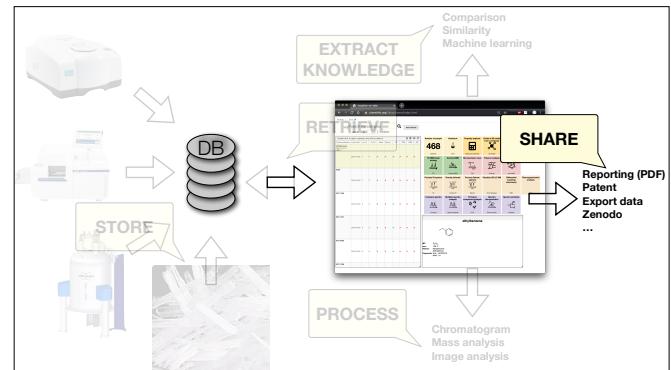
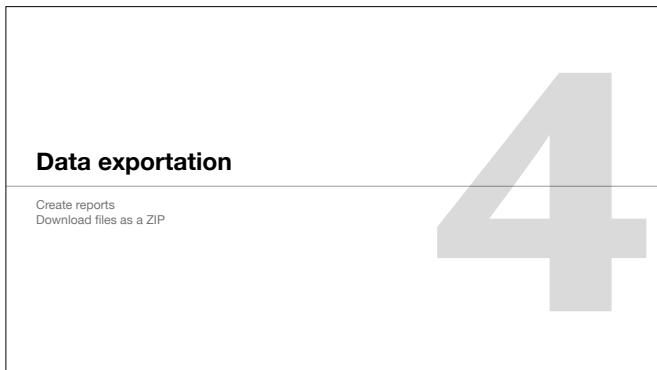
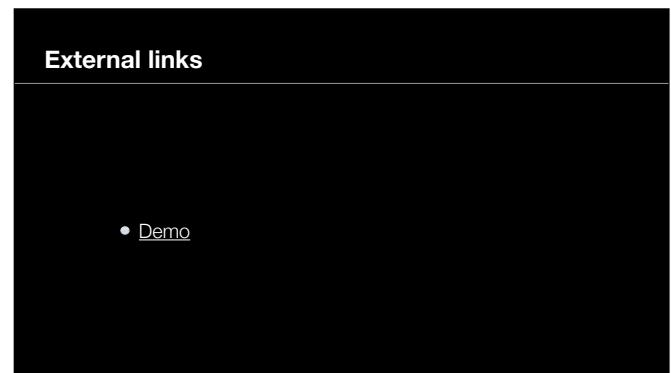
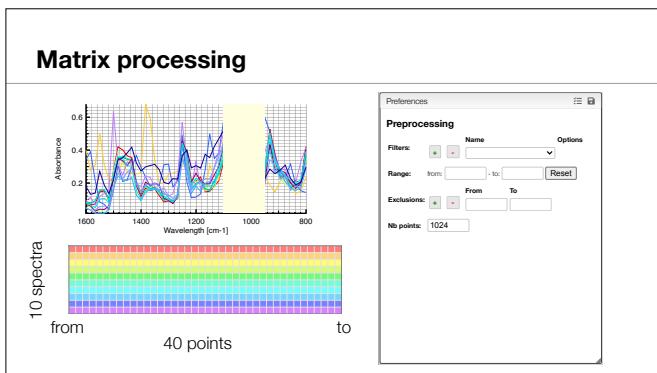
- Different ranges (from / to)
- Different units
- Different resolutions
- Different intensities
- Solvent / impurities

## Preprocessing: creation of a matrix



## Preprocessing: creation of a matrix





## External links

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- [Demo](#)