Supporting Information for

A Novel Strategy Using Peroxymonosulfate to Control the Formation of Iodinated Aromatic Products in Treatment of Phenolic Compounds by Permanganate

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Text S1. Description of the principle of the Precursor Ion Scan (PIS) and Multiple Reaction Monitoring (MRM) approach

The PIS approach has been developed by Zhang et al. [1-3] as an effective tool to selectively pick out polar halogen-containing compounds that are ionizable in negative ESI and its principle has been well elaborated by these authors. There are three quadrupoles of the mass spectrometer called Q_1 , Q_2 and Q_3 . The compounds in the samples would be firstly ionized by the electrospray ionization producing corresponding molecular ions. These ions then passed Q_1 in sequence with their m/z values scanned. As these ions entered collide chamber (Q_2) and collided with argon gas, fragment ions were then produced. By setting PIS of m/z 127 as conducted in this work, Q_3 would only selectively detect fragment iodide ion (m/z of 127) that generated in Q_2 . In this way, polar iodide-containing compounds could be quickly and selectively picked out. For MRM measurement, the combination of molecular ion and the iodide ion was used as the precursor/product ion pairs due to their high intensity.

References

[1] Zhang X., Talley J. W., Boggess B., Ding G., Birdsell D., Fast selective detection of polar brominated disinfection byproducts in drinking water using precursor ion scans, Environ. Sci. Technol., 2008, 42, 6598-6603.

[2] Gong T., Zhang X., Detection, identification, and formation of new iodinated disinfection byproducts in chlorinated saline wastewater effluents, Water Res., 2015, 68, 77-86.

[3] Ding G., Zhang X., A picture of polar iodinated disinfection byproducts in drinking water by (UPLC/)ESI-tqMS, Environ. Sci. Technol. 2009, 43, 9287-9293.