

Accepted Manuscript

Title: An approach to evaluate the information in chromatographic fingerprints: Application to the optimisation of the extraction and conservation conditions of medicinal herbs

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PII: S0021-9673(15)01464-8
DOI: <http://dx.doi.org/doi:10.1016/j.chroma.2015.10.020>
Reference: CHROMA 356935

To appear in: *Journal of Chromatography A*

Received date: 8-8-2015
Revised date: 7-10-2015
Accepted date: 8-10-2015

Please cite this article as: T. Alvarez-Segura, E. Cabo-Calvet, J.R. Torres-Lapasió, M.C. García-Álvarez-Coque, An approach to evaluate the information in chromatographic fingerprints: application to the optimisation of the extraction and conservation conditions of medicinal herbs, *Journal of Chromatography A* (2015), <http://dx.doi.org/10.1016/j.chroma.2015.10.020>

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1 **Highlights**

2 The article contains:

3 Unsupervised approach to evaluate the information content in fingerprints.

4 The peaks in the fingerprints were ranked based on the peak prominences.

5 The information content was established as the number of peaks that exceeds a threshold.

6 The extraction conditions were studied assisted by Plackett-Burman designs.

7 Solvent nature and concentration, ultrasonication time and temperature were studied.

8

9 **An approach to evaluate the information in chromatographic fingerprints: application** 10 **to the optimisation of the extraction and conservation conditions of medicinal herbs**

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14

15 **Abstract**

16 A new approach is reported for high-performance liquid chromatography to measure the
17 level of information in fingerprints. For this purpose, the concept of peak prominence, which
18 is the protruding part of each visible peak with regard to the valleys that delimit it, was used.
19 The peaks in the fingerprints are ranked according to the areas of the peak prominences, and
20 a threshold is established to discriminate between the significant peaks and those that are
21 irreproducible. The approach was applied to evaluate the impact of several extraction
22 conditions (solvent nature and composition, time and temperature of the treatment, amount of
23 sample, and time and temperature of conservation of the extracts) on the number of
24 significant peaks found in the fingerprints of a medicinal herb (a green tea sample), using
25 Plackett-Burman designs. Acetonitrile, ethanol and methanol were used for the extraction,

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