Wine fingerprinting of wine characteristic compounds profiles combined with multivariate analysis for wine authentication approaches

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The aim of this study was to fingerprint and identify the characteristic compounds of different red and white wines in order to discriminate wines according to grape variety and vintage.

Introduction

Authentication of high quality wines in order to protect the prestigious brands, represent a current challenge in research. Wines authentication in terms of geographical and varietal origins, vintage year, identifying fraud and determining the specifications of the product with the label are requirements of consumers and the European Community. Development and harmonization of validated analytical methods at national and European level represent international priorities.

Experimental

SD DV Murfatlar during 2009-2017

White wines:
- Muscat Ottonel
- Sauvignon Blanc
- Feteasca Regala
- Riesling Italian
- Pinot Gris
- Chardonnay
- Columbu

Red wines:
- Cabernet Sauvignon
- Pinot Noir
- Merlot
- Feteasca Neagra

UHPLC-MS fingerprinting of wine characteristic compounds profiles combined with multivariate analysis for wine authentication approaches

Results and discussions

Red wines: Principal Component Analysis discriminating different varieties

Identification of phenolic compounds in wines: positive ionization

<table>
<thead>
<tr>
<th>Nr. crt.</th>
<th>Compounds</th>
<th>Retention time (min)</th>
<th>Molecular ion [M]+</th>
<th>Fragments (m/z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Vanillic acid</td>
<td>3.30</td>
<td>169.0495</td>
<td>111.0444, 125.0598</td>
</tr>
<tr>
<td>2.</td>
<td>Caffeic acid</td>
<td>3.42</td>
<td>181.0495</td>
<td>163.0380</td>
</tr>
<tr>
<td>3.</td>
<td>Syringic acid</td>
<td>3.38</td>
<td>199.0601</td>
<td>140.0671, 155.0702</td>
</tr>
<tr>
<td>4.</td>
<td>Gallic acid</td>
<td>6.25</td>
<td>171.0288</td>
<td>116.9963, 130.9818</td>
</tr>
<tr>
<td>5.</td>
<td>p-coumaric acid</td>
<td>6.36</td>
<td>165.0546</td>
<td>147.0450</td>
</tr>
<tr>
<td>6.</td>
<td>Ferulic acid</td>
<td>7.70</td>
<td>195.0652</td>
<td>177.0544, 145.0284</td>
</tr>
<tr>
<td>7.</td>
<td>Chlorogenic acid</td>
<td>2.43</td>
<td>355.1023</td>
<td>163.0389</td>
</tr>
<tr>
<td>8.</td>
<td>p-hydroxybenzoic</td>
<td>4.10</td>
<td>139.0389</td>
<td>131.6150, 73.3923</td>
</tr>
<tr>
<td>9.</td>
<td>Catechin</td>
<td>6.17</td>
<td>289.0720</td>
<td>139.0389, 123.0441, 163.0389</td>
</tr>
<tr>
<td>10.</td>
<td>Epicatechin</td>
<td>6.54</td>
<td>289.0720</td>
<td>163.0389</td>
</tr>
</tbody>
</table>

PCA analysis based on quantitative UHPLC-MS / MS data (phenolic compounds) for: (A) white wines and (B) red wines

Conclusions

UHPLC-MS fingerprinting coupled with MVA provided sufficient discrimination power to discriminate three grape varieties of red wine (Feteasca Neagra, Cabernet Sauvignon, Merlot) and white wine (Chardonnay, Columbu, Muscat Ottonel, Riesling Italian, Sauvignon Blank), using positive ionization data.

UHPLC-MS fingerprinting coupled with MVA have a considerable potential for the discrimination of year of vintage for white and red wines, depending on wine variety. Old wines (2009, 2010 and 2011 years) can be differentiated from the others.

Additional qualitative software packages combined with online databases based on food are needed for rapid wine authentication and identification of specific compounds responsible for wine discrimination. Future studies will be performed using Compound Discoverer software for spectral data processing.

Acknowledgments

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