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IsotopeTrack: A fast and flexible application for the analysis of spICP-TOF-MS datasets

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Particle pollutants, including engineered nanoparticles and complex multi-element particles, are increasingly recognized as important drivers of biogeochemical cycling and contaminant transport across environmental compartments. Single-particle ICP-ToF-MS (spICP-ToF-MS) enables detailed compositional characterization of individual particles, yet existing data-processing applications remain constrained by vendor-specific formats, limited multi-sample handling, and insufficient visualization capacity for large datasets. At the same time, environmental studies increasingly generate datasets containing hundreds of thousands of particles, requiring automated interpretation, advanced visualization, and machine-assisted pattern recognition to support source identification and mechanistic understanding. To address these needs, we developed IsotopeTrack, an open-source Python-based platform for spICP-ToF-MS data processing with cross-platform compatibility (Windows and macOS). The software implements complete calibration procedures, including transport efficiency and sensitivity calibration, and incorporates compound Poisson log-normal modeling with element-specific parameter optimization. In addition, the platform integrates an interactive graphical workspace allows drag-and-drop construction of customized workflows, supports multiple file formats, and provides advanced visualization modules including elemental correlations, isotopic ratio distributions, ternary diagrams, and composition heatmaps. Parallelized processing reduced analysis time from hours to minutes and enabled rapid comparison of environmental samples containing very large particle numbers. By combining batch processing, AI-assisted, and interactive visualization, the platform facilitates source apportionment and mechanistic interpretation of particulate pollutants across atmospheric, aquatic, and biological matrices. This open-source framework therefore provides an analytical and computational bridge between single-particle measurements and environmental process understanding, enabling large-scale characterization of nanoparticle and particulate pollutant behavior in complex environmental systems.