



# Ion mobility spectroscopy and chemometrics for the analysis and discrimination of tomato sauce

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## AIMS AND METHODOLOGIES

In the present work, the volatile fraction of tomato sauce samples was analyzed by Gas-Chromatography (GC) coupled to a detector based on Ion-Mobility Spectroscopy (IMS). In the IMS system, the volatile molecules after the chromatographic run are ionized and pushed in an electric field inside a drift tube. Moreover, a gas (N<sub>2</sub>) flows in the drift tube in the opposite direction, bumping the volatile molecules. The combination of electric field and drift-gas aims at further separating the analytes.

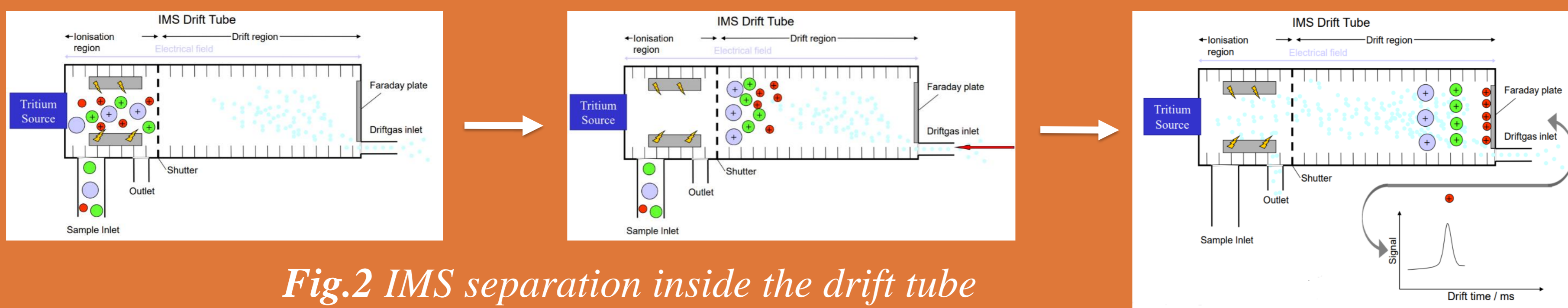


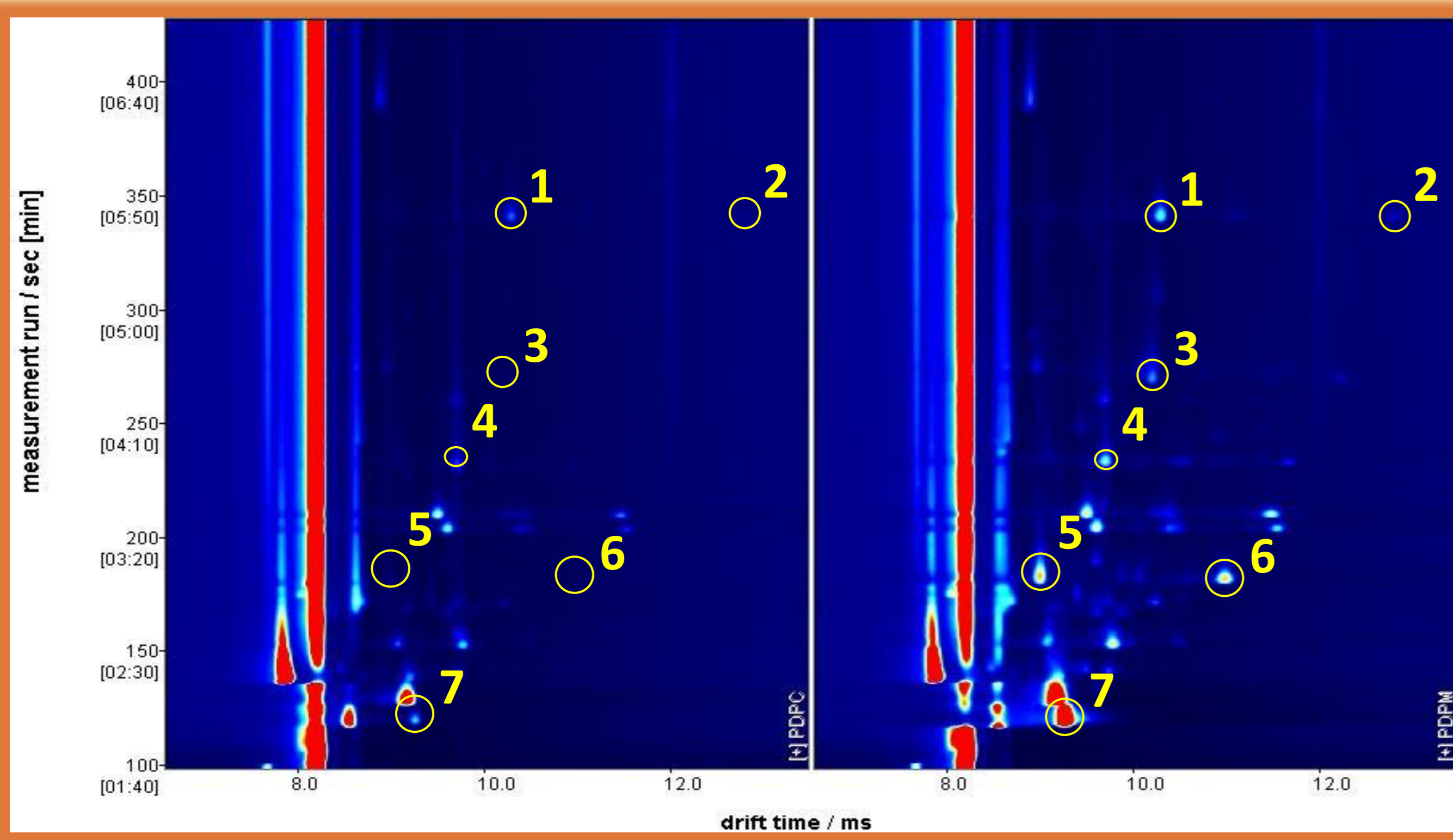
Fig.2 IMS separation inside the drift tube



Fig.1 GC-IMS system FlavourSpec® (GAS Dortmund)

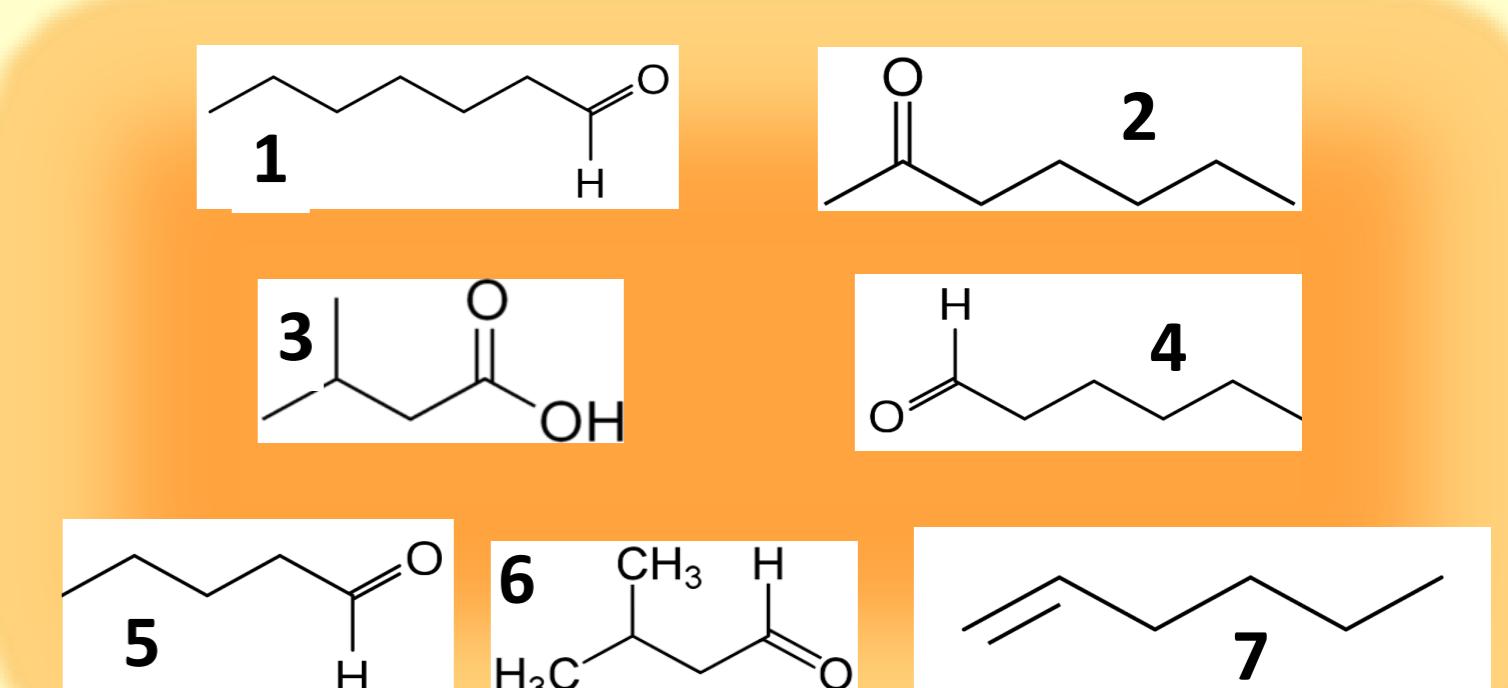
Sixteen commercial tomato sauce samples were analyzed by GC-IMS. These pertain to 6 commercial brands and 7 producers (named A to G). Two replicates were carried out for each sample. The aim of the work was to discriminate the tomato sauce samples based on brands and producers.

GC-IMS output is a 2D graph, in which the vertical and the horizontal axes represent the GC and the IMS separations.

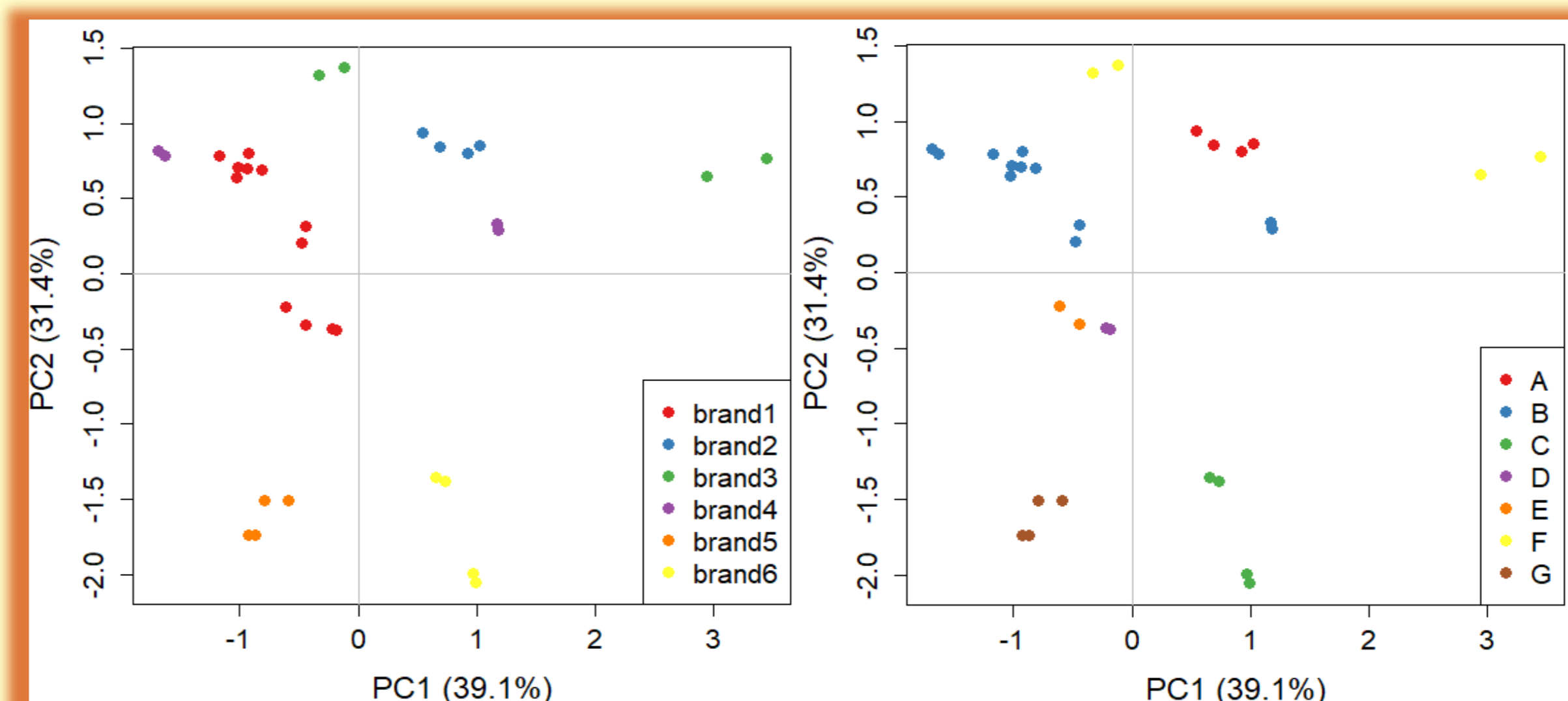


From PCA, it is possible to evaluate the GC-IMS areas that most influence the discrimination. GC-IMS database, then, allows a tentative attribution to specific molecules.

Peak	Attribution	Flavor
1	Heptanal	Fat, citrus, rancid
2	Heptan-2-one	Fruity, spicy
3	Isovaleric acid	--
4	Hexanal	Grass, tallow, fat
5	Pentanal	Green, grass
6	Methyl-butanal	Cocoa, almond, malt
7	1-hexene	--



GC-IMS 2D plots (the third dimension, represented by colors, is the peak intensities) are converted into 1D vectors for PCA. PCA grouping shows a good discrimination between brands and producers (except for brands 3 and 4).



## RESULTS AND CONCLUSIONS

GC-IMS analysis proved to be a valid method for the discrimination of tomato sauce samples, based on the commercial brand and the producers. The 2D analytes separation allowed also to evaluate possible molecules of the volatile fraction that can be mostly useful for such discrimination.

## BIBLIOGRAPHY

Zappi A., Marassi V., Kassouf N., Giordani S., Pasqualucci G., Garbini D., Roda B., Zattoni A., Reschiglian P., Melucci D. (2022) A Green Analytical Method Combined with Chemometrics for Traceability of Tomato Sauce Based on Colloidal and Volatile Fingerprinting. *Molecules*, 27, 5507. <https://doi.org/10.3390/molecules27175507>