

Article

Ion-trap Mass Spectrometric Analysis of Bisphenol A Interactions with Titanium Dioxide Nanoparticles and Milk Proteins

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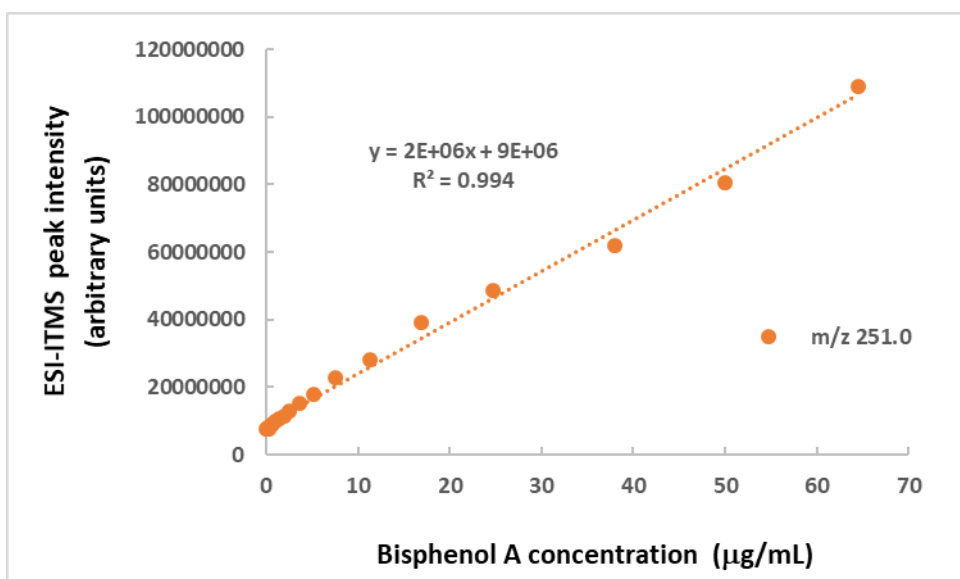


Figure S1. Standard calibration curve for determination of bisphenol A by ESI-ITMS, using m/z 251.0 for extracted ion monitoring in positive polarity. Relative standard deviation of each data point = 5%.

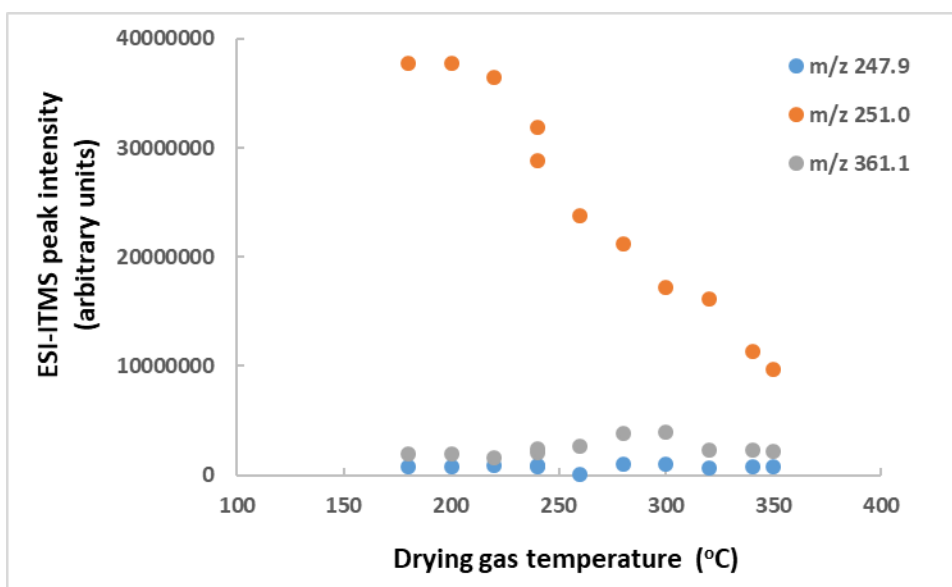


Figure S2. Optimization of drying gas temperature for TiO₂ nanopowder (428 g/mL) in BPA standard solution (1.8 g/mL) containing sodium formate (41 g/mL). Relative standard deviation of each data point = 5%.

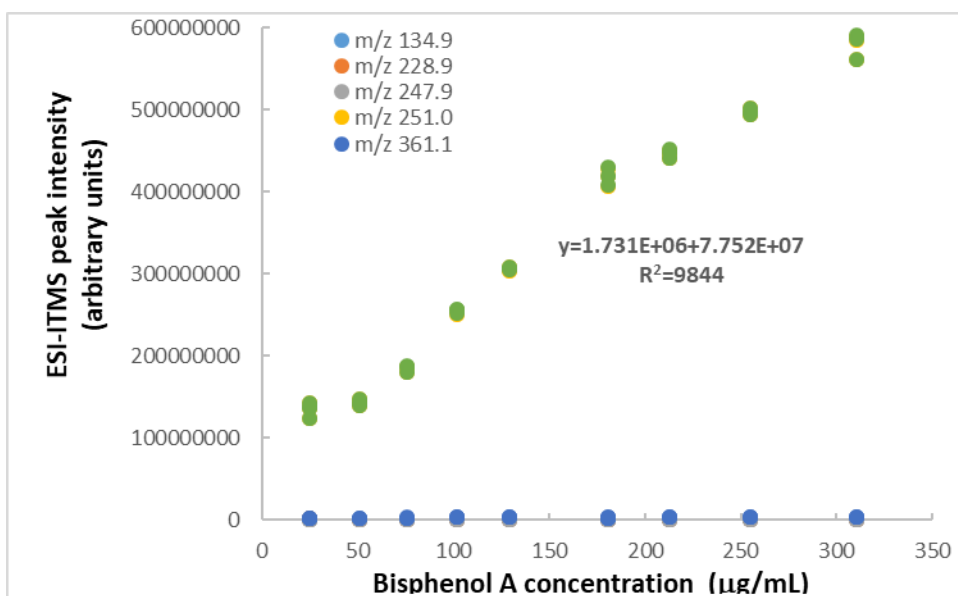


Figure S3. Addition of BPA into BPA solution (25 µg/mL) containing TiO₂ nanoparticles (104 µg/mL), L-glutamic acid (41 µg/mL) and sodium formate (260 µg/mL) for ESI-ITMS analysis. Relative standard deviation of each data point = 5%.

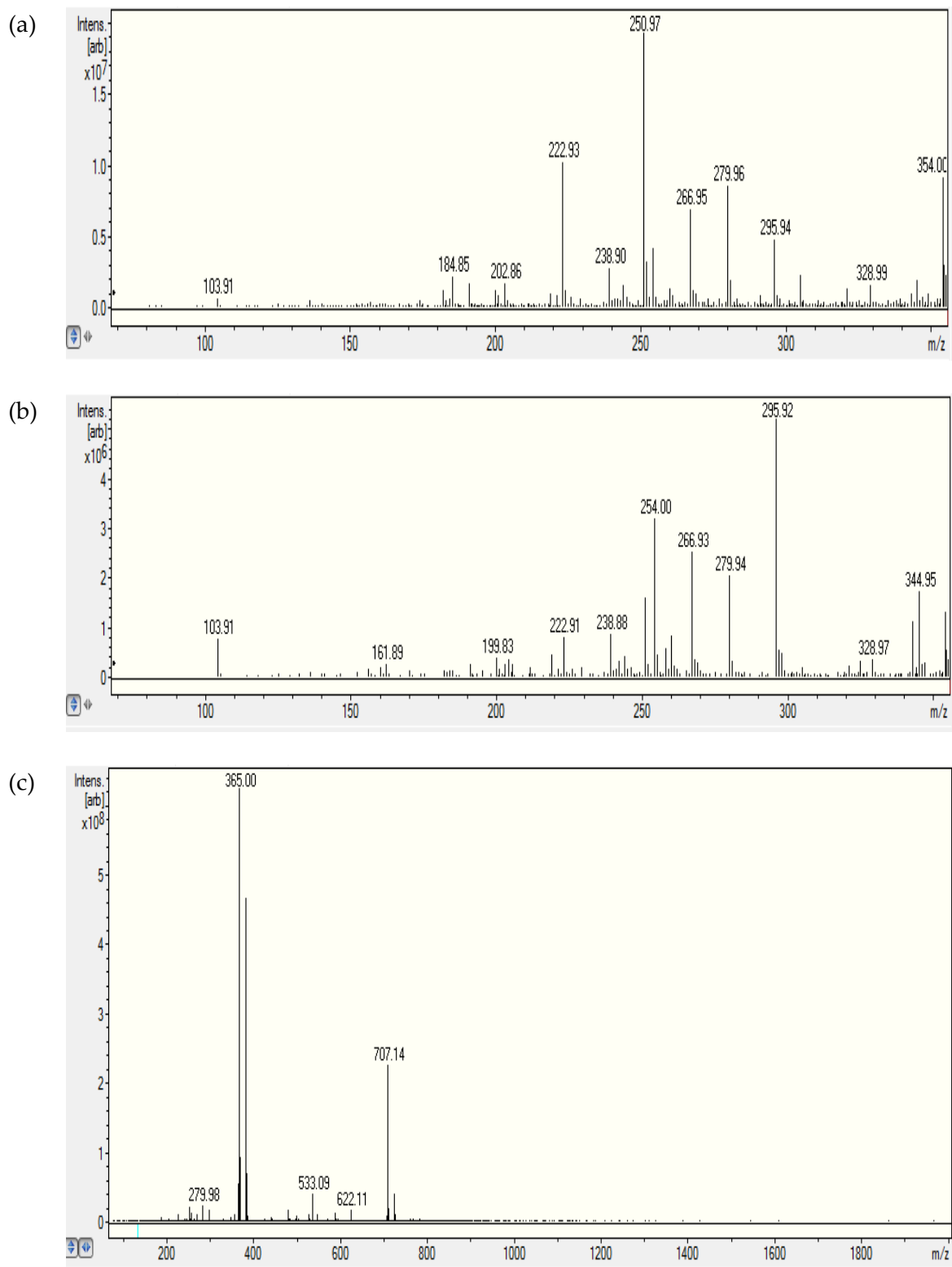


Figure S4. ESI-ITMS spectra: (a) 1.00 mL of BPA (1.8 g/mL) + 50 g/mL sodium formate, (b) 0.14 mL of milk + 1.00 mL of BPA (1.8 g/mL) + 50 g/mL sodium formate, (c) 0.14 mL of whey + 1.00 mL of BPA (1.8 g/mL) + 50 g/mL sodium formate.

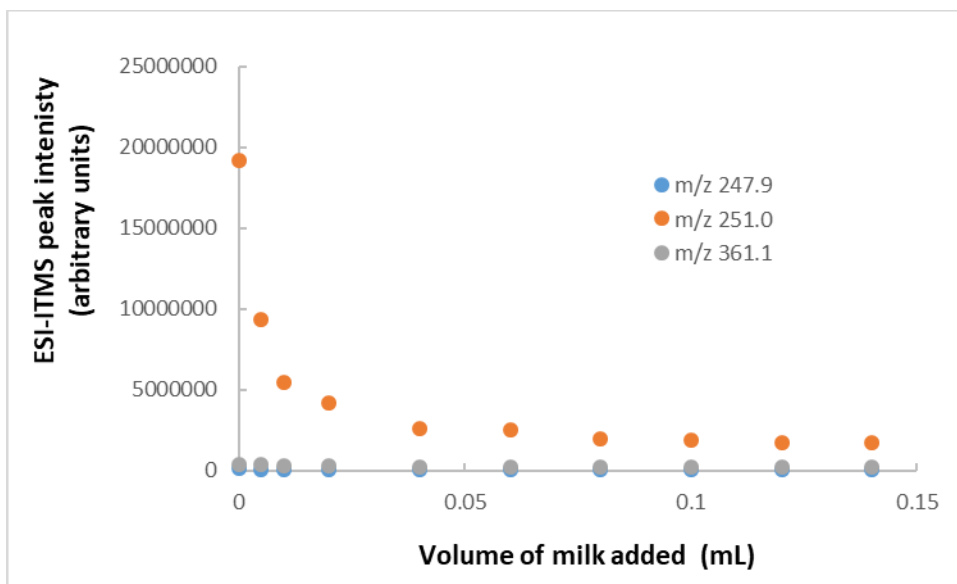


Figure S5. ESI-ITMS analysis of BPA (1.8 g/mL) standard solution containing sodium formate (41 g/mL) after adding different volumes of milk. Relative standard deviation of each data point = 5%.

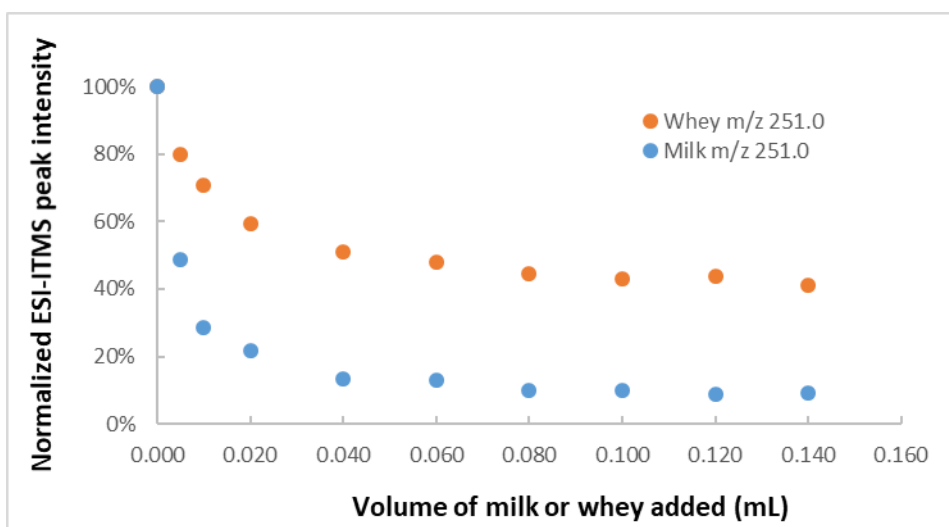


Figure S6. ESI-ITMS analysis of BPA (1.8 g/mL) standard solution containing sodium formate (41 g/mL) after adding different volumes of milk or whey. All peak intensities were normalized for easy comparison between milk and whey. Relative standard deviation of each data point = 5%.

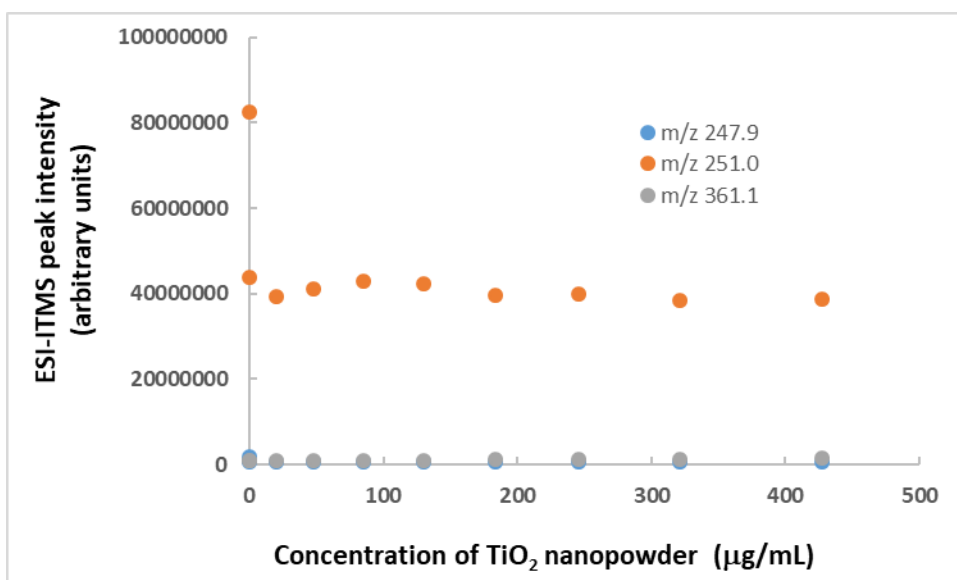


Figure S7. Effect of TiO₂ nanoparticles on BPA binding with whey proteins. Addition of whey (0.5 mL) to 1.8 mg/mL BPA standard solution (25 mL) initially at 0 g/mL TiO₂ decreased the ESI-ITMS intensity of m/z 250.1 for [BPA+Na]⁺ by approximately half. Relative standard deviation of each data point = 5%.

Table 1. Operational settings for ESI-ITMS analysis.

Mass Range Mode	UltraScan
Ion Polarity	positive
Mass scan range	70-2000 Da
Ion Source Type	ESI
Alternating Ion Polarity	off
Source (capillary/interface) temperature	250°C
Capillary (spray voltage)	4500 V
End plate offset	50 V
Nebulizer gas	N ₂ 99.9990% (0.5 bar)
Dry gas	N ₂ 99.9990% (4.0 L/min)
Dry gas temperature	180°C