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Nontarget screening exhibits a seasonal cycle of PM2.5 organic aerosol composition in Beijing

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The molecular composition of atmospheric particulate matter in the urban environment appears as extremely complex, and it remains a grand challenge to identify its sources and formation pathways. In this study, we applied a novel nontarget analysis to HPLC/(−)ESI-HRMS measurements of yearlong $PM_{2.5}$ filter samples from Beijing, and represent all detected compounds in comprehensive molecular fingerprints. Additionally, we used a hierarchical clustering analysis (HCA) for complexity reduction of the large dataset. The Van Krevelen-diagram indicate that the major compound clusters exhibit a unique molecular pattern. We found that organic aerosol (OA) in Beijing during summer features a higher degree of oxidation and a higher proportion of organosulfates (OSs) in comparison to OA during wintertime, which exhibits a high contribution from (nitro-)aromatic compounds. OSs appeared with a high intensity in summer-haze conditions, indicating the importance of anthropogenic enhancement of secondary OA in summer Beijing. We estimated the quantitative contribution of the main compound clusters to total OA based on calibrations using surrogate standards. With this approach, we are able to explain a small fraction of the OA monitored by the Time-of-Flight Aerosol Chemical Speciation Monitor (ToF-ACSM). However, we observe a strong correlation between the sum of the quantified clusters and OA measured by the ToF-ACSM, indicating that the identified clusters represent the major variability of OA seasonal cycles. This study highlights the potential of using nontarget screening in combination with HCA for gaining a better understanding of the molecular composition and the origin of OA in the urban environment.