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RANDOMIZED BLOCKED DESIGN APPLIED FOR THE MULTICRITERIA OPTIMIZATION OF HEADSPACE TRAP EXTRACTION OF FURAN AND FURFURAL FROM SPONGE CAKE

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Furan, a possibly carcinogenic compound to humans, and furfural, a naturally occurring aroma compound, can be produced in heat-processed foods [1,2]. Therefore, their simultaneous determination is important for food safety and quality purposes. Headspace techniques coupled to gas chromatography-mass spectrometry (GC-MS) are often used to analyze process-induced compounds. Although headspace trap (HS Trap) extraction has been recently used for furan quantitation in bread crust [3], this technique has not been used for the simultaneous determination of furan and furfural before. This work presents an optimal design of experiments (O-DOE) approach using random blocks for the multicriteria optimization of HS Trap extraction of furan and furfural from sponge cake for their quantification by GC-MS. A bias related to sample preservation was observed during preliminary tests and eliminated in further assays by considering it as a blocking factor. A tailor-made experimental plan including four instrumental factors (i.e. thermostating temperature and time, dry purge time, pressurization cycles) and two sample preparation variables (i.e. ratio of water and sample weight [dry basis] and total amount [dry basis]), considering the blocking factor was designed. Response surface models (P-value <0.0001; R^2 0.974 for all models) resulted in the identification of most linear and some quadratic terms and a few second order interactions as influencing the extraction of furan, furfural and their internal standards, *d4*-furan and *d4*-furfural. Interestingly, one of the sample preparation variables, namely the ratio of water and sample weight (dry basis), showed no effect on furfural extraction, while different profiles for furan and *d4*-furan were observed regarding this factor. A set of optimal conditions for a HS Trap extraction method was, for the first time, successfully defined by using the optimal design of experiments methodology and a desirability function.

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References:

- [1] J. Pico, J. Bernal, M. Gómez, Food Research International, 75, 200 (2015).
- [2] European Food Safety Authority, EFSA Journal, 9, 2347 (2011).
- [3] L. Huault, N. Descharles, B. Rega, S. Bistac, V. Bosc, P. Giampaoli, Food Addit Contam A, 33, 236, (2016).