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► To cite this version:

Mayela Cepeda Vasquez, David Blumenthal, Valérie Camel, Barbara Rega. Randomized blocked design applied for the multicriteria optimization of headspace trap extraction of furan and furfural from sponge cake. 16. Chemometrics in Analytical Chemistry - CAC 2016, Jun 2016, Barcelone, Spain. , 2016, XVI Chemometrics in Analytical Chemistry. hal-01449989

HAL Id: hal-01449989

<https://hal.science/hal-01449989>

Submitted on 3 Jun 2020

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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.

Acknowledgements: The authors wish to thank Nicolas Descharles and Jessica Malfaire for technical support. In addition, M. Cepeda-Vázquez wishes to thank the Mexican National Council for Science and Technology (CONACYT) for her doctoral grant.

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).