Different headspace solid phase microextraction – gas chromatography/mass spectrometry approaches to haloanisoles analysis in wine.

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Streszczenie

Three approaches in determination of six haloanisoles (2,4,6-trichloroanisole, 2,3,4-trichloroanisole, 2,3,6-trichloroanisole, tetrachloroanisole, pentachloroanisole and 2,4,6-tribromoanisole) in wine were compared. Comprehensive gas chromatography - time of flight mass spectrometry (GC×GC-ToF-MS) was described for the first time for this application and compared to gas chromatography-tandem mass spectrometry (GC-MS/MS) using triple quadrupole instrument. These techniques were compared with "standard" analytical approach using GC-MS(SIM). SPME method was developed and used for all separation methods (DVB/PDMS fiber, 70 °C, 30%NaCl, 20 min extraction). Extraction dependence on matrix was discussed using model wines with different ethanol contents (8%, 12%, and 18%) as well as water and different wines (dry white, dry red and sweet liqueur), with the lowest sensitivities obtained for highest ethanol contents in model wine and for liqueur wine. Limits of detection for GC×GC-ToF-MS method were 0.09-2.92 ng/L depending on the examined compound and matrix (compared to 0.1-13.3 ng/L obtained using GC/MS(SIM)). For GC-MS/MS method lower detection limits were achieved than for the GC×GC method (0.01-0.1 ng/L), however comprehensive gas chromatography-mass spectrometry provides full spectral information on analyzed compounds. Both methods had limits of detection far below odor thresholds of haloanisoles in wine, good linearity up to 2000 ng/L tested and good precision, what makes them suitable for analysis of these compounds in low ppt levels.

Słowa kluczowe

Haloanisoles, molecule, Wine, SPME, GC×GC, MS/MS

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