RealCOW, a warping approach for the systematic determination of markers in GC-MS data

Saïd Abou El Karam, Jérémy Ratel, Nathalie Kondjoyan, Erwan Engel

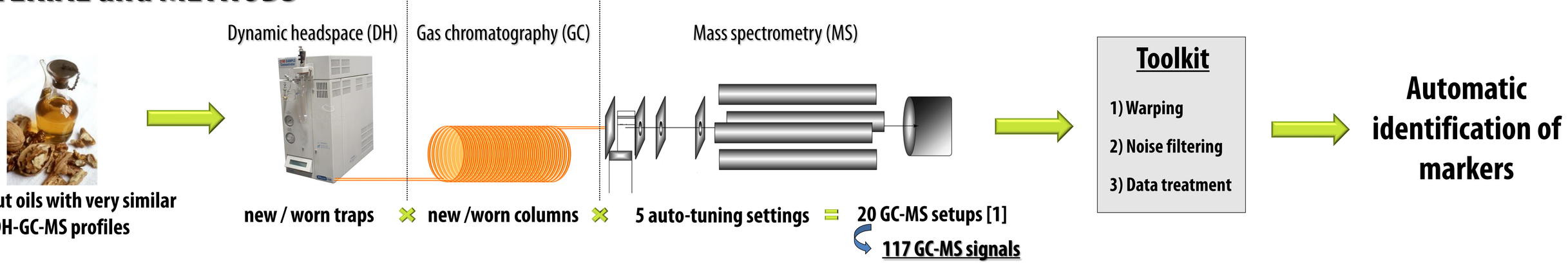
REALCOW, A WARPING APPROACH FOR A SYSTEMATIC DETERMINATION OF MARKERS IN GC-MS DATA

S. ABOU EL KARAM, J. RATEL, N. KONDJOYAN, E. ENGEL*

INRA, UR370 QuaPA, MASS Group, F-63122 Saint-Genès-Champanelle, France. *e-mail : erwan.engel@clermont.inra.fr

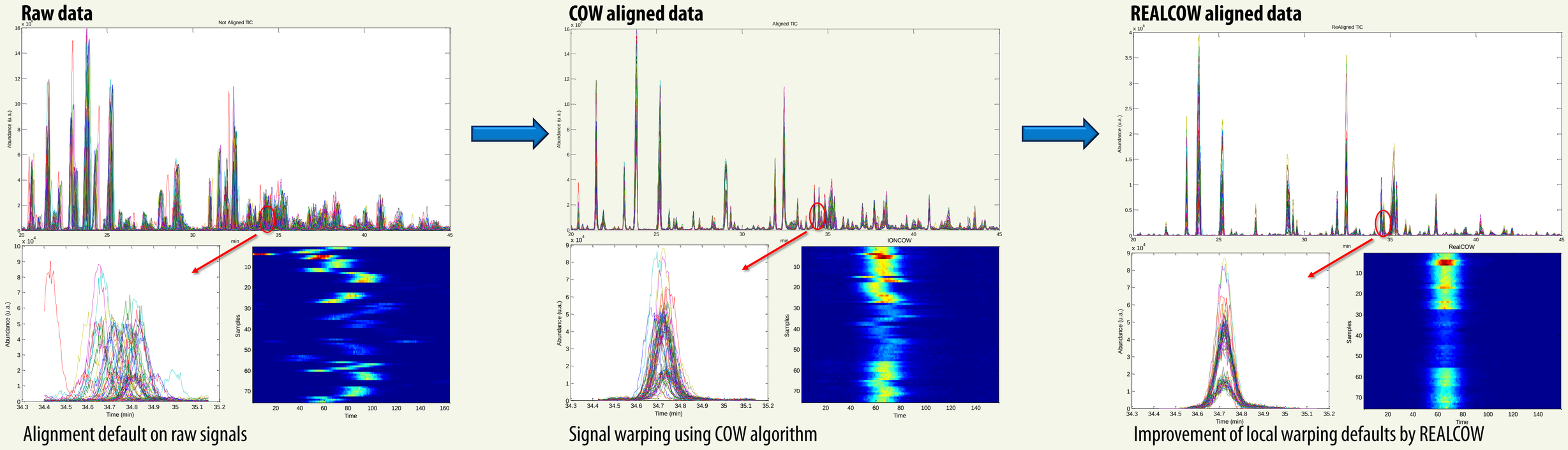
CONTEXT and OBJECTIVES The development of automated tools for systematic research of markers in the gas chromatography-mass spectrometry signals requires breaking down the barriers posed by the signal treatment and more particularly by the alignment. The present study proposes a toolkit including a novel alignment approach based on the COW method [3] which was upgraded for correcting unresolved local distortions. The determination of the discriminative markers from the realigned signals was based on an original data normalisation method [1] combined with a recent deconvolution software [2]. In order to assess the performance of our developed systematic strategy (REALCOW), the toolkit was applied to a data set giving the composition in volatile compounds of vegetable oils. Each oil was analysed with 20 different analytical setups of the same GC-MS system in order to mimic instrumental drifts and to make difficult the identification of volatile markers of oil samples.

MATERIAL and METHODS



RESULTS

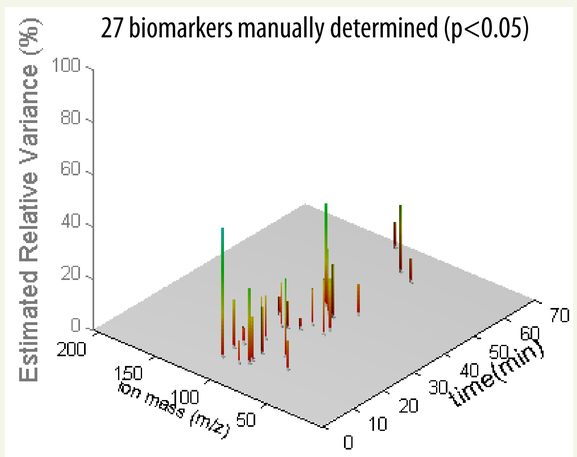
Warping of GC-MS signals



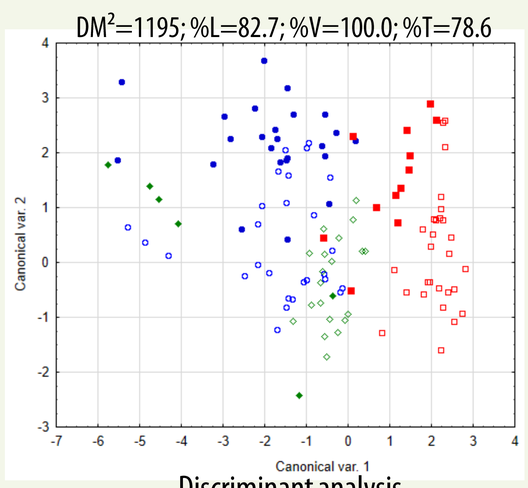
Alignment default on raw signals — Signal warping using COW algorithm — Improvement of local warping defaults by REALCOW

Determination of biomarkers

Expert method (manual approach)

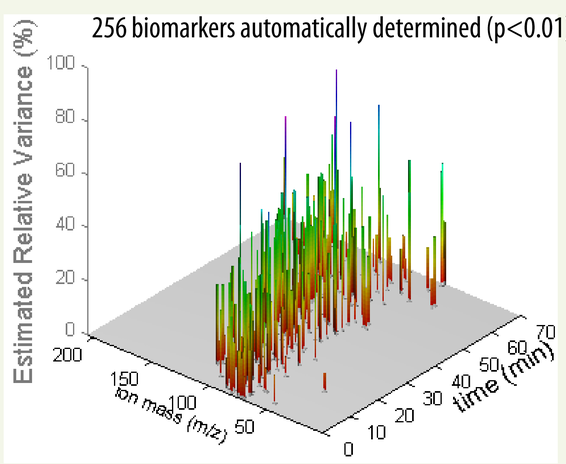


Anovagram

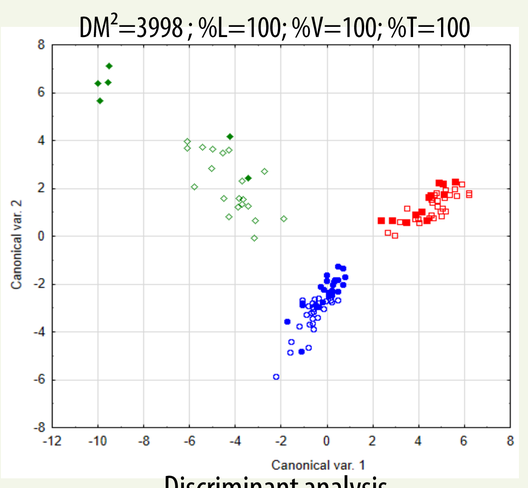


Discriminant analysis (3 best variables among 27)

Systematic method using REALCOW (automatic approach)



Anovagram



Discriminant analysis (3 best variables among 256)

CONCLUSIONS The markers identified by expert were also found by the developed systematic method which in turn offered much more markers with higher discriminative power. The performance of the REALCOW method was demonstrated on a data set affected by important instrumental drifts. Further investigation on other data sets is now needed to assess the robustness of the REALCOW method.

REFERENCES [1] Deport, C., Ratel, J., Berdague, J.L., Engel, E. (2006). Comprehensive combinatory standard correction: A calibration method for handling instrumental drifts of gas chromatography-mass spectrometry systems. *Journal of Chromatography A, 1116*, 248-258.
[2] Mass Spectra Separation Software (MS3), IDDN.FR.001.270012.000.R.P.2010.000.10800. INRA, UR QuaPA, F-63122 Saint Genès Champanelle, France.
[3] Tomasi, G., van den Berg, F., Andersson, C. (2004). Correlation optimized warping and dynamic time warping as preprocessing methods for chromatographic data. Journal of Chemometrics, 18, 231-241.

38th International Symposium on Capillary Chromatography (ISCC), 2014, Riva del Garda, Italy.

Centre de Clermont-Theix-Lyon
63122 Saint Genès Champanelle – France,
www.clermont.inra.fr