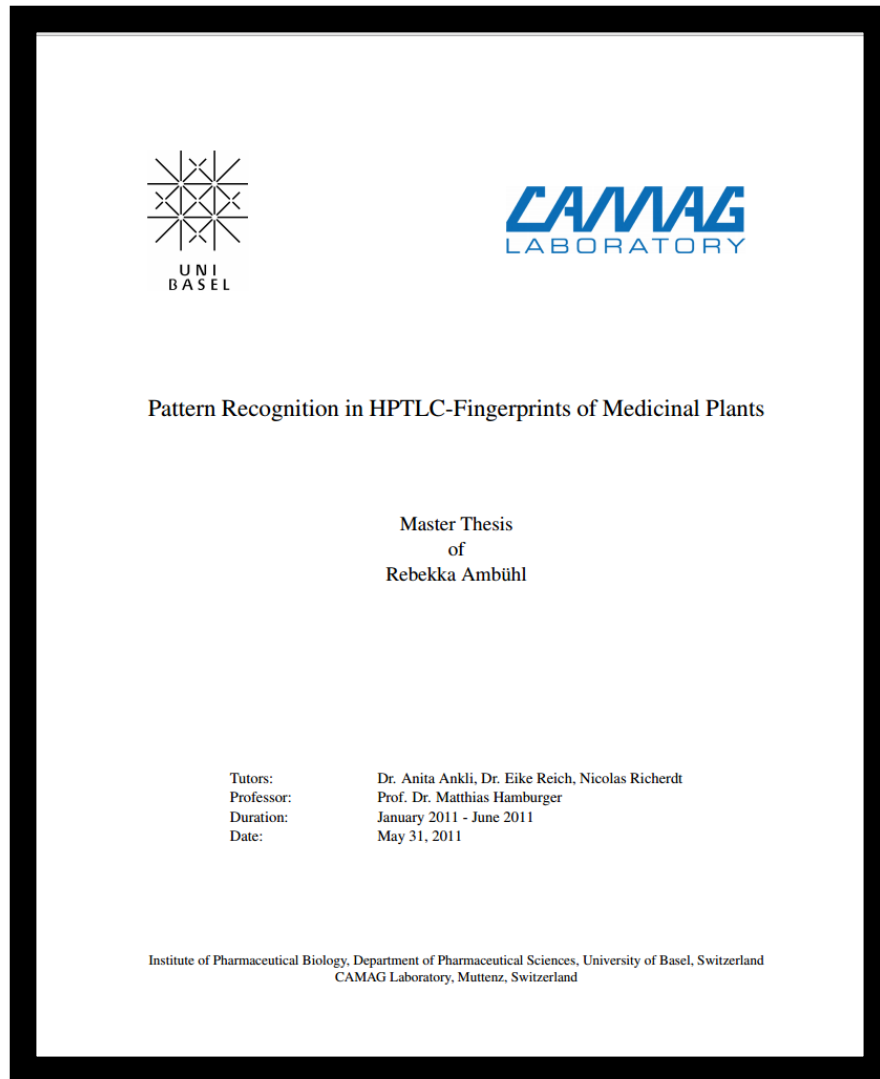# ChromCorr v 0.1: A toolbox for HPTLC data processing.

Grégory Genta-Jouve

International Symposium for High Performance Thin Layer Chromatography
Lyon, 2nd – 4th July 2014

Laboratoire de Pharmacognosie et de Chimie des Substances Naturelles
UMR CNRS 8638 COMETE – Université Paris Descartes
www.pharmacognosie-parisdescartes.fr

The beginning of the story…

Pattern Recognition in HPTLC-Fingerprints of Medicinal Plants

Master Thesis
of
Rebekka Ambühl

Tutors:	Dr. Anita Ankli, Dr. Eike Reich, Nicolas Richerdt
Professor:	Prof. Dr. Matthias Hamburger
Duration:	January 2011 - June 2011
Date:	May 31, 2011

Institute of Pharmaceutical Biology, Department of Pharmaceutical Sciences, University of Basel, Switzerland
CAMAG Laboratory, Muttenz, Switzerland

Conclusion:

« HPTLC fingerprints can be stored as images and provide a source to compare and identify substances»

« A limitation of this work was the missing possibility for an alignment of the retardant factor »

Let's do it then!

Metabolomics pipelines as an inspiration

Metabolomics is the scientific study of chemical processes involving metabolites.

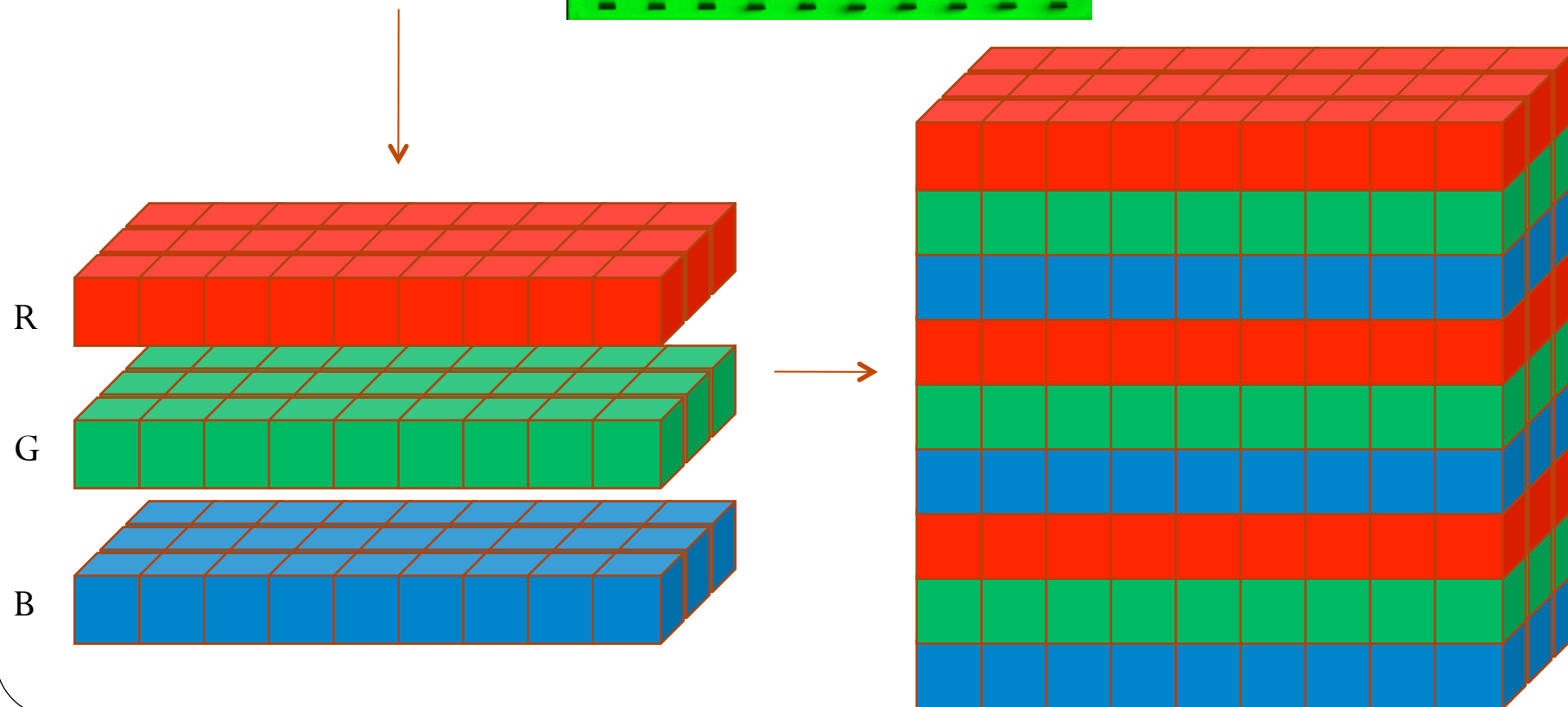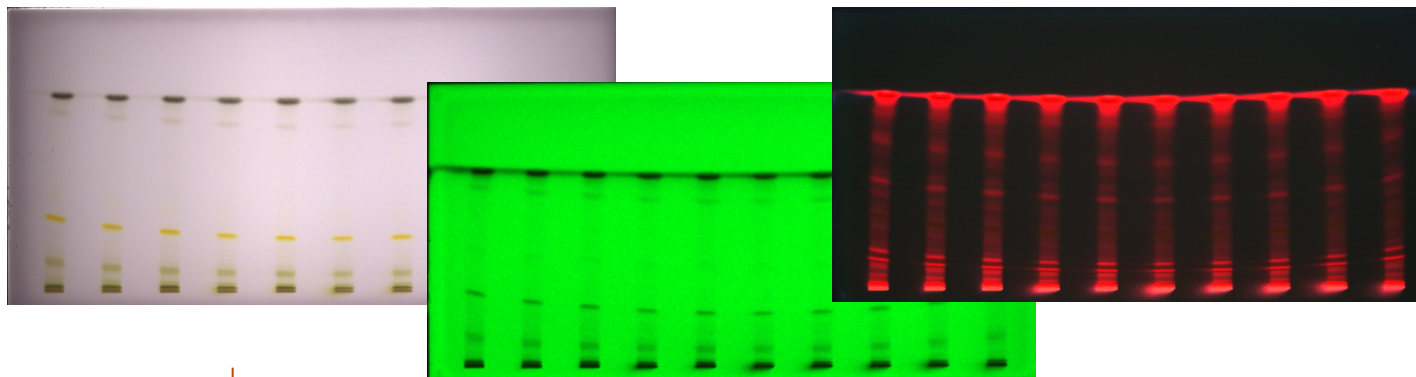Several techniques are usually used such as NMR and MS.
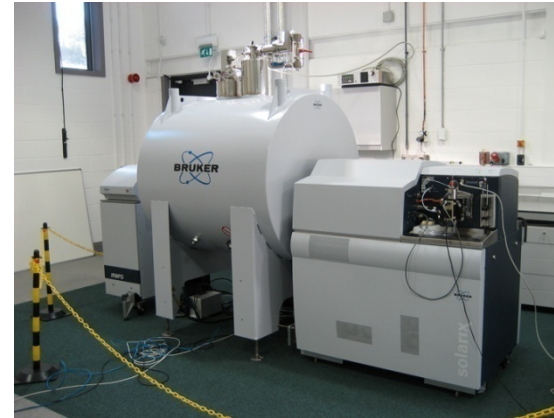
Brief description of the workflow:
- ❑ data acquisition
- ❑ data correction
- ❑ features detection
- ❑ spectral/chromatogram alignment
- ❑ features selection
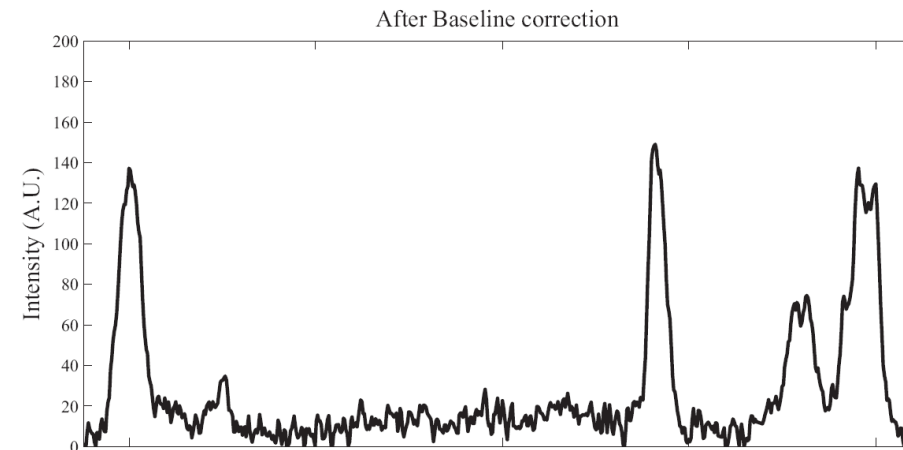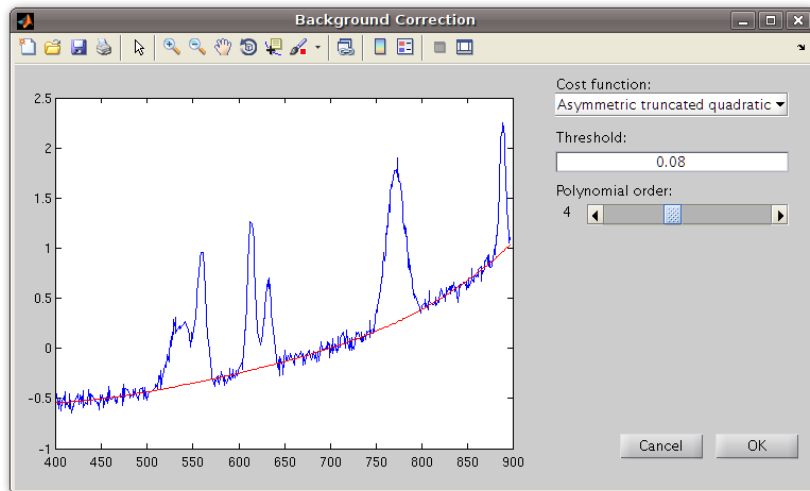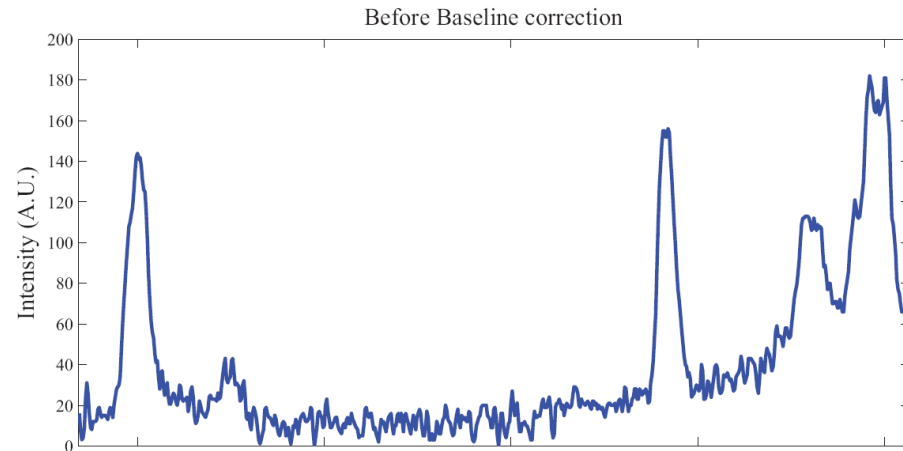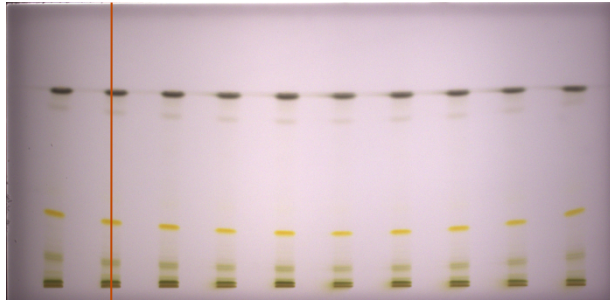- ❑ missing values imputation
- ❑ data normalisation
- ❑ statistical analyses
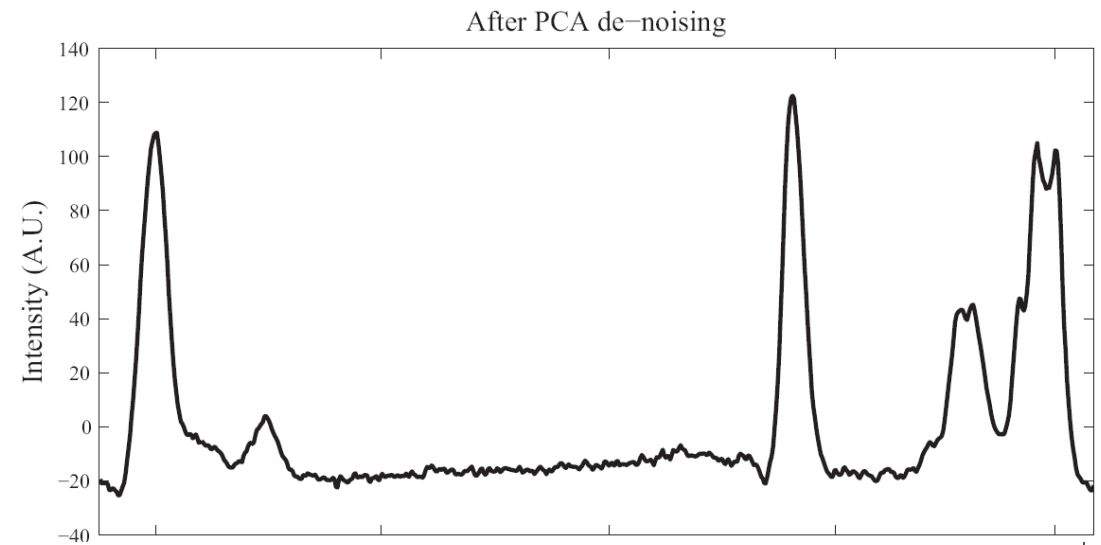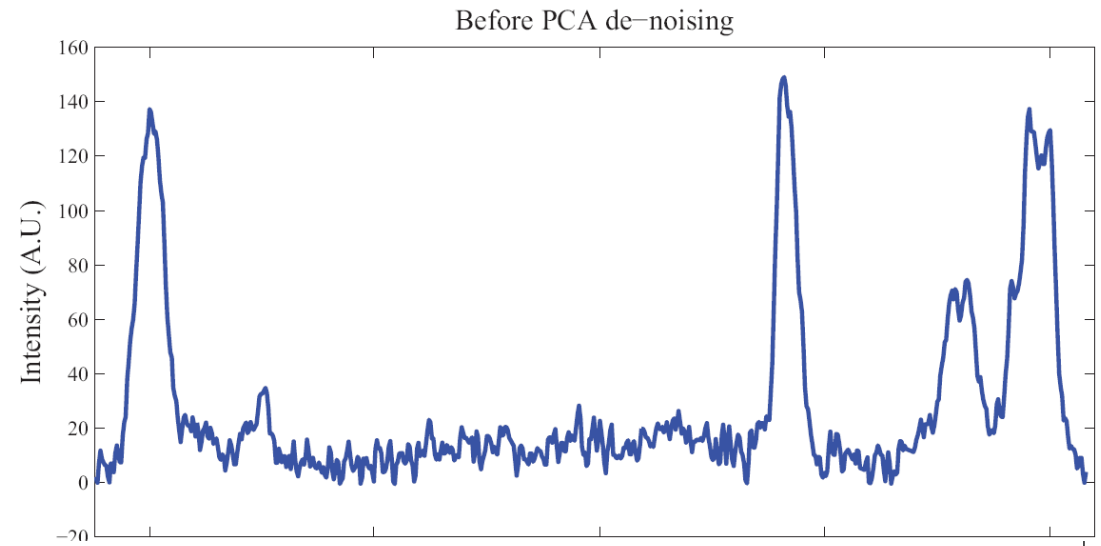
What can be done with HPTLC?
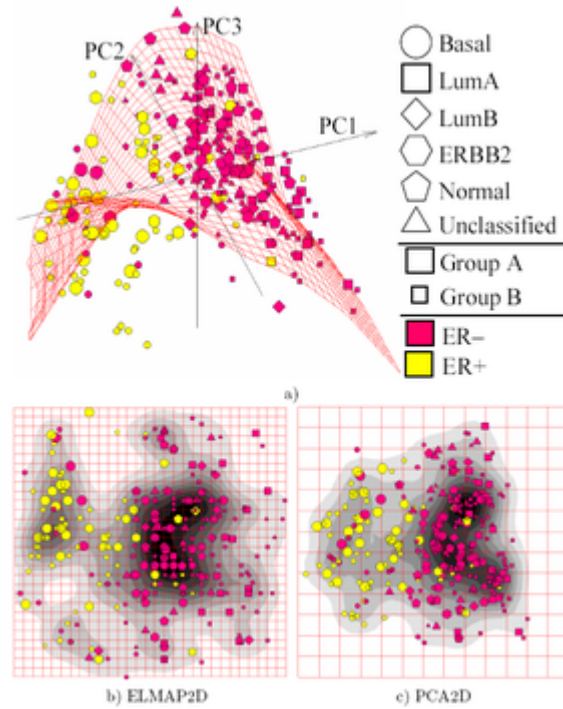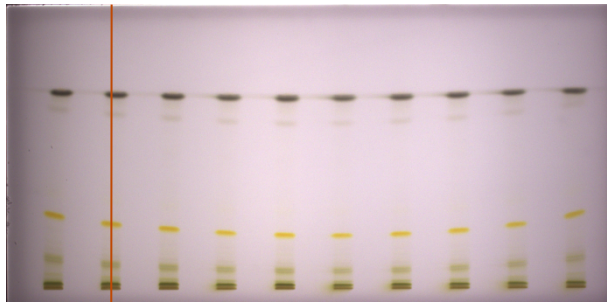
Data acquisition: simple images
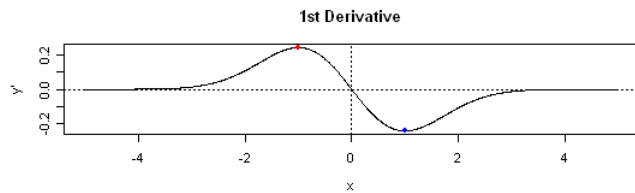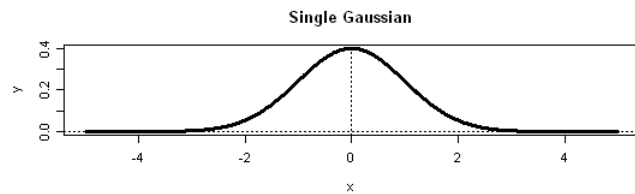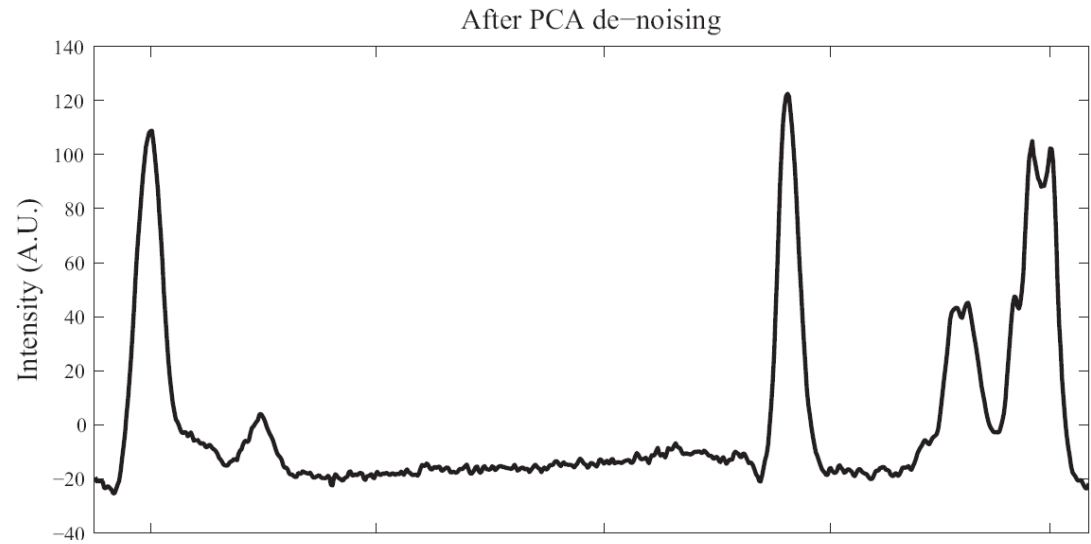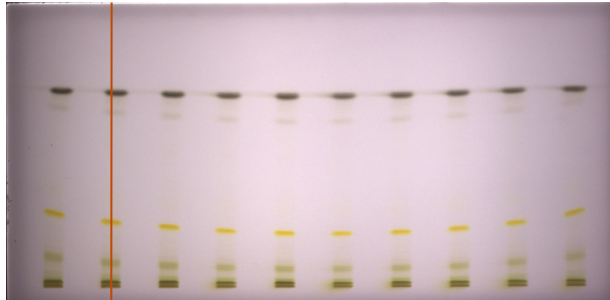
What can be done with HPTLC?

Data correction: baseline correction

Before Baseline correction

After Baseline correction

V. Mazet, C. Carteret, D. Brie, J. Idier, B. Humbert.*Chemometrics and Intelligent Laboratory Systems*, vol. 76, no. 2, p. 121-133, april 2005.

What can be done with HPTLC?

Data correction: de-noising

What can be done with HPTLC?

Peak detection

After PCA de−noising

Single Gaussian

1st Derivative

Rf	0	…	1
R(254 nm)	$I_{(1,1)}$	…	$I_{(1,n)}$
G(254 nm)	…	…	…
…	$I_{(m,1)}$	…	$I_{(m,n)}$

What can be done with HPTLC?

Chromatogram alignment

Before drift diffusion correction
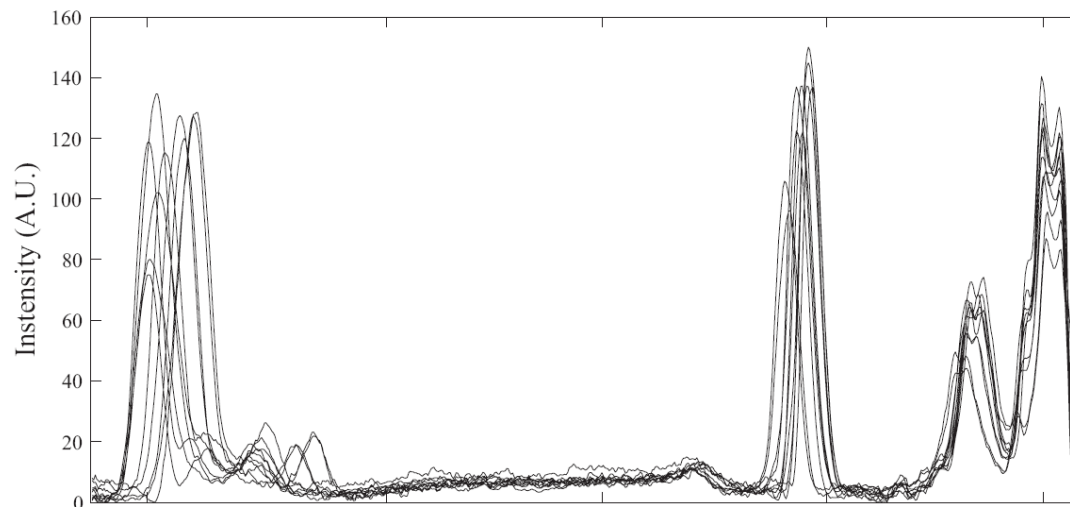
Visible

254 nm

Each peak has a 9 bits code for the identification

Correlation optimized warping is used to align chromatograms

366 nm

Raw BPC Data

COW Aligned BPC Data

What can be done with HPTLC?

Chromatogram alignment

Visible

254 nm

366 nm

The ChromCorr toolbox

Proof of the concept:
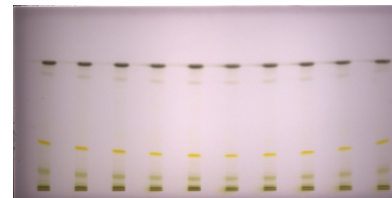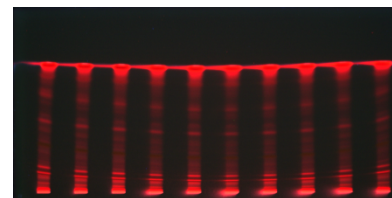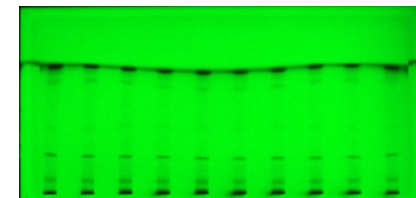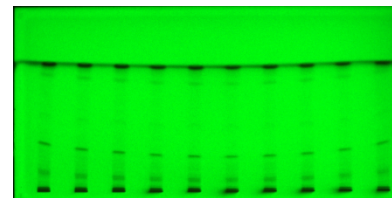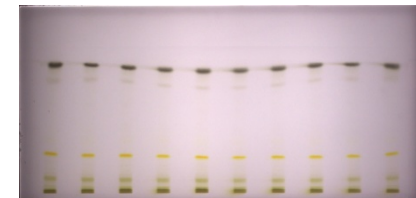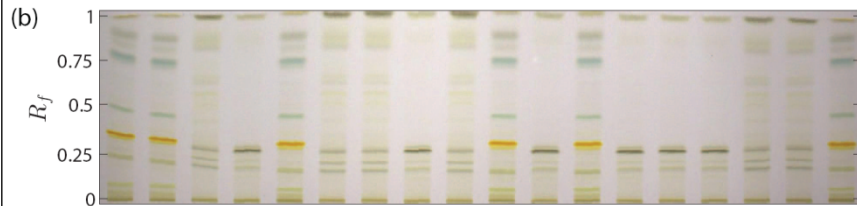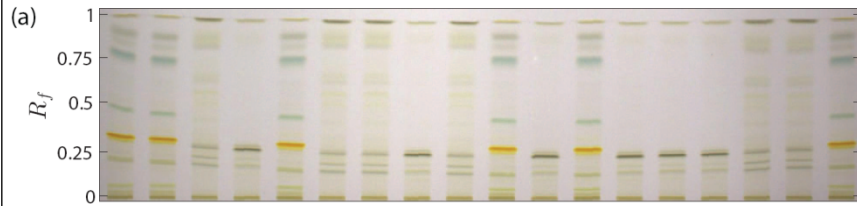 application of 10 times the same extract on the plate
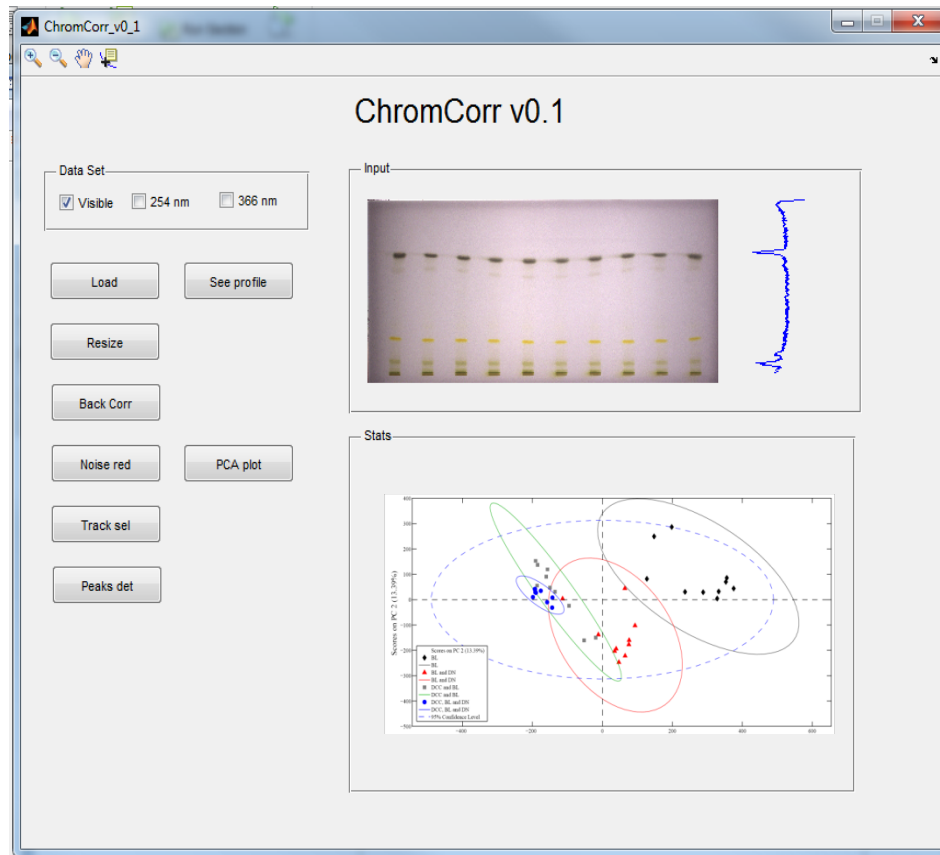
Before   After
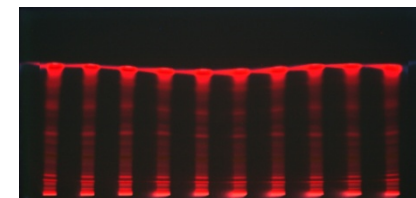
Major issue! There is no biological meaning.

The ChromCorr toolbox
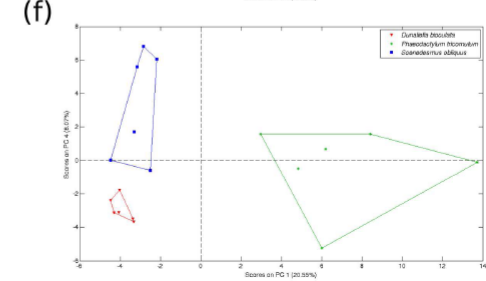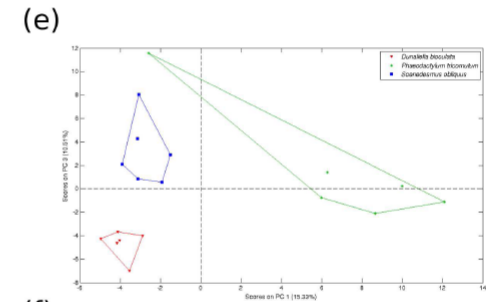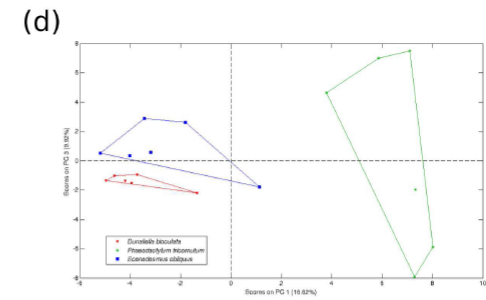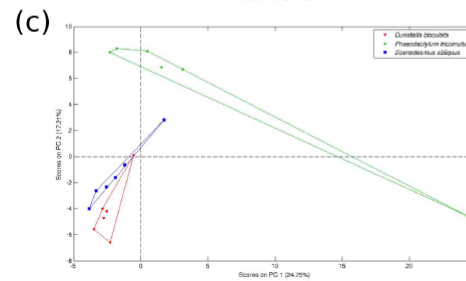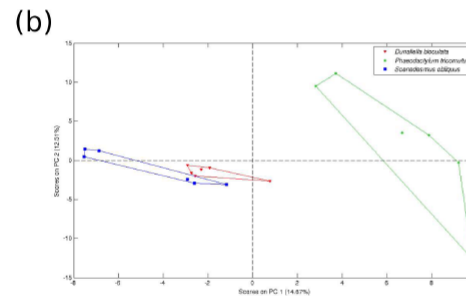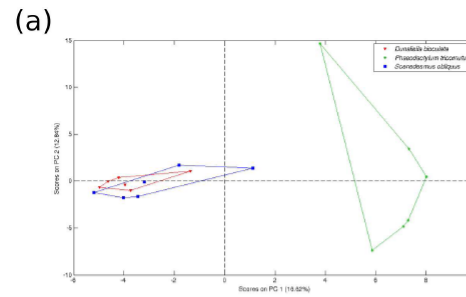
Another test:

application of 4 times 3 different micro algal extracts on the plate

Nice improvement of the
clustering

Conclusion

❑We demonstrated that HPTLC can be used to cluster natural extracts.
❑Implementation of new algorithms is possible.

❑One major drawback: ChromCorr is implemented in the Matlab environment. The development will be move to a free platform: Galaxy (web based environment).

❑To become more popular, HPTLC needs to have standards:
❑   -in processing data (data correction, etc…)
❑   -in reporting results (hptlcML files ?)

❑New developments in the field need to be supported by the HPTLC community.

Acknowledgments

Chanel Parfums Beauté

Coralie Audoin
Vincent Cocandeau
Lionel Weinberg
Serge Holderith
Nicola Fuzzati

Université Paris Descartes

Sylvie Michel

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Thank you for your kind attention!