Supplementary Information

Non-target analysis and characterisation of nanoparticles in spirits via single particle ICP-ToF-MS

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Python script:

https://github.com/djdt/djdt.github.io/blob/feece3a08b1ff90131bbd9d618ba778509941467/scripts/non_target_screening_script.py (updated 28.09.2023)

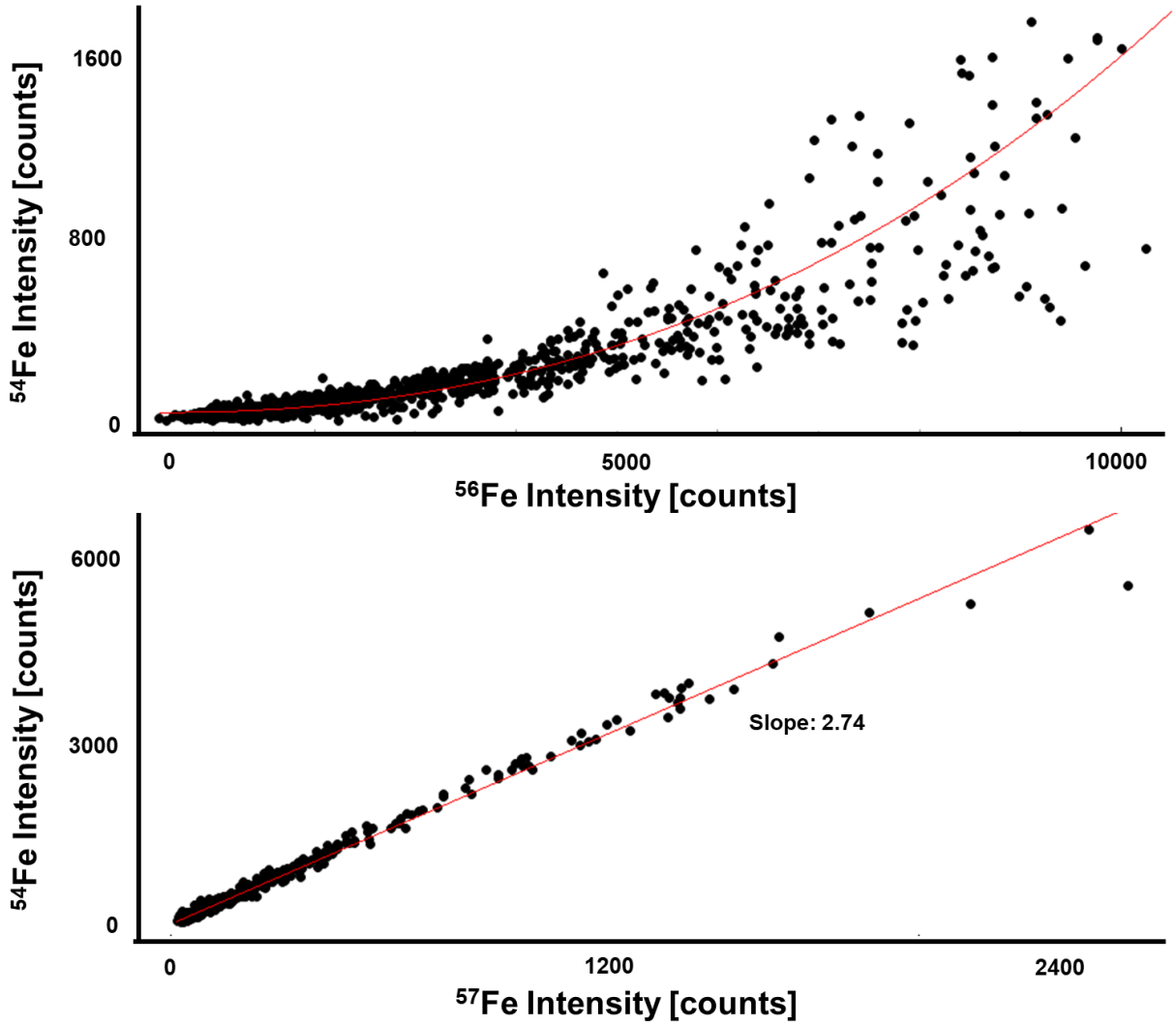

Figure S1. The ratio of ^{54}Fe and ^{56}Fe was investigated in all detected NPs (top). The ratio was found to be drifting at high ^{56}Fe intensities due to a limited dynamic range. The $^{54}Fe/^{57}Fe$ plot (bottom) shows isotope ratios independent from signal intensities. ^{56}Fe was used to count particles, ^{54}Fe was used to determine sizes and masses.

Table S1. Overview of NP characteristics in all samples.

Sample NP entities	PNC (x10^3)	Ionic Bkg (ng/L)	Mean mass (fg)	Mean size (nm)	sDL (nm)
Tap water					
Fe_2O_3	14.2 ± 1.1	77.1 ± 20.0	0.95 ± 1.90	58.6 ± 25.0	31.9
CuO	42.6 ± 1.9	268 ± 160	1.43 ± 2.60	64.5 ± 24.0	28.3
ZnO	91.0 ± 1.1	940 ± 1100	4.20 ± 4.70	100 ± 36	36.4
W1					
TiO_2	4.19 ± 0.59	3140 ± 5100	4.13 ± 7.90	94.6 ± 53.0	50
Fe_2O_3	38.0 ± 1.8	57600 ± 460000	4.82 ± 6.90	113 ± 28	87
Ag	9.21 ± 0.85	14.2 ± 2.6	0.208 ± 0.30	30.9 ± 8.5	17
Au	6.14 ± 0.69	0.53 ± 0.02	0.31 ± 0.41	28.1 ± 9.6	13

W2					
TiO_2	6.43 ± 0.72	201 ± 83	5.93 ± 9.90	105 ± 63	38
Fe_2O_3	12.4 ± 1.0	10300 ± 36000	5.13 ± 9.00	108 ± 40	59
Ag	8.46 ± 0.83	34.3 ± 9.4	0.35 ± 1.10	34.2 ± 12.0	17
SnO_2	39.5 ± 1.8	200 ± 56	3.45 ± 4.20	89.0 ± 29.0	39
Au	7.35 ± 0.78	0.63 ± 0.02	0.37 ± 0.59	29.3 ± 11.0	14
W3					
TiO_2	18.8 ± 1.4	983 ± 880	9.1 ± 20.0	116 ± 74	43
MnO	8.64 ± 0.91	2210 ± 4900	1.28 ± 1.70	68.3 ± 24.0	40
Fe_2O_3	34.1 ± 1.8	42.1 ± 210	105 ± 110	300 ± 110	88
Ag	8.26 ± 0.80	8.50 ± 1.30	0.60 ± 1.00	41.4 ± 16.0	17
SnO_2	9.60 ± 0.88	93.8 ± 19.0	1.88 ± 2.60	71.4 ± 26.0	37
Au	4.40 ± 0.58	0.23 ± 0.02	0.77 ± 1.10	36.0 ± 15.0	13
W4					
TiO_2	3.80 ± 0.60	2530 ± 3600	1.76 ± 4.60	69.1 ± 39.0	48
Fe_2O_3	13.3 ± 1.0	46200 ± 320000	6.87 ± 5.62	114 ± 28	81
Ag	13.7 ± 1.0	14.9 ± 2.8	0.19 ± 0.21	30.3 ± 7.4	17
Au	12.5 ± 1.0	0.60 ± 0.02	0.36 ± 0.57	28.5 ± 12.0	14
W5					
TiO_2	2.20 ± 0.42	220 ± 96	7.25 ± 15.0	107 ± 69	38
MnO	0.77 ± 0.22	2210000 ± 6000000	121 ± 43	34.6 ± 3.7	33
Fe_2O_3	6.43 ± 0.72	5380 ± 13000	4.90 ± 11.0	97.9 ± 47.0	50
Ag	5.86 ± 0.67	43.1 ± 13.0	0.60 ± 0.74	43.3 ± 14.0	18
Au	4.86 ± 0.61	0.61 ± 0.02	0.54 ± 0.86	31.7 ± 14.0	13
W6					
TiO_2	4.46 ± 0.61	3180 ± 5300	2.84 ± 5.00	84.8 ± 46.0	50
Fe_2O_3	71.7 ± 2.4	58300 ± 470000	4.89 ± 7.00	105 ± 26	86
Ag	6.26 ± 0.71	14.4 ± 2.7	0.24 ± 0.42	31.4 ± 9.7	16
Au	6.25 ± 0.69	0.511± 0.02	0.47 ± 0.70	28.7 ± 14.0	13
W7					
TiO_2	5.94 ± 0.70	407 ± 240	6.95 ± 11.0	101 ± 54	40
MnO	1.08 ± 0.29	1310000 ± 2600000	0.12 ± 0.10	34.0 ± 6.4	31
Fe_2O_3	6.43 ± 0.72	17000 ± 76000	4.90 ± 8.6	104 ± 42	63
Ag	9.03 ± 0.84	33.2 ± 9.2	0.41 ± 0.65	37.0 ± 13.0	18
Au	7.79 ± 0.78	0.54 ± 0.02	0.50 ± 0.73	31.3 ± 13.0	14
V1					
Fe_2O_3	5.86 ± 0.69	805 ± 690	2.45 ± 6.60	77.8 ± 36.0	37
SnO_2	7.24 ± 0.77	162 ± 43	2.98 ± 2.70	86.7 ± 26.0	38
G1					
Fe_2O_3	4.88 ± 0.63	334 ± 190	2.71 ± 5.30	85.3 ± 37.0	35
CuO	4.71 ± 0.63	412 ± 300	0.56 ± 0.65	50.5 ± 15.0	29
SnO_2	2.62 ± 0.45	20.1 ± 1.9	8.17 ± 9.20	113 ± 48	34
L1					
TiO_2	32.8 ± 1.6	623 ± 460	6.53 ± 6.80	128 ± 46	42
MnO	1.08 ± 0.29	61400 ± 80000	77.6 ± 55.4	29.3 ± 4.8	28
Fe_2O_3	44.8 ± 1.9	5040 ± 1200	2.39 ± 3.02	87.8 ± 26.0	49
Ag	4.17 ± 0.57	21.9 ± 5.0	0.58 ± 0.56	44.4 ± 11.0	17
SnO2	5.17 ± 0.66	1850 ± 1600	6.68 ± 9.70	109 ± 39	45
Au	2.78 ± 0.46	869 ± 35	0.33 ± 0.20	39.9 ± 7.3	13

L2					
TiO_2	4.78 ± 0.61	4330 ± 890	5.31 ± 7.30	115 ± 47	54
MnO	0.93 ± 0.27	1010000 ± 1800000	0.11 ± 0.84	32.4 ± 6.6	30
Fe_2O_3	1.85 ± 0.38	18500 ± 91000	7.08 ± 15.00	108 ± 55	65
Ag	2.31 ± 0.42	26600 ± 6700	0.34 ± 0.30	37.5 ± 8.6	17