

# Chemometric approaches in spectroscopy for food analysis

## Fingerprints examples

### EEM (fluorescence)

Pretreatment  
(normalization, 1<sup>ST</sup> and  
2<sup>ND</sup> derivative or  
others)

Variable selection (VIP,  
UVE-PLS or others)

Data exploration (PCA,  
PP)

PARAFAC,  
Classification  
tools (LDA,  
SIMCA, SVM,  
NPLS-DA or  
others)

Regression  
tools (NPLS,  
ANN, SVMR  
or others)

### FTIR, NIR, NMR, UV- Vis...

Noise filtering

Peak detection and  
deconvolution

Overlapping peaks  
(HELP, SFA, OPA or  
others)

Pretreatment (mean  
centering, normalisation  
or others)

Variable selection (VIP,  
UVE-(PLS) or others)

Data decomposition  
(MCR-ALS, PARAFAC2  
or others)

Data exploration (PCA)

Classification  
tools (LDA,  
SIMCA, SVM, PLS-  
DA or others),  
MCR-ALS

Regression  
tools (PLS,  
OPLS, SVMR  
or others),  
MCR-ALS

### HSI

Pretreatment (mean  
centering, normalisation  
or others)

Alignment (COW, DTW or  
others)

Variable selection (VIP,  
UVE-PLS or others)

Data exploration (PCA,  
PP)

Classification  
tools (LDA,  
SIMCA, SVM,  
PLS-DA or  
others)

Regression  
tools (PLS,  
OPLS, SVMR  
or others)

# Modern Food Analysis

**Frank Leslie Hart, Harry Johnstone  
Fisher**



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