

Chemometric approaches in spectroscopy for food analysis

Fingerprints examples

EEM (fluorescence)

Pretreatment
(normalization, 1ST and
2ND 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

Clemens Wendtner



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