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Isolation and identification of vitamin D_3 oxidation products in simulated whole milk powder by liquid chromatography mass spectrometry

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In a successful fortification program, the stability of micronutrients added to the food is one of the most important factors. The added vitamin D_3 is known to sometimes decline during storage of fortified milk powders, and oxidation through fatty acid lipoxidatoin is suspected as the likely cause. The main objective of this study is to find a method to extract and to identify vitamin D_3 oxidation products (VDOPs) in stored whole milk powder. Identification of VDOPs in natural foods is a challenge due to the low amount of their contents. An extraction method using a liquid-liquid extraction (LLE) followed by a solid phase extraction (SPE) was optimized to extract VDOPs. The bottleneck of the VDOPs' identification could not be overcome without mass spectra prediction tools. The fragmentation trees and MS^n spectral trees provided by Mass Frontier software gave reliable methods to identify vitamin D_3 unknown compounds such as VDOPs. Methods based on high mass accuracy MS^2 and MS^n analysis have been developed for the identification of vitamin D_3 and its oxidation products. The multi stage mass spectrometry (MS^n) spectra can help to propose plausible schemes for unknown compounds and their fragmentations. This study was focused on identifying the fragmentation rules for some VDOPs by incorporating MS data with in silico calculated MS fragmentation pathways. Diels-Alder derivatization was used to enhance the sensitivity and selectivity for mass spectrometry data collection. Finally, the confirmed PTAD derivatize target compounds were separated and analyzed using ESI(+)-UHPLC-MS/MS in multiple reaction monitoring (MRM) mode in model samples.

Biography

Fatemeh Mahmoodani is currently a PhD student at the School of Chemical Sciences, University of Auckland, New Zealand. Her current research focuses on vitamin D_3 degradation in whole milk powder and identification of vitamin D_3 isomerization and oxidation products. Her PhD project is collaboration with Fonterra Cooperative Group Ltd. and funded by the Primary Growth Partnership Program of New Zeeland.

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