Polyaniline Based Materials as a Method to Eliminate Haloanisoles in Spirits Beverages

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In this research, the abilities of two polyaniline-based materials (PANI-EB and PANI-ES) were evaluated as potential fining agents to eliminate 2,4,6-trichloroanisole (TCA) and 2,4,6-tribromoanisole (TBA). The results showed that the retention percentages of TCA and TBA were higher than 68% for all the materials tested in methanol, and they vary according to the interaction time and the quantity of polymer used. The polymers were also tested in whisky following the same procedures and considering the results obtained in the methanol tests. The analyses indicated that polyaniline-based materials are effective in removing TBA and TCA, with retention percentages around 75% and 13%, respectively. Electronic structure calculations and molecular dynamics simulations helped to gain insight on the behavior of the PANI polymers in methanol and simulated whiskey solution (ethanol/water) and their interactions with each haloanisole. Finally, the main compounds present in the whisky were characterized in order to demonstrate that the purification process did not modify significantly the aromatic profile of the product and the total phenolic content.