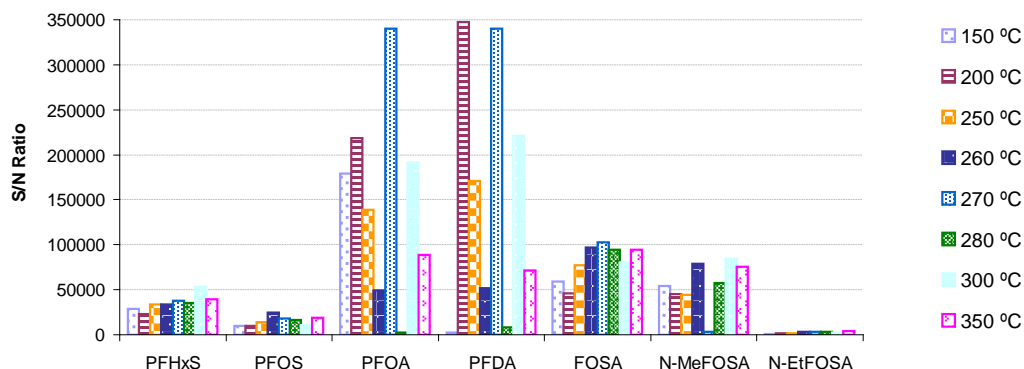


Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Analysis of perfluorinated alkyl substances in Spanish sewage sludge by liquid chromatography-tandem mass spectrometry

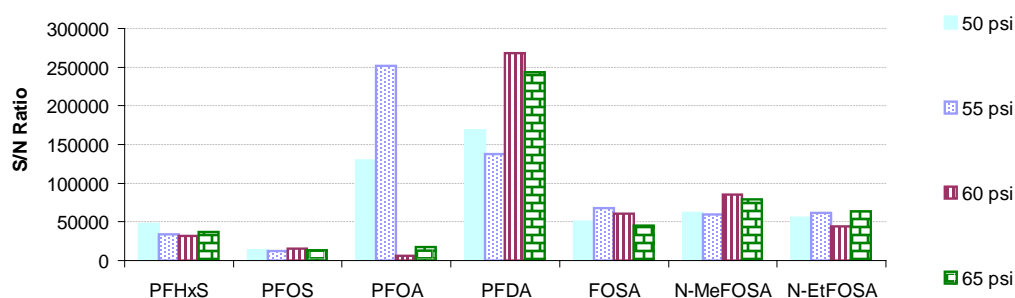
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The nebulizing gas pressure was evaluated in the range of 50-65psi, being 55psi the pressure providing the best results for most of the compounds studied. In the case of 60psi and 65psi the signal of PFOA decreased although the values for the rest of the compounds were acceptable (Fig. S3).

Fig. S3

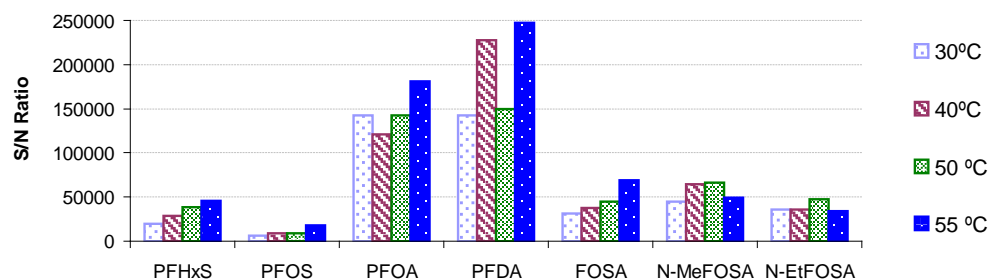
Evaluation of the N₂ nebulizing gas pressure in the analysis of PFAS.



Spray chamber temperature was tested between 30°C and 60°C. In this case, 55°C provided the best S/N ratio for most of the compounds; higher temperatures did not allow a good ionization (Fig. S4).

Fig. S4

Study of the effect of the spray chamber temperature in the analysis of PFAS.



Spray chamber temperature was evaluated in a range from 30 to 60°C.
At 60°C, operational problems appeared, indicating that this temperature was not adequate.

The spray shield voltage facilitates the introduction of the ions formed in the spray chamber toward the mass spectrometer. This parameter was ranged from -300 to -600v, and the value selected was -450v. The X-Y position and voltage of the spray needle was necessary to maximize the nebulization efficiency and optimize the sensitivity and maximum robustness. The needle voltage was ranged from -1000 to -4000v; in this case, -2000v was considered as optimal value.

Some MS/MS parameters were optimized to achieve the suitable collision induced dissociation (CID) of the parent ions for formation of the product ions. The collision gas pressure was tested in the range of 1.6 and 2mTorr; 1.8mTorr provided good results for most of the analytes (Fig. S5).

Fig. S5

Study of the effect of the collision gas pressure in the analysis of PFAS.

