

Aberystwyth University

An Analytical Pipeline for Quantitative Characterization of Dietary Intake

Garcia-Perez, Isabel; Posma, Joram M; Chambers, Edward S.; Nicholson, Jeremy K.; Mathers, John C.; Beckmann, Manfred; Draper, John; Holmes, Elaine; Frost, Gary

Published in:

Journal of Agricultural and Food Chemistry

DOI:

[10.1021/acs.jafc.5b05878](https://doi.org/10.1021/acs.jafc.5b05878)

Publication date:

2016

Citation for published version (APA):

Garcia-Perez, I., Posma, J. M., Chambers, E. S., Nicholson, J. K., Mathers, J. C., Beckmann, M., Draper, J., Holmes, E., & Frost, G. (2016). An Analytical Pipeline for Quantitative Characterization of Dietary Intake: Application To Assess Grape Intake. *Journal of Agricultural and Food Chemistry*, 64(11), 2423-2431.

<https://doi.org/10.1021/acs.jafc.5b05878>

General rights

Copyright and moral rights for the publications made accessible in the Aberystwyth Research Portal (the Institutional Repository) are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

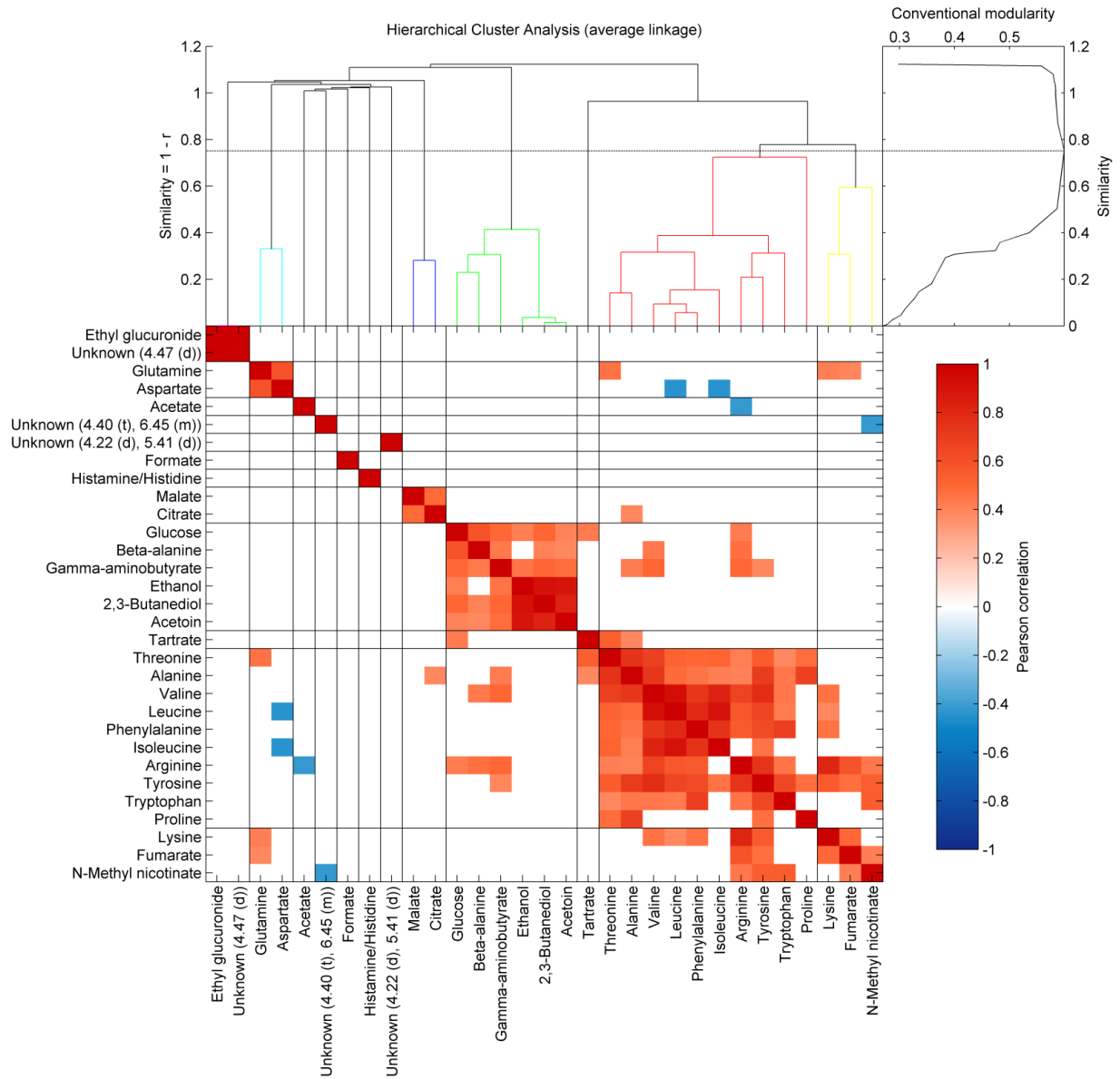
- Users may download and print one copy of any publication from the Aberystwyth Research Portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the Aberystwyth Research Portal

Take down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

tel: +44 1970 62 2400
email: is@aber.ac.uk

Supplementary Figure 1: Correlation of 31 identified compounds in ¹H-NMR global profiles of red and green grapes visualized in a heat map with hierarchical clustering applied.



Supplementary Table 1: Mean values of quantified tartaric acid in different varieties of red and green grapes from different countries.

red grape variety	mean tartaric acid (mMol)	SD
Sharad (India)	0.88	0.03
Red Globe (Peru)	0.59	0.09
Ralli (Chile)	0.81	0.04
Pink Muscat (Chile)	0.81	0.04
Flame (Chile) (1)	0.93	0.05
Flame (Chile) (2)	0.85	0.05
Crimson (Chile)	1.11	0.09
Black Princess (Chile)	0.98	0.00
Jack's Salute (South Africa)	0.71	0.08
Magenta (South Africa)	0.79	0.03
Crimson (South Africa)	0.81	0.04
total	0.84	0.03
green grape variety	mean tartaric acid (mMol)	SD
Thompson (India) (1)	1.11	0.14
Thompson (India) (2)	0.71	0.04
Thompson (Namibia)	0.82	0.04
Thompson (Chile)	0.76	0.03
Sugraone (Chile)	0.91	0.09
Thompson (South Africa)	0.80	0.11
total	0.85	0.08