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Classification of Mineral Sunscreen and Naturally Occurring Particles via Two-dimensional Hierarchical Clustering in River Water using single-particle ICP-TOFMS

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Single-particle inductively coupled plasma mass spectrometry (spICP-MS) is a sensitive and high throughput technique for the analysis of nanoparticles (NPs) and submicron particles (µPs) at the individual particle level. Using a time-of-flight (TOF) mass analyzer, the mass amounts of multiple elements and isotopes across the atomic mass range (from ^{6}Li to ^{238}U) can be determined in individual particles. For the analysis of particle-rich environmental samples, spICP-TOFMS produces a large amount of data with many single-element and multi-element particles types recorded. From these files, data reduction techniques such as hierarchical clustering analysis (HCA) can be used to extract particle-population-level information. HCA is a technique that separates data into groups or clusters based on measured similarities between data points and has been used previously to predict the presence of anthropogenic NPs in complex samples.[1]

In this study, we characterized neat suspensions of natural stream water and sunscreen by spICP-TOFMS. Titanium dioxide (TiO_2) and zinc oxide (ZnO) engineered nanoparticles (NPs) are used in some sunscreen products as mineral-based filters to produce broad-band protection from UV light. River waters can become contaminated with mineral-based sunscreens due to human recreational activities such as bathing, swimming and other water sports. Following initial spICP-TOFMS analyses, we spiked stream water with different concentrations of sunscreen particles and used two-dimensional HCA to identify clusters distinct to river water and sunscreen particles in the spICP-TOFMS data. Clustering is based on recorded element mass amounts in particles. We found that HCA produced two clusters of Ti-rich and Zn-rich particles that were distinct to sunscreen particles. These sunscreen-derived NPs are isolated from naturally occurring NPs and µPs that are rich in Fe, Al, Mn, Ti, Mg, Zn, Ce, La, and/or Pb. Via HCA, we demonstrate the classification of sunscreen-derived Ti and Zn NPs across more than two orders of magnitude and at PNCs up to 50 times lower than that of naturally occurring Ti and Zn NPs.

1. K. Mehrabi, R. Kaegi, D. Günther and A. Gundlach-Graham, *Environ. Sci.: Nano*, 2021, **8**, 1211-1225.