

Supplementary material:

ICP-MS as a contributing tool to non-target screening (NTS) analysis for environmental monitoring

Jörg Feldmann^{1,*}, Helle Rüz Hansen^{2,*}, Thomas Molnár Karlsson^{3,*}, Jan H. Christensen^{3,*}

¹TESLA-Analytical Chemistry, Institute of Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria

²Danish Environmental Protection Agency, Tolderlundsvej 5, 5000, Odense C, Denmark

³Department of Plant and Environmental Sciences, University of Copenhagen, 1871 Frederiksberg C, Denmark

*Corresponding authors: joerg.feldmann@uni-graz.at, herha@mst.dk, tmmk@plen.ku.dk, jch@plen.ku.dk

Table of content:

Figure S1: *Web of Science bibliographic search, sum of publications with topic matching “non-target screening”, “suspect screening” or “non-target analysis” between 1991-2023, February 2024.*

Figure S2: Percentage of compounds containing heteroatoms which can be selectively detected by ICP-MS (from the NORMAN list of Emerging contaminants current status 106).

Figure S3: Identification Level scheme modified from Schymanski et al. 2014 by introducing ICP-MS information to the scheme as level 4b.

Figure S4: Confidence level scheme for quantification using NTS.

Figure S1.: Web of Science bibliographic search, sum of publications with topic matching “non-target screening”, “suspect screening” or “non-target analysis” between 1991-2023, February 2024.

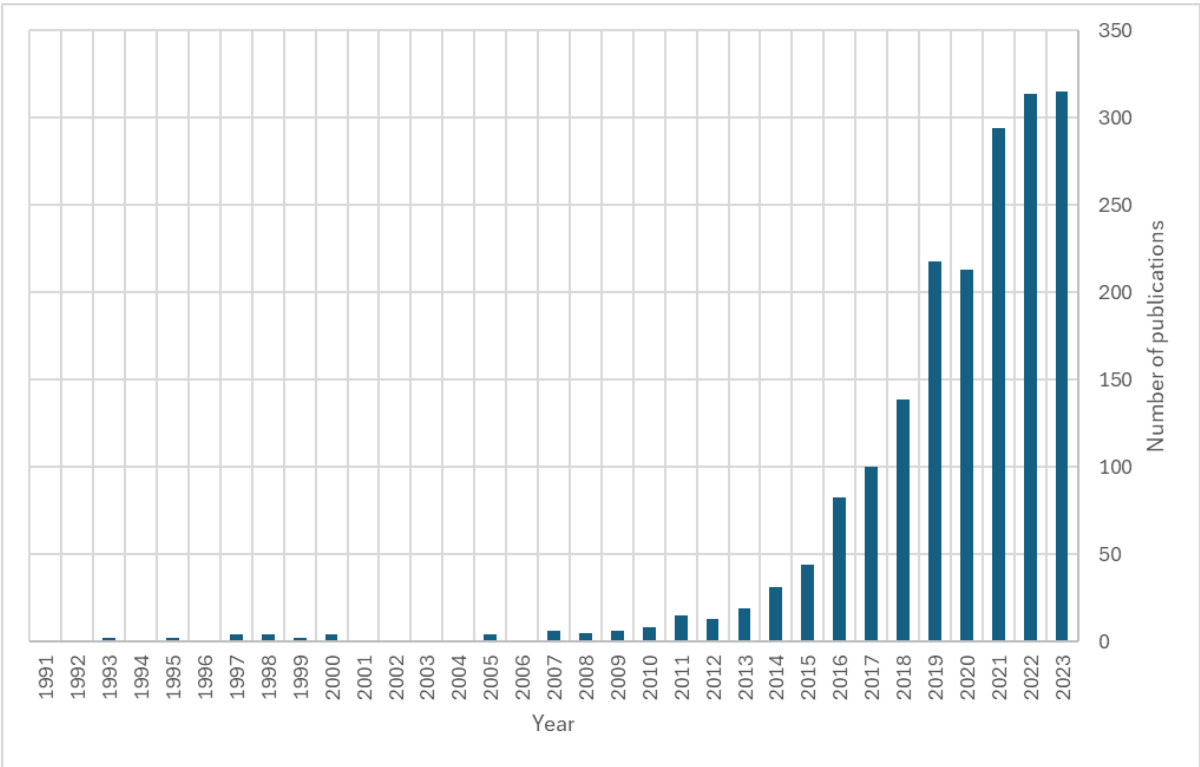


Figure S2: Percentage of compounds containing heteroatoms which can be selectively detected by ICP-MS (from the NORMAN list of Emerging contaminants current status 106).

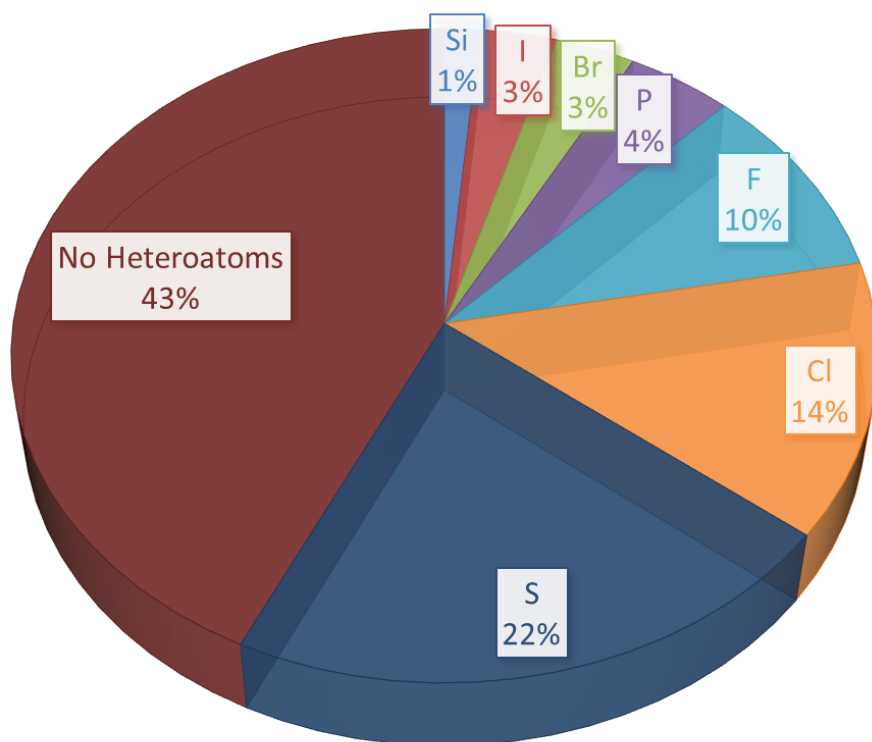


Figure S3: Identification Level scheme modified from Schymanski et al. 2014 by introducing ICP-MS information to the scheme as level 4b. Its element-specific parallel detection enhances the confidence for the unequivocal molecular formulae.

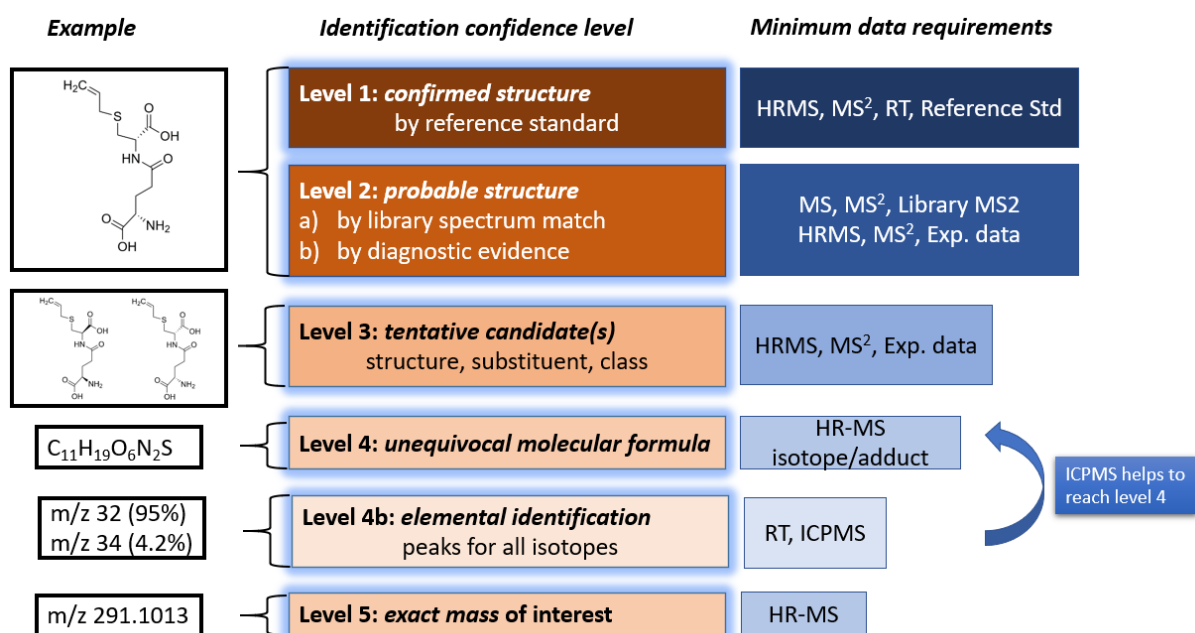


Figure S4: Confidence level for quantification using NTA. We suggest six levels of confidence in quantitative data. Level 6 uses a surrogate standard and has the lowest level of confidence, while level 5 uses an identical standard for external calibration. Using ICP-MS can increase the confidence because of its element-specific detection with low matrix effect of compounds that contain a hetero-atom detectable with ICP-MS. Level 2 and 1 are using isotopically-labelled standards spiked at different times to the sample workflow.

