

Supplementary Materials: Elemental Profiles of Whisk(e)y Allow Differentiation by Type and Region

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Table S1. Calibration curve details ($y = ax + b$), detection limits (LOD), accuracy and precision for all elements, measured by ICP-MS and MP-AES. Accuracy, expressed as percent recovery, and precision, expressed as relative standard deviation (RSD), are calculated from spiking experiments. All elements were determined by ICP-MS, except for Ca, K, Mg, Na, and Si which were measured by MP-AES.

Element	a	b	R	LOD ($\mu\text{g/L}$)	Recovery	RSD	Element	a	b	R	LOD ($\mu\text{g/L}$)	Recovery	RSD
27 Al	0.00028	0.0036	0.9999	0.442	114%	15%	140 Ce	0.0149	0.00004	0.9998	0.0006	n.d. ¹	n.d.
47 Ti	0.00053	0.00003	1.0000	0.146	112%	38%	141 Pr	0.0184	0.000008	0.9998	0.0003	n.d.	n.d.
51 V	0.0056	0.0002	1.0000	0.007	78%	19%	146 Nd	0.0032	0.000006	0.9999	0.0013	n.d.	n.d.
52 Cr	0.0062	0.0509	0.9947	10.1	87%	9%	147 Sm	0.0026	0.0000009	0.9999	0.0005	n.d.	n.d.
55 Mn	0.007	0.0007	1.0000	0.019	89%	19%	153 Eu	0.0059	0.000002	0.9999	0.0003	n.d.	n.d.
56 Fe	0.0068	0.0375	0.9994	7.01	126%	11%	157 Gd	0.002	0.0000009	0.9999	0.0006	n.d.	n.d.
58 Ni	0.0036	0.0006	1.0000	0.027	91%	19%	163 Dy	0.0029	0.000002	0.9999	0.0004	n.d.	n.d.
59 Co	0.0064	0.00003	1.0000	0.002	94%	22%	165 Ho	0.0113	0.000001	0.9999	0.0001	n.d.	n.d.
63 Cu	0.0035	0.0014	1.0000	0.022	97%	15%	166 Er	0.0037	0.0000005	0.9999	0.0002	n.d.	n.d.
66 Zn	0.0012	0.0035	1.0000	0.125	77%	19%	169 Tm	0.0112	0.000003	0.9999	0.0002	n.d.	n.d.
71 Ga	0.0033	0.000008	1.0000	0.002	115%	27%	172 Yb	0.0024	0.0000006	0.9999	0.0004	n.d.	n.d.
75 As	0.0029	0.00005	1.0000	0.002	100%	25%	175 Lu	0.0113	0.0053	0.9998	0.024	n.d.	n.d.
82 Se	0.0003	0.00003	1.0000	0.016	96%	2%	178 Hf	0.0031	0.00001	0.9998	0.008	n.d.	n.d.
85 Rb	0.0059	0.00008	1.0000	0.013	90%	19%	181 Ta	0.0124	0.000008	1.0000	0.002	n.d.	n.d.
88 Sr	0.0094	0.0015	1.0000	0.009	88%	21%	182 W	0.0032	0.00001	1.0000	0.006	n.d.	n.d.
90 Zr	0.0072	0.0006	0.9999	0.010	99%	10%	185 Re	0.0042	0.0000008	1.0000	0.0004	n.d.	n.d.
93 Nb	0.0122	0.00003	1.0000	0.002	70%	14%	193 Ir	0.005	0.000002	1.0000	0.014	115%	28%
97 Mo	0.0013	0.00005	1.0000	0.007	83%	40%	195 Pt	0.0019	0	1.0000	0.007	121%	26%
101 Ru	0.0023	0.0000006	1.0000	0.001	101%	24%	197 Au	0.003	0.0000001	1.0000	0.015	108%	30%
103 Rh	0.012	0.0001	1.0000	0.002	104%	25%	205 Tl	0.0064	0.00001	1.0000	0.001	85%	19%
105 Pd	0.0027	0.0025	1.0000	0.041	107%	50%	208 Pb	0.0018	0.0003	1.0000	0.004	80%	14%

107 Ag	0.0054	0.0001	1.0000	0.004	96%	14%	232 Th	0.0151	0.00006	0.9999	0.001	100%	1%
114 Cd	0.0027	0.00007	1.0000	0.003	77%	16%	238 U	0.0089	0.000008	1.0000	0.001	81%	19%
118 Sn	0.0031	0.00008	1.0000	0.006	106%	32%	Ca	837.34	0	0.99995	2.79	102%	1%
123 Sb	0.0038	0.00004	1.0000	0.004	107%	18%	K	121.40	0	0.99959	9.74	117%	4%
125 Te	0.0005	0.0000006	1.0000	0.002	102%	26%	Mg	340.47	0	0.99997	7.66	104%	3%
133 Cs	0.0113	0.00002	1.0000	0.002	78%	18%	Na	678.13	0	0.99998	8.87	114%	7%
137 Ba	0.0016	0.0002	1.0000	0.016	65%	17%	Si	9.17	0	0.99998	49.6	107%	5%
139 La	0.0151	0.00003	0.9999	0.0005	n.d.	n.d.							

¹n.d., not detected.