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A novel comprehensive analysis approach based on liquid chromatography-mass spectrometry for lipid oxidation of rapeseed oil

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Background:

Lipid oxidation of rapeseed oil can lead to the deterioration of nutrition and cause huge economic losses. The chlorophyll content in rapeseed oil greatly accelerates photooxidation and has become a core quality parameter of rapeseed oil.

Objective:

To reveal and understand the oxidation mechanism of rapeseed oil on the molecular level, is very important for improving the quality and nutritional value of rapeseed oil by solving the technical bottleneck of antioxidant of rapeseed oil.

Methods:

Qualitative and quantitative analysis and structural identification of the oxidation products formed during lipid oxidation of rapeseed oil by different pathways, such as autoxidation and photooxidation, were carried out by the established comprehensive analytical method with high coverage, high throughput, high sensitivity, and high specificity for oil oxidation products, based on high resolution mass spectrometer combined with chiral derivatization approaches to label the hydroxyl group, carbonyl group, and carboxyl group containing oxidation products. The oxidative reaction mechanism and kinetics of rapeseed oil was revealed by identification of oxidation quality markers of rapeseed oil using the chemometrics approach.

Results:

1. In this research, the novel methods were established by combining chemical derivatization (CD)-based retention index (RI) algorithm and mass spectrometric fragmentation annotation (CD-RI-LC-MS/MS) for identification and quantification of oxidation products of rapeseed oil. After derivatization, the detection sensitivities could be improved significantly compared with underived compounds at most 5112 folds. The RIs algorithm was established to compensate for retention time variances and assist the structural elucidation of oxidation products from LC retention level during LC-MS analysis with excellent reproducibility and accuracy (RSD < 1%).
2. By using methods motioned above, more oxidation products could be detected, including hydroperoxide, epoxidized, and hydroxylated compounds when chlorophyll was added in rapeseed oil and exposed to light radiation (10000 lux, 4°C).
3. Quality markers of pathways and stage of rapeseed oil oxidation were identified through data analysis by using the chemometrics approach.
4. Reaction kinetics of lipid photooxidation of rapeseed oil has been deduced. Lipid oxidation rate of rapeseed oil is accelerated significantly.

Conclusions:

The more precise and detailed molecular information of lipid oxidation of rapeseed oil related distinct pathways and stages could be provided by the novel approaches established by this research work, compared with conventional methods to assess lipid oxidation that measure primary and secondary oxidation products such as peroxide value, iodine values, diene conjugate and malondialdehyde. Oxidation mechanism of rapeseed oil, especially photooxidation induced by chlorophyll, was studied based on the molecular information of lipid oxidation of rapeseed oil, such as hydroxyl group, carbonyl group, and carboxyl group containing oxidation products. This research work could provide methodology, molecular structure database, and crucial theoretical support for studying the molecular mechanism of rapeseed oil oxidation deterioration during its processing and storage.

References:

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