ChromCorr v 0.1: A toolbox for HPTLC data processing.

Grégory Genta-Jouve

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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…

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

R
G
B
What can be done with HPTLC?

Data correction: baseline correction

What can be done with HPTLC?

Data correction: de-noising

Lei Zhang, Weisheng Dong, David Zhang, Guangming Shi Pattern Recognition, Volume 43, Issue 4, April 2010, Pages 1531-1549
What can be done with HPTLC?

Peak detection

After PCA de-noising

<table>
<thead>
<tr>
<th>Rf</th>
<th>0</th>
<th>...</th>
<th>1</th>
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<td>R(254 nm)</td>
<td>I_{(1,1)}</td>
<td>...</td>
<td>I_{(1,n)}</td>
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<tr>
<td>G(254 nm)</td>
<td>...</td>
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</tr>
<tr>
<td>...</td>
<td>I_{(m,1)}</td>
<td>...</td>
<td>I_{(m,n)}</td>
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</tbody>
</table>
What can be done with HPTLC?

Chromatogram alignment

Each peak has a 9 bits code for the identification

Correlation optimized warping is used to align chromatograms

What can be done with HPTLC?

Chromatogram

Visible 254 nm

366 nm

Giorgio Tomasi, Frans van den Berg and Claus Andersson
Journal of Chemometrics
What can be done with HPTLC?

Chromatogram alignment

Giorgio Tomasi, Frans van den Berg and Claus Andersson Journal of Chemometrics Volume 18, Issue 5, pages 231–241, 2004
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.
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