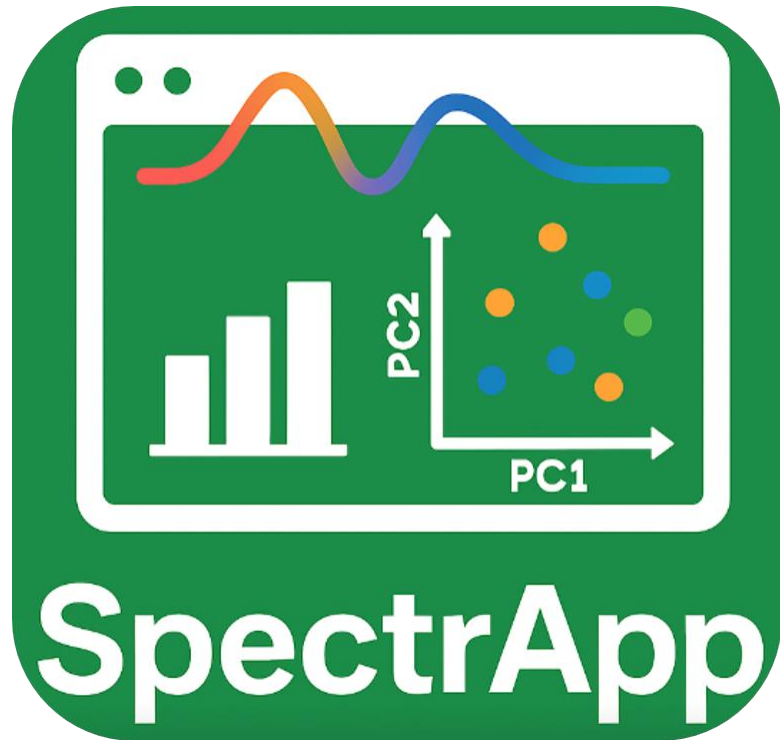# SpectrApp

Applications that facilitates to perform statistical analysis.

It aims to be an alternative to paid solutions (e.g., Matlab, STATA,...) providing a user-friendly interface of R routines for many common tasks.

Login SpectrApp

Username

Enter your username

Password

Enter your password

→] Login

© Spectrapp - Developed by the Department of Chemistry of the University of Turin and DataBloom Srl

Username: *eafs*

Password: *2025*

SpectrApp pipeline

Import data

Import data

Type of file:

.csv ▾

Data:

Upload… | eafs2025_blood.csv

Upload complete

⚙▾

☁ Import

30
Rows

602
Columns

⚙

→ Next step → Edit

Once imported, click on "Next step"

↗ — ↗

Search:

ID	Blood_source	700	701	702	703	704	705	706	707	70
	All	All	All	All	All	All	All	All	All	All
S_1	Blood_1	0.839248598	0.83859545	0.8373409510000001	0.836078405	0.835126758	0.834991634	0.835918605	0.837677121	0.840327

Edit data

Data pre-processing

Spectra / Time / Numeric Variables

☐ Select ranges

All data selected.

Choose pre-processing technique(s):

Background (row)
Baseline
Continuum Removal

Row Scaling
Standard Normal Variate (SNV)
SNV + Detrend
Extended Multiplicative Signal Correction (EMSC)

With spectra, select the variable range

Select one or more pre-processing from the list (N.B. the order is significant)

Data pre-processing

Spectra / Time / Numeric Variables

☐ Select ranges

All data selected.

Choose pre-processing technique(s):

Extended Multiplicative Signal Correction (EMSC) ×

Preprocessing Settings

↔ **Range scaling**

≋ **Smoothing**

⊞ **Binning**

🖌 **Background / Baseline**

⊡ **Row scaling & EMSC**

Edit settings *ad hoc* for specific pre-processing

⚙ Preprocess

→ Next step →
Chemicals

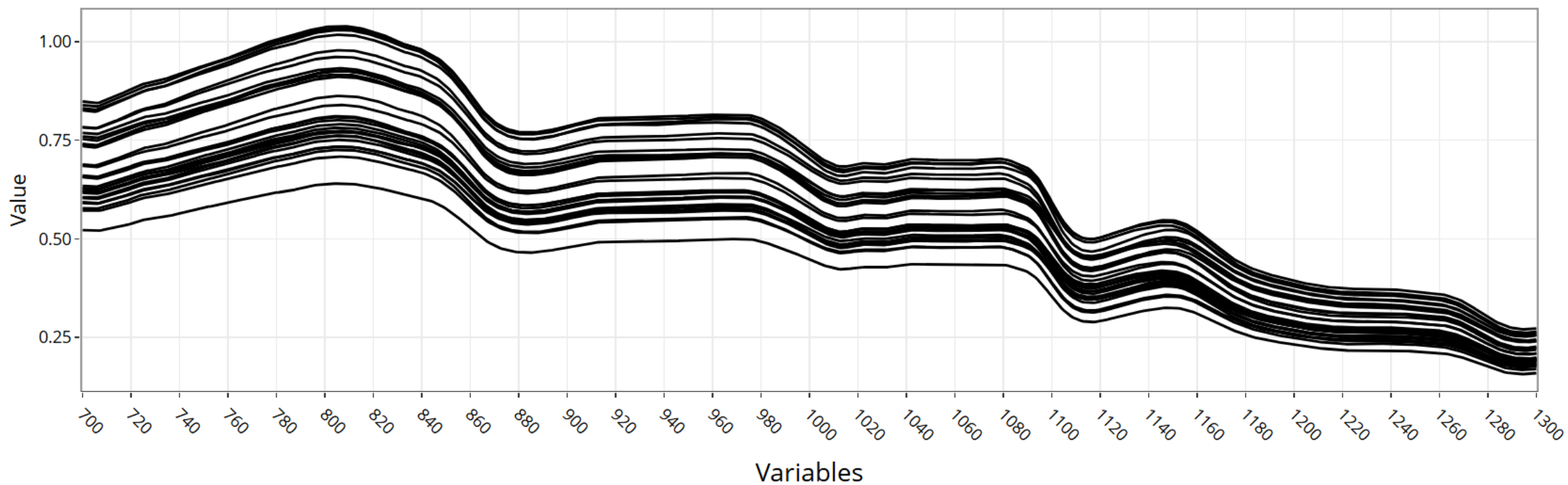# Data pre-processing

Compare raw and
pre-processed

Original data

Click to enter Plot title

Data pre-processing

Data pre-processing

Edit graphs settings

Original data

Pre-processed data

Click to enter Plot title

Value

0.04

0.00

-0.04

700 732 763 795 826 858 889 921 953 984 1016 1047 1079 1111 1142 1174 1205 1237 1268 1300

Variables

Blood_source — Source_1 — Source_2 — Source_3

Data pre-processing

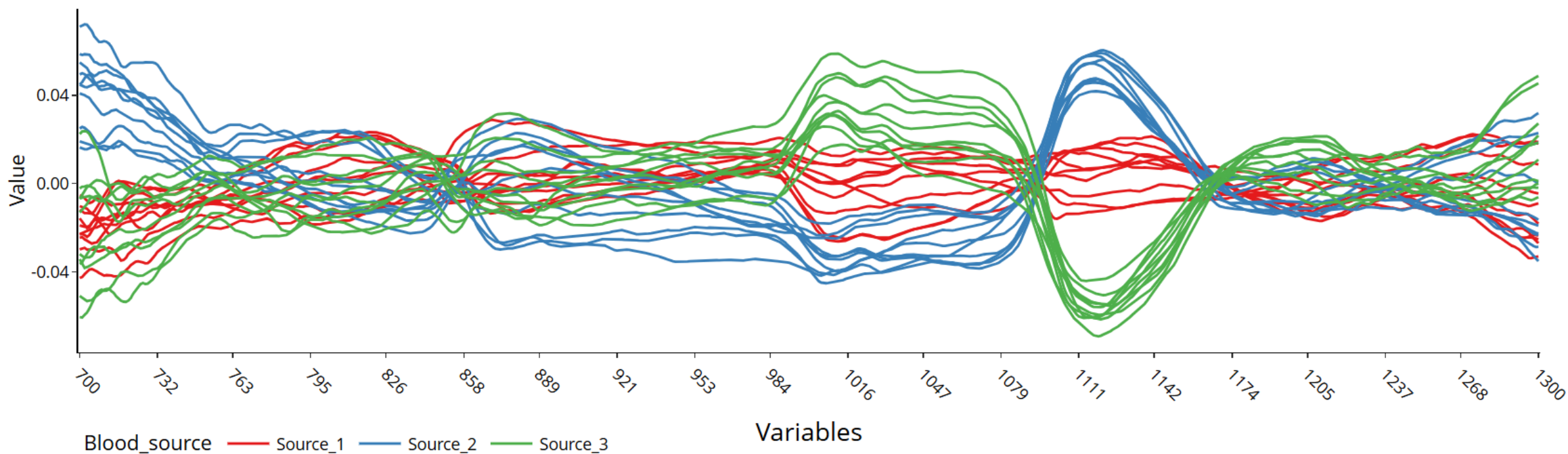## Pre-processed data

Show [10 ∨] entries   Search: [   ]

	Blood_source	Instrument	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720
S_1	Source_1	A	-0.024	-0.024	-0.025	-0.026	-0.027	-0.027	-0.027	-0.027	-0.025	-0.024	-0.022	-0.021	-0.019	-0.018	-0.016	-0.016	-0.015	-0.014	-0.013	-0.014	-0.015
S_2	Source_1	B	-0.010	-0.011	-0.011	-0.011	-0.013	-0.014	-0.014	-0.015	-0.016	-0.017	-0.016	-0.016	-0.015	-0.014	-0.014	-0.014	-0.014	-0.015	-0.014	-0.014	-0.014
S_3	Source_1	A	-0.005	-0.006	-0.007	-0.008	-0.009	-0.008	-0.008	-0.007	-0.007	-0.007	-0.008	-0.009	-0.009	-0.010	-0.009	-0.009	-0.009	-0.009	-0.009	-0.007	-0.007
S_4	Source_1	B	-0.030	-0.030	-0.029	-0.030	-0.030	-0.030	-0.030	-0.031	-0.031	-0.030	-0.030	-0.030	-0.029	-0.029	-0.030	-0.032	-0.034	-0.035	-0.035	-0.034	-0.032
S_5	Source_1	A	-0.012	-0.013	-0.013	-0.013	-0.014	-0.014	-0.013	-0.011	-0.009	-0.007	-0.005	-0.003	-0.002	-0.001	0.000	0.001	0.001	0.001	0.001	0.001	0.001
S_6	Source_1	B	-0.023	-0.023	-0.023	-0.024	-0.023	-0.021	-0.019	-0.017	-0.016	-0.015	-0.016	-0.016	-0.017	-0.017	-0.016	-0.014	-0.013	-0.011	-0.010	-0.009	-0.009
S_7	Source_1	A	-0.016	-0.017	-0.019	-0.020	-0.020	-0.018	-0.016	-0.015	-0.013	-0.010	-0.009	-0.007	-0.005	-0.002	-0.000	0.001	0.001	0.001	0.001	-0.000	-0.001
S_8	Source_1	B	-0.019	-0.019	-0.020	-0.020	-0.019	-0.018	-0.017	-0.016	-0.017	-0.018	-0.020	-0.022	-0.023	-0.023	-0.022	-0.021	-0.020	-0.018	-0.018	-0.018	-0.017
S_9	Source_1	A	-0.043	-0.042	-0.041	-0.040	-0.039	-0.039	-0.039	-0.040	-0.041	-0.041	-0.042	-0.041	-0.041	-0.042	-0.042	-0.042	-0.042	-0.041	-0.040	-0.039	-0.038
S_10	Source_1	B	-0.023	-0.022	-0.022	-0.021	-0.021	-0.021	-0.020	-0.020	-0.019	-0.019	-0.018	-0.019	-0.019	-0.019	-0.019	-0.019	-0.018	-0.017	-0.016	-0.016	-0.015

Showing 1 to 10 of 30 entries   Previous [1] 2 3 Next

If the pre-process is fine, you can start building the models

30	**2**	**601**	**0**
Samples	Factor variables	Numeric variables	Chemical variables

⧬ → Unsupervised   ⊕ → Discrimination   ▤ → Class Modelling   ⯗ → Regression

Unsupervised models

Exclude these variables from modeling:

Nothing selected ▾

Remove vars from computation

| PCA | HCA | K-means | DBSCAN | t-SNE | UMAP |

PCA model

Nr. of PCs for PCA model:

10

Select PCA methodology:

SVD ▾

🖩 Calculate

Unsupervised models

Unsupervised models

This approach works for both unsupervised and supervised models

Supervised models - discrimination

Supervised models - regression

MLR   PCR   PLS

Available models

PLS model

Select response (Y):

700.00

Nr. of components:

10

Select validation:

None

🧮 Calculate

Credits

Eugenio Alladio, PhD

Eugenio Alladio, PhD

Assistant Professor at the Department of Chemistry, University of Turin.

Alberto Mazzoleni

Alberto Mazzoleni

PhD student at the Department of Chemistry, University of Turin.

Giovanni Solarino

Giovanni Solarino

PhD student at the Department of Chemistry, University of Turin.

Lorenzo Castellino
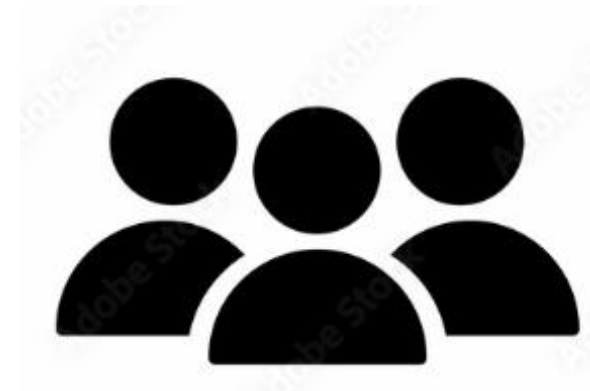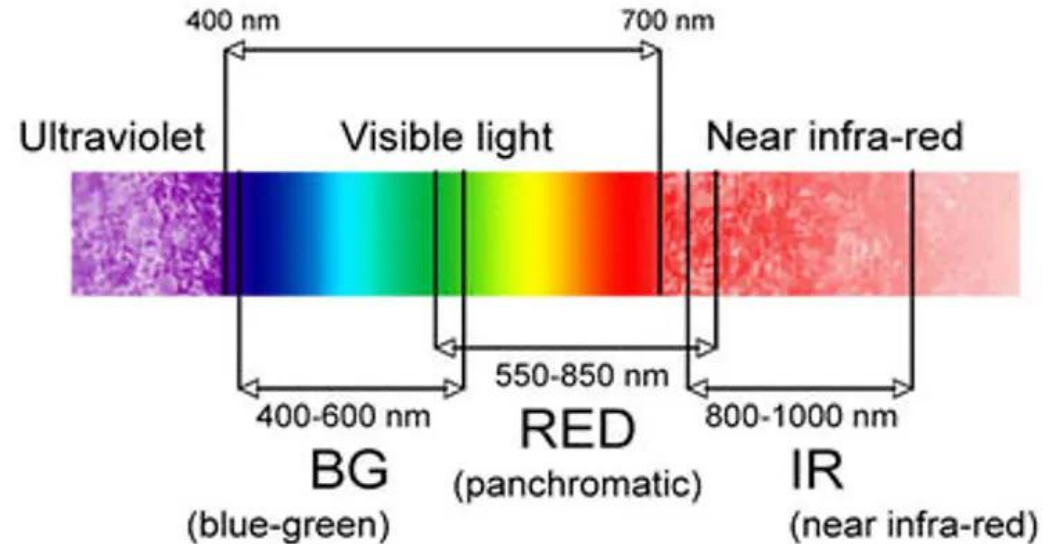
Lorenzo Castellino

PhD student at the Department of Chemistry, University of Turin.
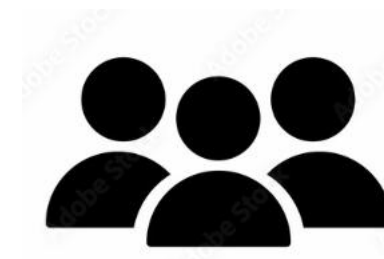
eafs2025_full_example.csv

- **Features:** NIR wavelengths + concentration.

- **Classes:** 2 types, 3 operators.
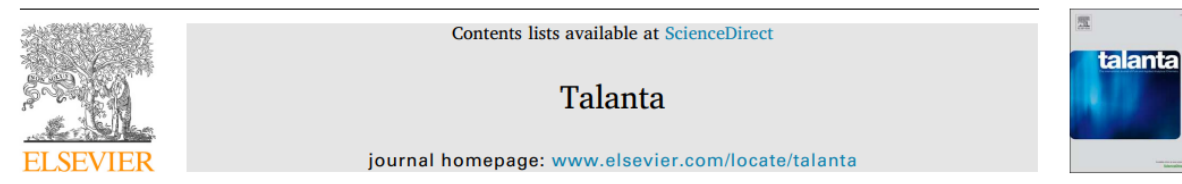
- **Samples:** training + test.

SpectrApp – workshop datasets

eafs2025_blood.csv

- **Features:** 600 NIR wavelengths.

- **Classes:** 3 subjects, 2 instruments.

- **Samples:** 30 samples.

Toward a novel framework for bloodstains dating by Raman spectroscopy:
How to avoid sample photodamage and subsampling errors

Alicja Menżyk[a,*], Alessandro Damin[b], Agnieszka Martyna[a], Eugenio Alladio[b,c], Marco Vincenti[b,c], Gianmario Martra[b], Grzegorz Zadora[a,d]

[a] Institute of Chemistry, University of Silesia in Katowice, Szkolna 9, 40-007, Katowice, Poland
[b] Department of Chemistry, University of Torino, Via P. Giuria 7, 10125, Torino, Italy
[c] Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Regione Gonzole 10/1, 10043, Orbassano, Torino, Italy
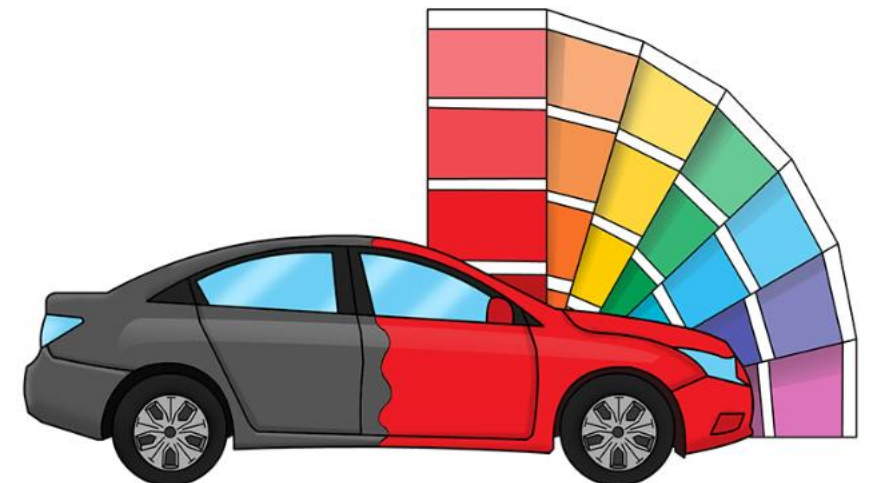[d] Institute of Forensic Research, Westerplatte 9, 31-033, Krakow, Poland

SpectrApp – workshop datasets

eafs2025_carpaints.xlsx

- **Features:** 175 NIR wavelengths.

- **Classes:** 2 classes, 4 replicates
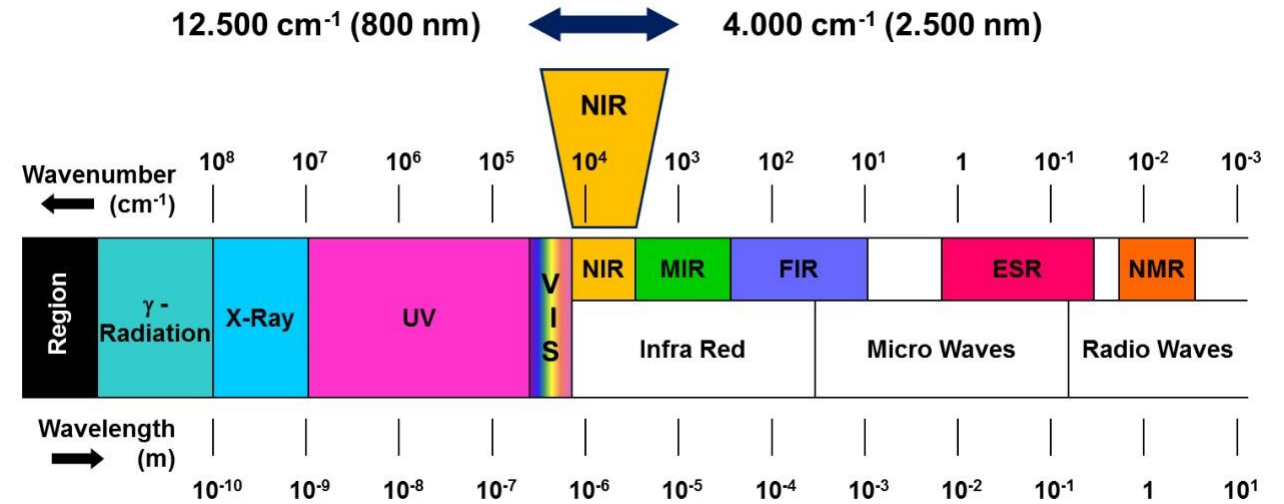
- **Samples:** 48 samples.

eafs2025_spraypaints.xlsx

- **Features:** UV-Vis, FTIR and micro-Raman wavelengths (3 spreadsheets).

- **Classes:** Spray brands, fluo vs. non-fluo.

- **Samples:** ~30 samples.
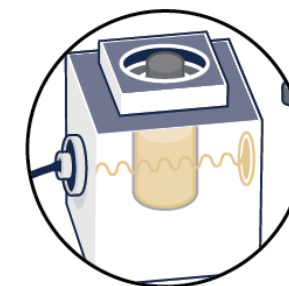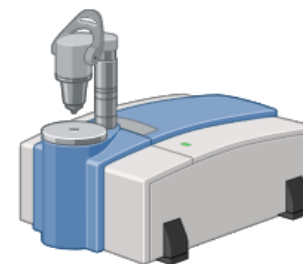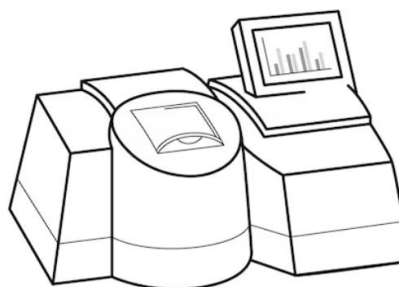
SpectrApp – workshop datasets

eafs2025_gsr.xlsx

- **Features:** SEM/EDX for gunshot residue analysis (elements) concentration.

- **Classes:** stubs and data from hands, barrell, cartridge and hammer.

- **Samples:** ~80 samples.

eafs2025_glass.csv

- **Features:** µ-XRF elements composition from glass samples + refraction index

- **Classes:** samples from 3 classes (lightbulb, windows, car).

- **Samples:** 105 samples.

SpectrApp – workshop datasets

eafs2025_ICP_MS.csv

- **Features:** ICP-MS elements composition from glass samples

- **Classes:** samples from 4 classes.

- **Samples:** training and test datasets.

SpectrApp – workshop datasets

eafs2025_gasoline.csv

- **Features:** gasoline samples with known Octane numbers were measured between 900 and 1700 nm using NIR.

- **Response:** Octane number rating.

- **Samples:** 60 samples.

eafs2025_wines.csv

- **Features:** set of covariates described in Forina et al. (1986).

- **Class:** 3 Italian wines – Barolo, Barbera, Grignolino.

- **Samples:** 178 samples.

Data | PDF Available

Wines M.Forina, C.Armanino, M.Castino, M.Ubigli, "Multivariate data analysis as discriminating method of the origin of wines", Vitis, 25, 189-201 (1986)

January 1986
DOI:10.13140/2.1.4312.6560

Authors:

Michele Forina
Università degli Studi di Genova

SpectrApp

Cost-effective: As an alternative to paid solutions like Matlab or STATA, SpectrApp offers a cost-effective option for performing statistical analysis, particularly for users or organizations with budget constraints.

User-friendly interface: SpectrApp provides a user-friendly interface, making statistical analysis accessible to users with varying levels of expertise. This can lower the barrier to entry for individuals or teams who may not have extensive programming skills.

Wide range of analysis techniques: SpectrApp offers a comprehensive set of analysis techniques, including decomposition methods like PCA and PLS, unsupervised models such as clustering, and supervised models like regression (e.g., multivariate regression) and classification (e.g., kNN). This breadth of functionality caters to diverse analytical needs.

Updates and maintenance: SpectrApp's development team must consistently update and maintain the application to ensure compatibility with new R releases, address bugs or security vulnerabilities, and add features or improvements. Failure to do so could lead to usability issues or a stagnant feature set over time.

Learning curve for new users: Despite its user-friendly interface, SpectrApp still requires users to understand statistical concepts and the underlying methodology behind the analysis techniques it offers. New users may need to invest time in learning how to interpret results and make informed decisions based on the outputs generated by the application.

SpectrApp – future perspectives
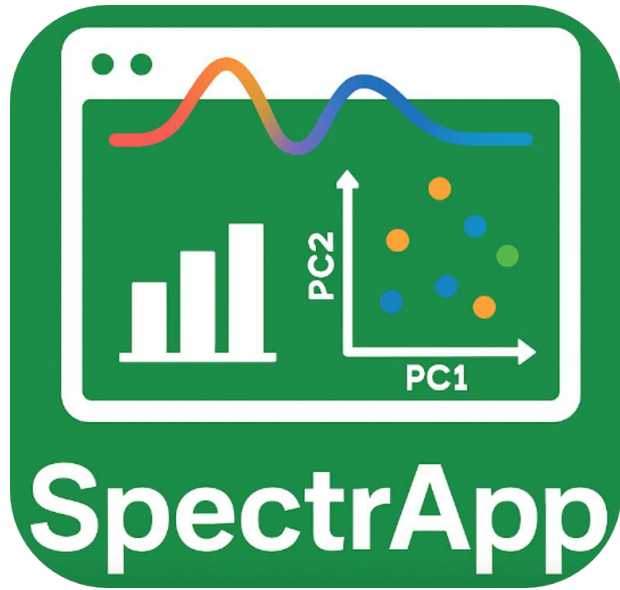
- **Enhanced integration and compatibility**;

- **Advanced chemometrics modules**: Continuously expanding the repertoire of statistical analysis techniques within SpectrApp can enhance its utility for users across diverse domains.

- **Scalability and performance optimization**: Investing in scalability and performance optimization;

- **Community engagement and support**: an article is in the making with the intention of release to general public shortly after (GitHub code will be available, too)!

- **Cross-platform compatibility**;

- **Continuous improvement and innovation**.

Let's Keep
in Touch

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