rTLC: Open source software for multivariate analysis of HPTLC data

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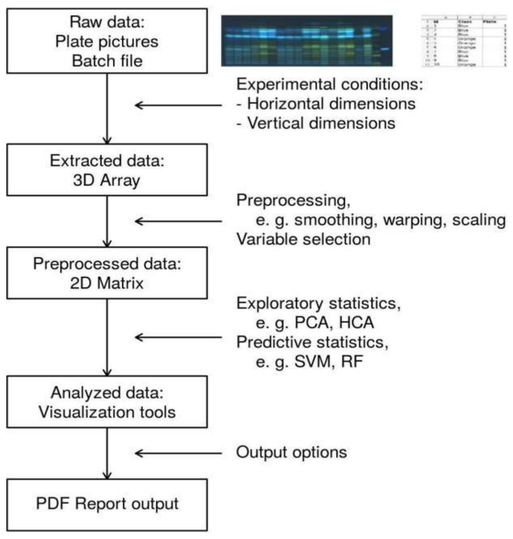

Fig. 1 Pipeline of rTLC [1]

Highlights

- *HPTLC is especially suited for multivariate data analysis (MVDA) [1].*
- *rTLC, an open-source software dedicated to TLC/HPTLC, was developed to streamline MVDA [2] (Fig. 1):*
  - *Written in R [3] with the shiny package [4] provided a web-based user interface (Figs. 2 and 3)*
  - *Visualization tools and a user-friendly interface substantially fastened the analysis (Figs. 4 and 5)*
  - *Preprocessing algorithms mitigated experimental variations (Fig. 6)*
  - *Both unsupervised (Figs. 7, 8 and 9) and supervised statistics (Tables 1 and 2) as supported tools.*
- *German propolis was used to demonstrate its capabilities.*
- *The software was released open-source to encourage reuse and improvement [5].*

Fast and intuitive data preparation

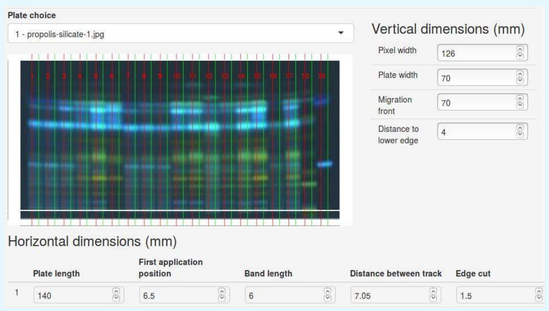

Fig. 2 Video densitogram extraction made automatic using parameters and dimensions of prior analysis

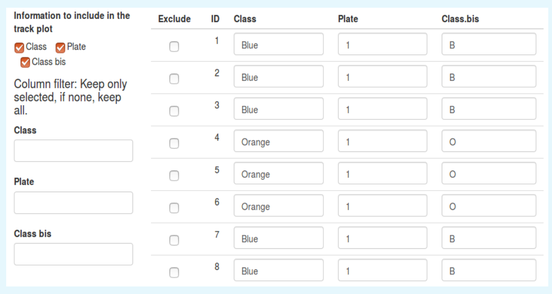

Fig. 3 Information on each sample can be added via an excel file and edited inside the software

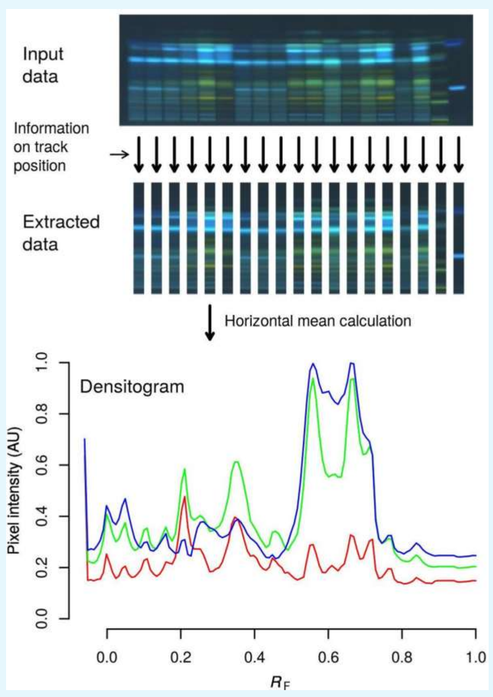

Fig. 4 Processing of experimental parameters for extraction of HPTLC chromatograms to obtain HPTLC densitograms

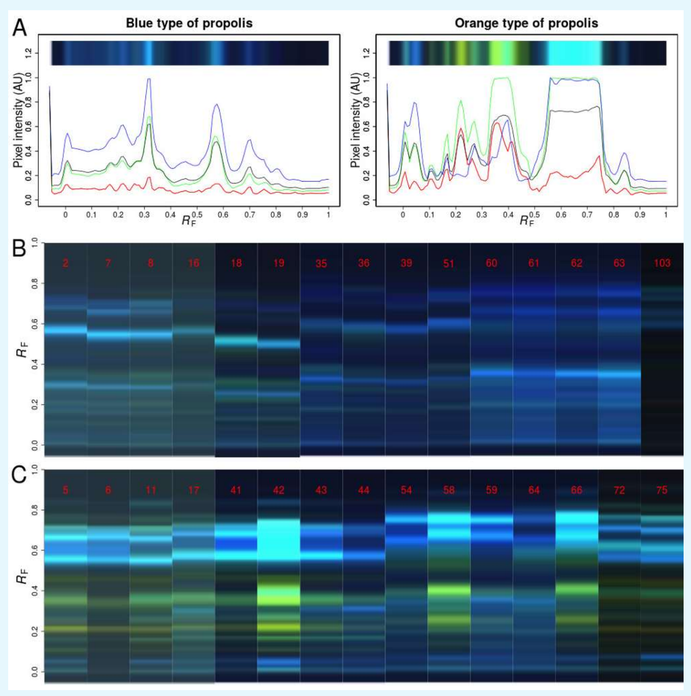

Fig. 5 RGB channel densitograms (A) and HPTLC chromatograms of the phenolic profiles of blue-type (B) and orange-type (C) German propolis samples

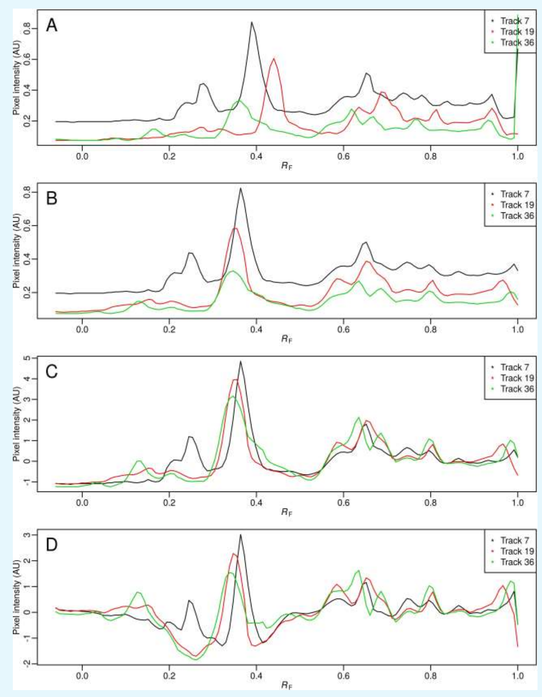

Fig. 6 Effect of preprocessing on the green channel densitograms of 3 blue propolis: Original data (A) realigned with parametric time warping (B), standard normal variate (C) and mean centering (D)

Powerful data analysis tools

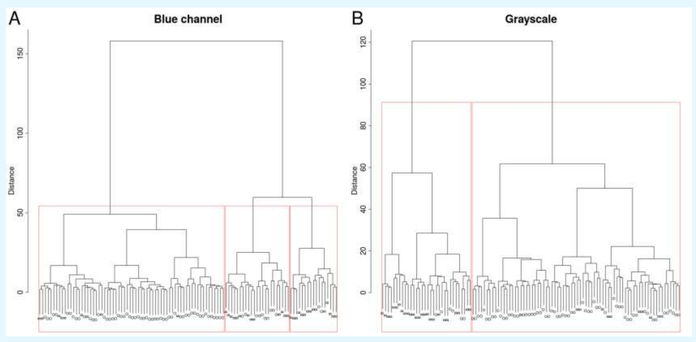

Fig. 7 Dendrograms for blue channel (A) and grayscale (B) image evaluation of German propolis samples

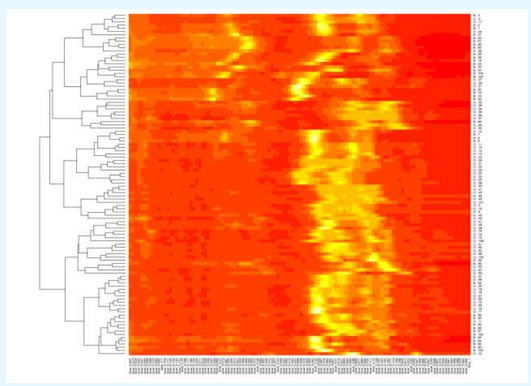

Fig. 8 Heat map analysis for the blue channel

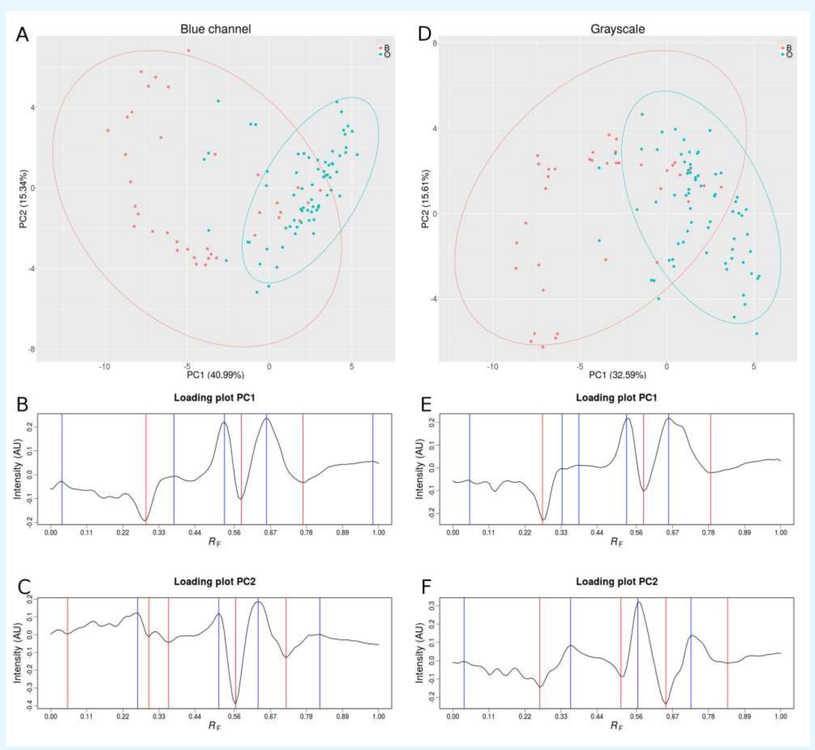

Fig. 9 PC scores (A and D) and loading plots according to the blue channel (B and C) and grayscale image (E and F) evaluation

		Cross validation set					
Channel	**Type**	**Blue-type**	**Orange-type**	**Accuracy**	**Blue-type**	**Orange-type**	**Accuracy**
Red	Blue	6	6	0.7143	19	6	0.7692
	Orange	2	14		12	41	
Green	Blue	8	4	0.8214	18	7	0.8077
	Orange	1	15		8	45	
Blue	Blue	9	3	0.8214	17	8	0.7564
	Orange	2	14		11	42	
Gray	Blue	8	4	0.8517	18	7	0.8590
	Orange	0	16		4	49	

Table 1 Supervised statistic results with support vector machine

		Cross validation set					
Channel	**Type**	**Blue-type**	**Orange-type**	**Accuracy**	**Blue-type**	**Orange-type**	**Accuracy**
Red	Blue	6	6	0.7857	14	11	0.8077
	Orange	0	16		4	49	
Green	Blue	9	3	0.8571	16	9	0.8590
	Orange	1	15		2	51	
Blue	Blue	9	3	0.8929	17	8	0.8333
	Orange	0	16		5	48	
Gray	Blue	9	3	0.8929	16	9	0.8590
	Orange	0	16		2	51	

Table 2 Supervised statistic results with random forest

References [1] G.E. Morlock, P. Ristivojević, E.S. Chernetsova, J. Chromatogr. A, 1328 (2014) 104–112. [2] D. Fichou, P. Ristivojevic, G. Morlock, Anal. Chem. 88 (2016) 12494-12501. [3] R Core Team, R - a language and environment for statistical computing, R Foundation for Statistical Computing, Vienna, Austria, 2016, www.R-project.org. [4] W. Chang, J. Cheng, J. Allaire, Y. Xie, J. McPherson, Shiny - web application framework for R, 2016, wwww.CRAN.R-project.org/package=shiny. [5] https://github.com/DimitriF.

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