

**CLOVER**  
BioSoft



## Use Cases of Clover MSDA Software

Keywords: Clover MSDA software, data analysis, MALDI-TOF, mass spectrometry, profiling, classification, discrimination, identification, statistics



**Clinical proteomics:**  
Biomarker  
discovery



**Clinical proteomics:**  
Oncology



**Clinical proteomics:**  
Neurology



**Biopharma**  
development



**Food &**  
beverage

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## About Us

# Clover BioSoft

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Clover BioSoft develops innovative tools for mass spectrometry data analysis, empowering researchers to unlock the full potential of MALDI-TOF profiling across the life sciences.

## Get in Touch

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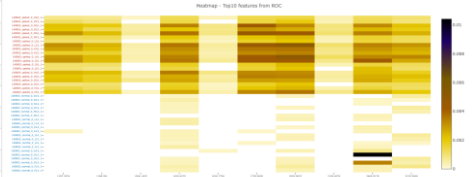
# Clinical proteomics: Biomarker discovery

Protein profiling aiming for identification of biomarkers separating plasma spiked with standard peptides from non-spiked control (CTRL) samples

## 1 Discover

Top 10 m/z features from ROC analysis all represent spiked peptides (including oxidized versions)

Peak #	AUC (s = 0.8)	Appearance #	Positive Category #	Mass #	p value *	q value (FDR adjusted p value) #
1297.3074	1	21/40	20/20	1620.4375	9.156e-11	5.033e-10
1348.581	1	20/40	20/20	2093.9652	1.081e-10	5.033e-10
1620.4375	1	36/40	20/20	1348.581	1.510e-10	5.033e-10
1759.9656	1	22/40	20/20	1759.9656	3.523e-10	8.807e-10
2093.9652	1	32/40	20/20	1297.3074	1.890e-9	3.779e-9
3150.5668	1	30/40	20/20	2109.4076	1.852e-7	3.006e-7
2109.4076	0.95	18/40	18/20	1636.7706	2.654e-6	3.792e-6
1636.7706	0.9188	18/40	17/20	3150.5668	1.638e-5	1.968e-5
2466.9178	0.9025	33/40	20/20	1364.1455	1.771e-5	1.968e-5
1364.1455	0.85	14/40	14/20	2466.9178	1.068e-2	1.068e-2



## 2 Build a feature table

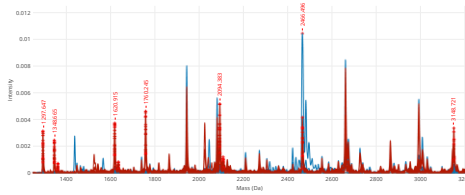
Parameters

Preprocessing parameters

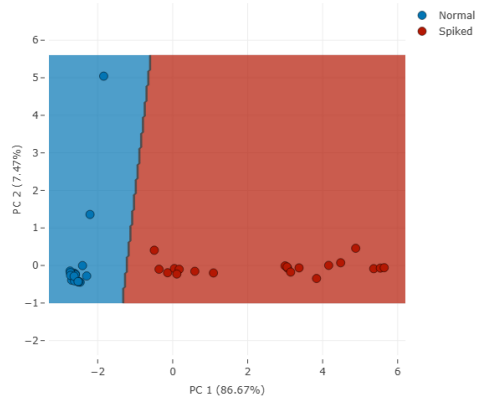
- Savitzky-Golay
  - Window length: 31
  - Polynomial order: 3
- Baseline
  - Tophat filter, Factor: 0.02
- Mass filtering
  - Replicated

Feature Table parameters

- Alignment
  - Allowed shift: High
  - Binning (fSD): On
  - Constant Mass tolerance (Da): 5
  - Linear Mass tolerance (ppm): 600
- Blank scanning
- Normalization
  - TIC
- Find Peaks
  - Minors: 1297.3074 - 1348.581 - 1364.1455 - 1620.4375 - 1636.7706 - 1759.9656 - 2093.9652 - 2109.4076 - 2466.9178 - 3150.5668
  - Relative (threshold): 0.04
  - Maximum: Peak INTENSITY
  - Constant Mass tolerance (Da): 5
  - Linear Mass tolerance (ppm): 600
- Peak shape
  - Prominence: 0.01
  - Width: 0
  - Distance: 1
- Merge
  - Constant Mass tolerance (Da): 5
  - Linear Mass tolerance (ppm): 600



## 3 Train the classifier



## 4 Predict

Name	Predicted Category ↓	Estimated Prob.
140803_0_F15_1	Spiked	99.43%
140803_0_G15_1	Spiked	82.58%
140803_0_G16_1	Spiked	98.86%
140803_0_H15_1	Spiked	99.35%
140803_0_H16_1	Spiked	99.58%
140803_0_I15_1	Spiked	70.93%
140803_0_N14_1	Normal	88.06%
140803_0_O13_1	Normal	84.53%
140803_0_O14_1	Normal	88.06%



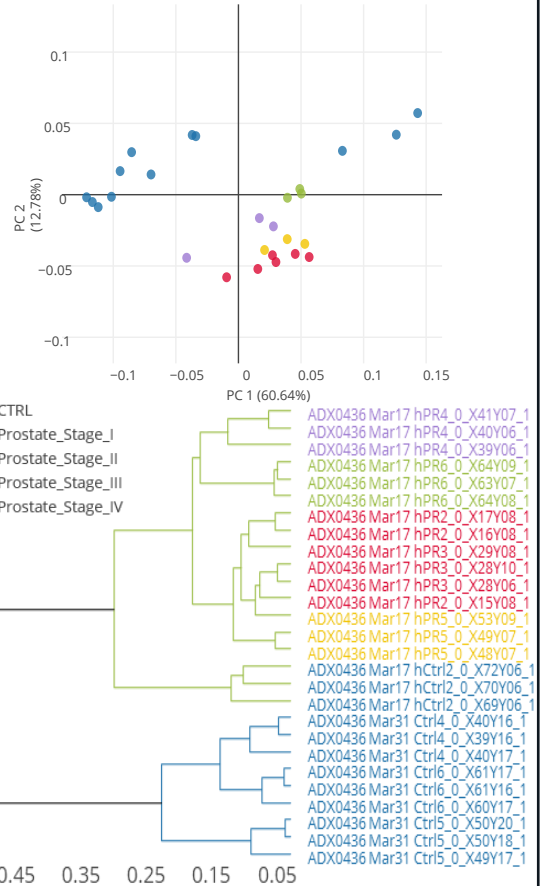
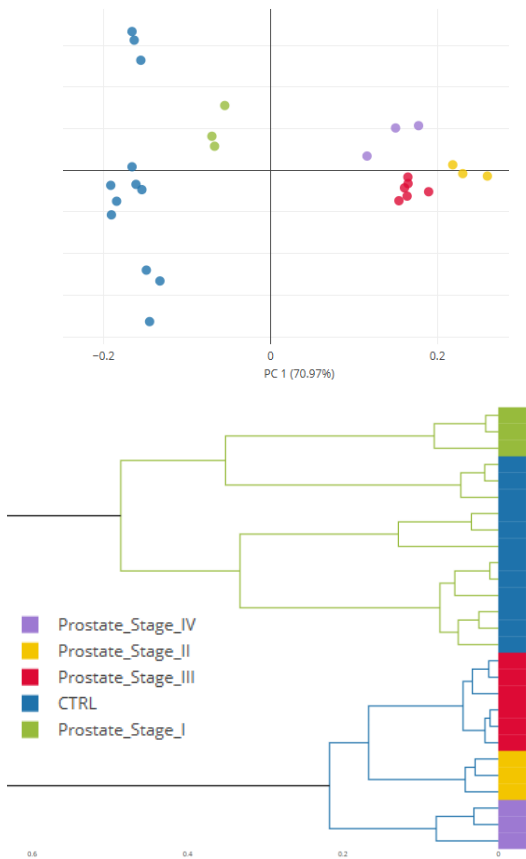
# Clinical proteomics: Oncology

Multimic *ex*BAMS-MALDI-TOF EV/exosome profiling for classification of prostate cancer stages

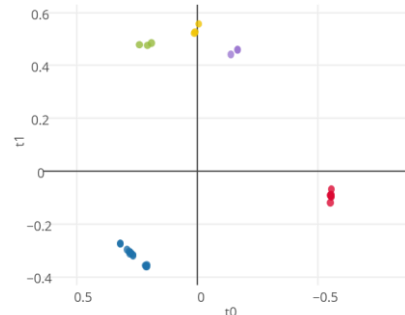
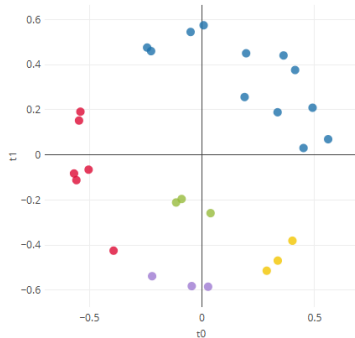
## Protein profiling

## Peptide profiling

Unsupervised multivariate analysis  
Hierarchical clustering & PCA:



Supervised ML Prediction Models  
LightGBM

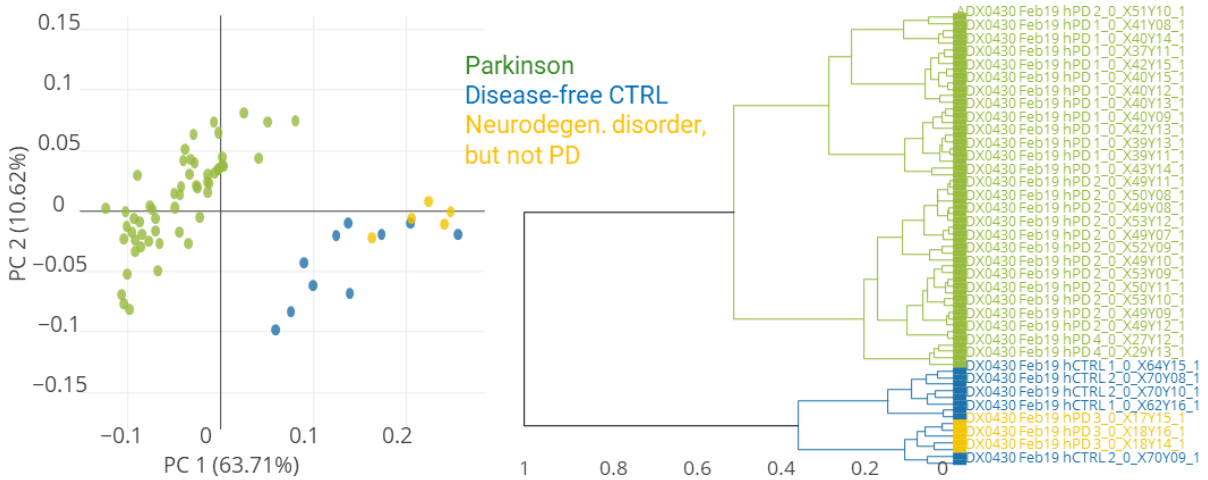




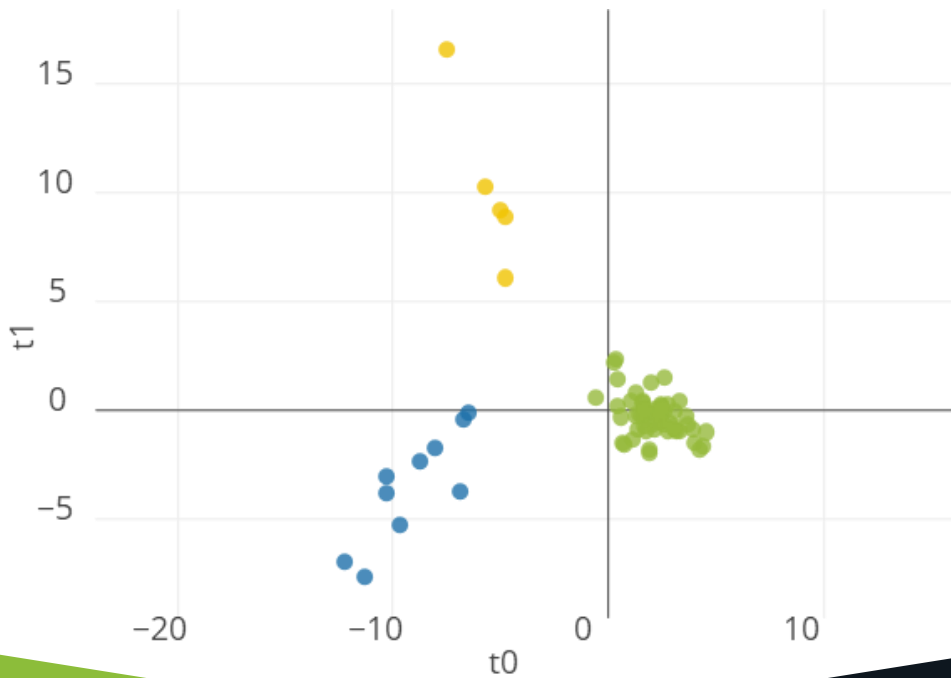
# Clinical proteomics: Neurology

*exo*BAMS-MALDI-TOF EV/exosome **protein profiling** discriminates between Parkinson's disease (PD), other neurodegenerative disorders, and disease-free CTRL samples

Unsupervised multivariate analysis  
Hierarchical clustering & PCA:



Supervised ML Prediction Models  
PLS-DA

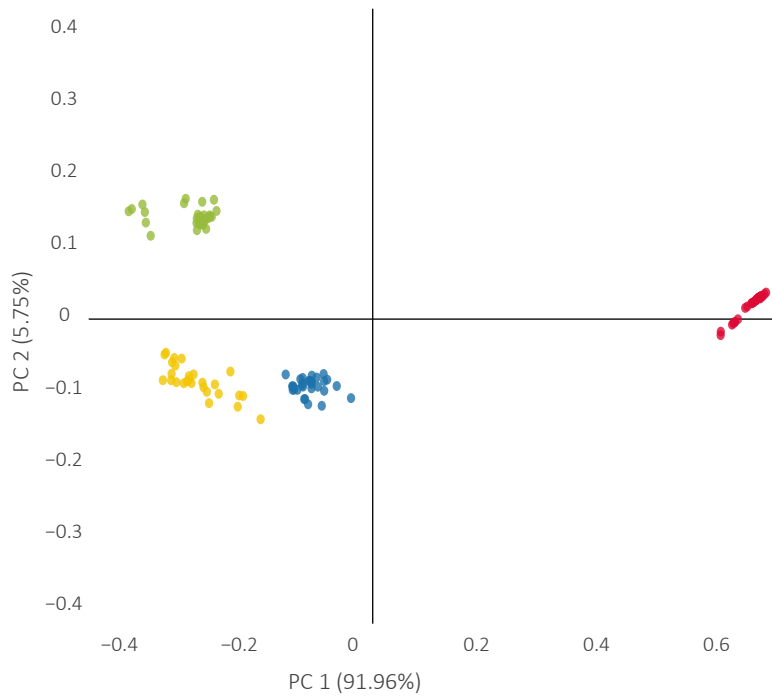




# Biopharma development: Biosimilar classification

Classification of nivolumab biosimilars based on N-glycan profiles

Unsupervised multivariate analysis  
Hierarchical clustering & PCA:

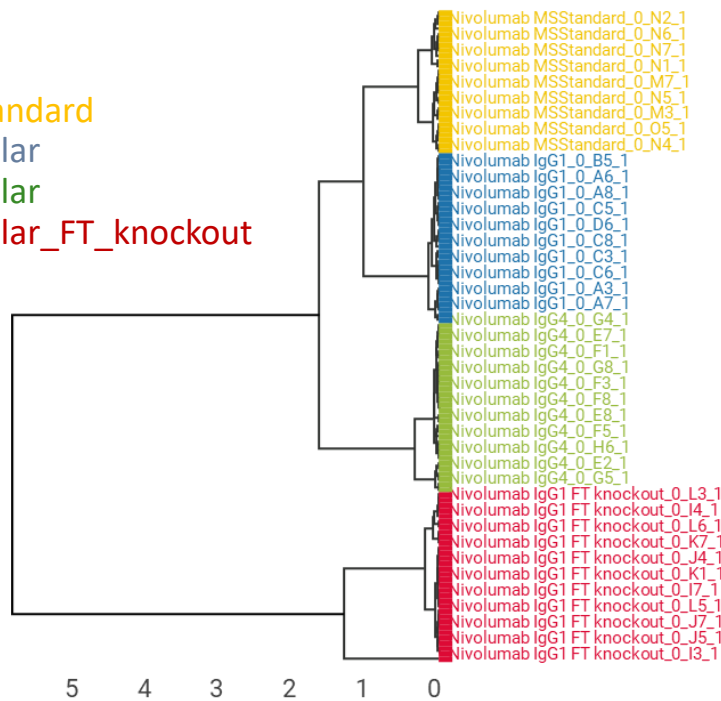


IgG1\_MS\_Standard

IgG1\_Biosimilar

IgG4\_Biosimilar

IgG1\_Biosimilar\_FT\_knockout

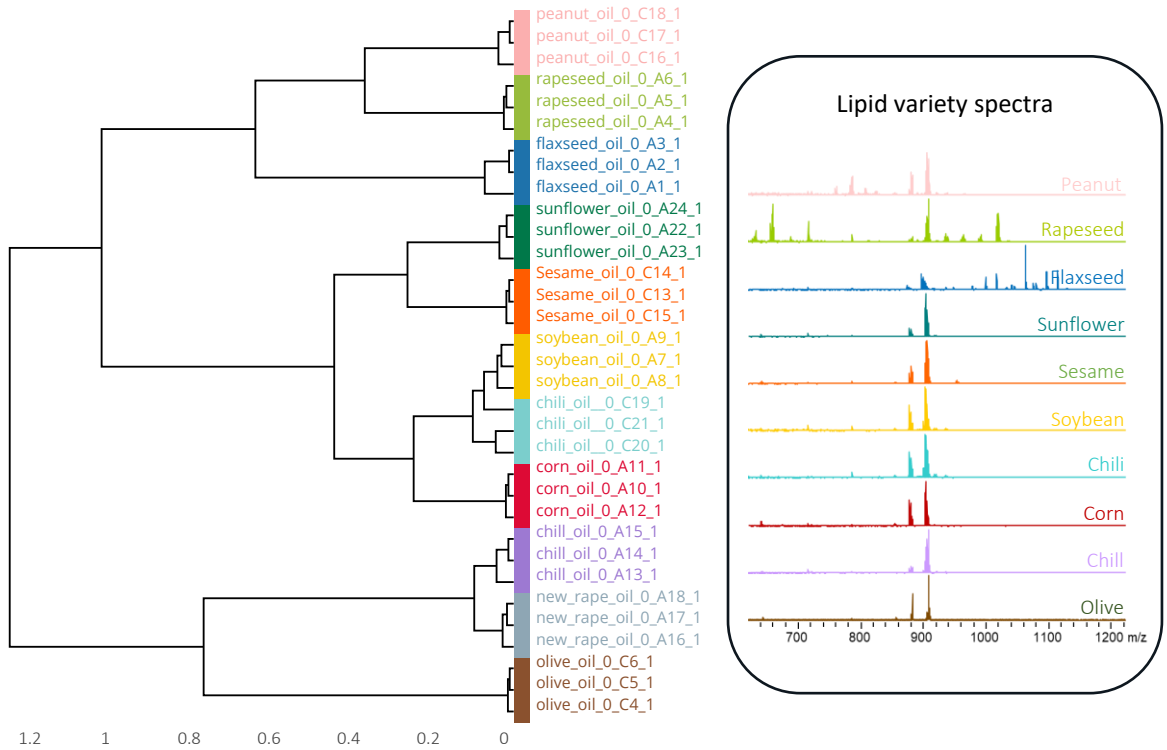




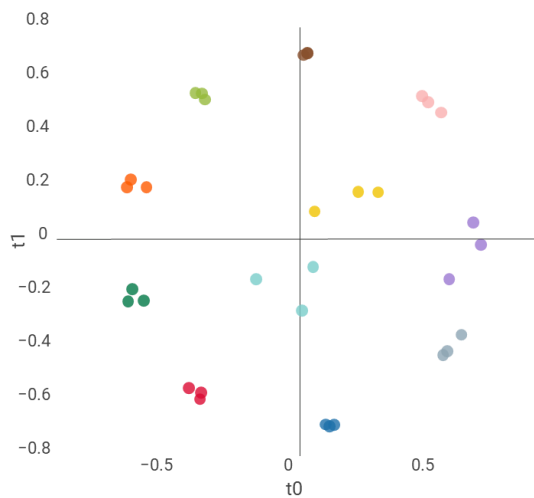
# Food & beverage: Food authenticity

## Classification of edible oils based on lipid profiles

### Unsupervised multivariate analysis Hierarchical clustering & PCA:



### Supervised ML Prediction Models Random Forest (RF)



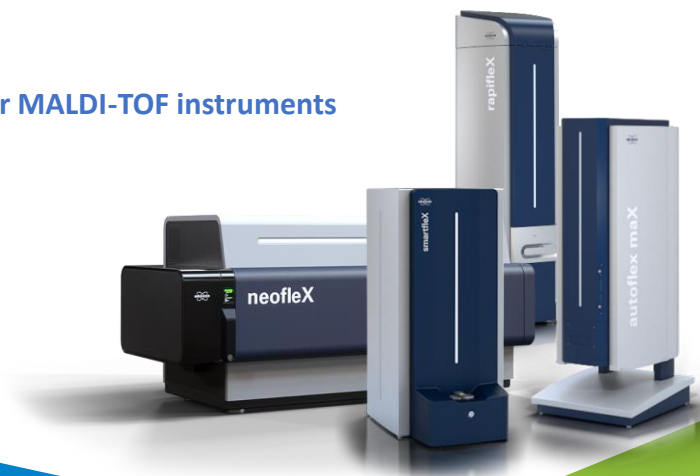
Sample courtesy: Chengdu Institute of Food Inspection, Chengdu, China; Data courtesy: Hong Kong Polytechnic University, Hong Kong, China

## Conclusions

- Clover MSDA software provides a powerful statistical toolbox to efficiently leverage the discriminative power of MALDI-TOF MS profiling data originating from biological samples.
- The software provides access to a wide range of statistical methods via an intuitive, workflow-oriented web interface. It features user management, project and experiment-driven data management, as well as detailed reporting of results.
- Clover MSDA software supports tailored data analysis workflows, allowing for time-efficient analysis of large cohorts of MALDI-TOF spectra with minimal effort and providing tremendous benefit to biomarker discovery as well as classification and identification tasks across a broad range of life science applications.

For Research Use Only. Not for use in clinical diagnostic procedures.

### Compatible with all Bruker MALDI-TOF instruments



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