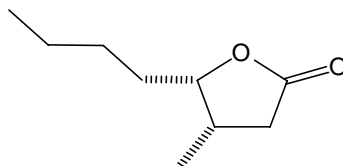


SCREENING OF OAK LACTONE PRECURSORS USING LC-MS/MS COMBINED WITH INFORMATION DEPENDENT ACQUISITION (IDA)

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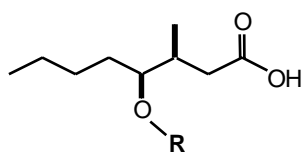
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The separation and identification of new flavour compounds in wine and spirits has been greatly aided by the ever-increasing sophistication of MS techniques. GC-MS has facilitated the identification of some 200 oak-derived volatile compounds in wine and spirits fermented and/or matured in oak barrels. Of these, the most important volatile compound is considered to be the (4S,5S) *cis*-isomer of 5-butyl-4-methyl-4,5-dihydro-2(3H)-furanone, more commonly known as '*cis*-oak lactone' or 'whisky lactone'. The aroma of *cis*-oak lactone in wine can be described as 'coconut' and 'vanilla'.



cis-oak lactone

Previous studies have showed increases in the concentration of extractable *cis*-oak lactone resulting from oak seasoning, drying and/or barrel heating. This suggested the presence of precursor forms in untreated oak samples. Several possible candidates for such precursors have been suggested and synthesized in our laboratory.



R: β -D-glucopyranoside, galloyl β -D-glucopyranoside and/or gallate

Proposed structures of oak lactone precursors

These candidates were then characterized using tandem mass spectrometry in negative and positive mode. The common characteristic fragmentation of the precursors was investigated so that it could be used for the screening of natural oak lactone precursors.

The screening of the potential natural precursors in oak extracts was carried out using LC-MS/MS combined with the Information Dependent Acquisition (IDA) technique. Precursor or neutral loss scan was used to generate a peak list of all ions present. The peak list was subjected to a set of user-defined criteria to filter out unwanted ions. The remaining ions, which are possibly derived from the oak lactone precursors, were then submitted for MS/MS. As a result, the potential oak lactone precursors, including the proposed compounds, were found in all oak extracts from French and American origins. The details of this study will be presented.