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Further insights on the carotenoid profile of tagetes patula flowers

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Identification of carotenoid esters is a challenge and much more difficult and laborious than that of free carotenoids in saponified extracts since the number of possible carotenoid esters found in plant materials is quite high. Xanthophylls can have 1 or 2 hydroxyl groups in the molecule which can be acylated or not with several fatty acids. We carried out a comprehensive identification of the carotenoids from marigold petals by LC-APCI-MS/MS and identified 56 carotenoids: 6 free carotenoids, 20 monoesters and 30 diesters. This was the first time that esters of auroxanthin, zeinoxanthin and β -cryptoxanthin were identified in marigold petals, while lutein esters were the major carotenoids, as expected. Differentiation between lutein mono-or heterodiester isomers was based on the different intensities of the ion fragments in the MS spectrum due to the loss of the substituent attached to the β -ring (more stable and more intense m/z signal) and the one attached to the β -ring. Moreover, the heterodiester with the fatty acid of the highest molecular mass acylated at the 3'-O-position eluted before the correspondent 3-O-regioisomer. For instance, both lutein 3-O-laurate-3'-O-myristate and lutein 3-O-myristate-3'-O-laurate presented in their MS spectrum, the fragment ions at *m/z* 733 [M+H-myristic acid]+ and *m/z* 761 [M+H-lauric acid]; however, in the first diester MS spectrum, the fragment ion at *m/z* 733 was more intense than at *m/z* 761 and the contrary occured for the other isomer.

Biography

Daniele Bobrowski Rodrigues has a Bachelor's degree in Pharmacy and a Master's degree in Food Science and Technology. She is a PhD student in the Food Science Department at University of Campinas-Brazil. The main themes of her research are extration and identification of pigments by HPLC-DAD-MS/MS, antioxidant capacity and carotenoid bioaccessibility.

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