

Supporting Information

TOFHunter—Unlocking Rapid Untargeted Screening of Inductively Coupled Plasma–Time-of-Flight–Mass Spectrometry Data

Hunter B. Andrews,^{1*} Lyndsey Hendriks,² Sawyer B. Irvine,³ Daniel R. Dunlap,⁴ Benjamin T. Manard⁴

¹Radioisotope Science and Technology Division, Oak Ridge National Laboratory, USA

²TOFWERK AG, Switzerland

³Nuclear Nonproliferation Division, Oak Ridge National Laboratory, USA

⁴Chemical Science Division, Oak Ridge National Laboratory, USA

*Corresponding author: (H.B.A.) andrewshb@ornl.gov

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The TOFHunter script is available as a digital download at:<https://github.com/andrewshb/TOFHunter>.

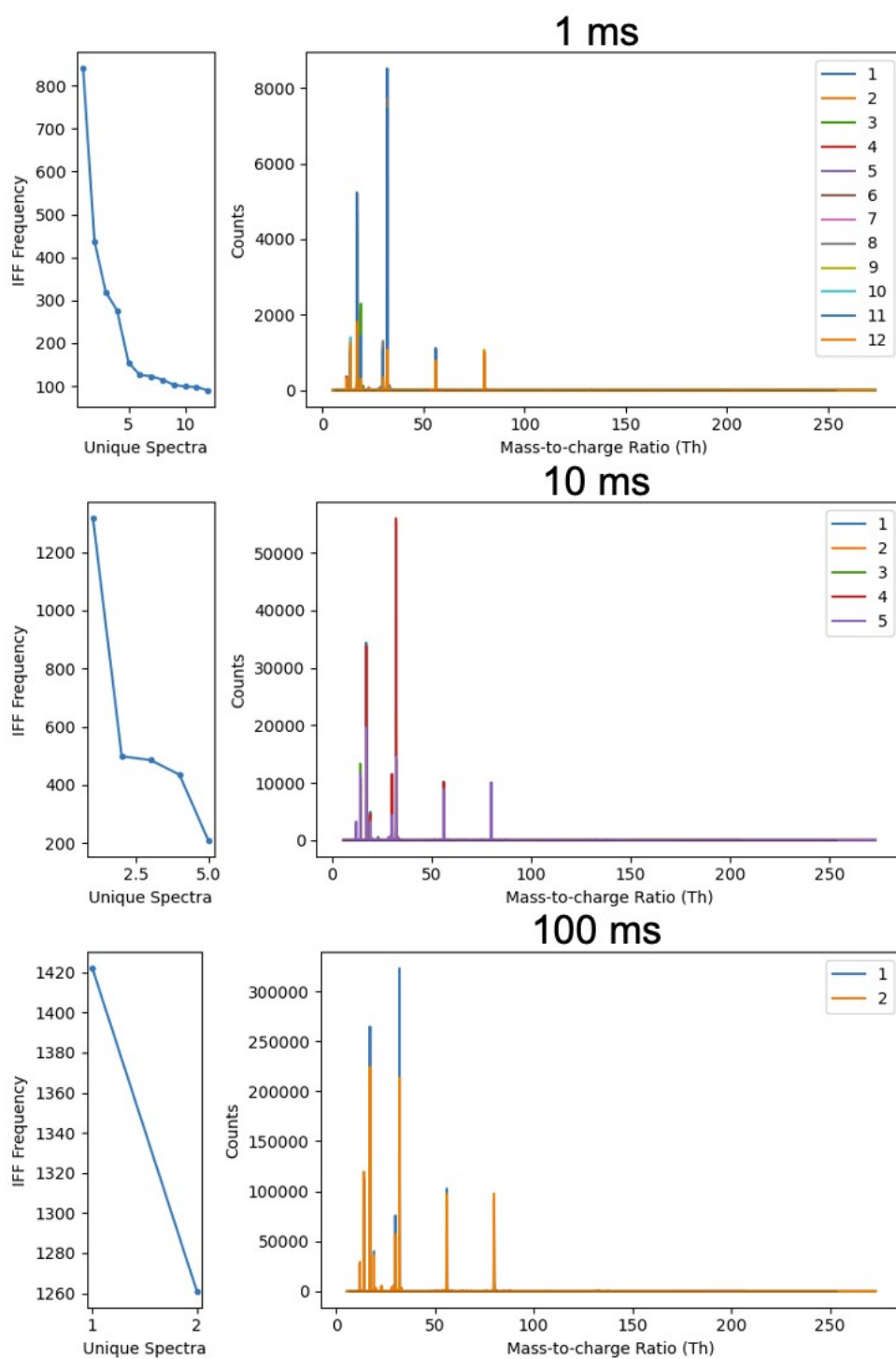


Figure S1. Change in IFF-detected unique features as a function of integration time when measuring a multielement standard.

Table S1. Abbreviated Peak Summary from Nanoplastic Example.^a

#	m/z	Intensity (a.u.)	Nuclide Matches	Potential Interferences
1	19.0	364	¹⁹ F	H ₃ O ⁺
1	21.0	60	²¹ Ne	
1	23.0	453	²³ Na	⁴⁶ Ca ⁺⁺ , ⁷ Li ¹⁶ O, ⁶ Li ¹⁶ O ¹ H, ⁶ Li ¹⁷ O, ⁴⁶ Ti ⁺⁺
1	24.0	146	²⁴ Mg	¹² C ¹² C, ⁴⁸ Ca ⁺⁺ , ⁷ Li ¹⁶ O ¹ H, ⁷ Li ¹⁷ O, ¹⁰ B ¹⁴ N, ⁶ Li ¹⁸ O, ...
1	29.0	777	²⁹ Si	⁵⁸ Fe ⁺⁺ , ¹¹ B ¹⁸ O, ¹¹ B ¹⁷ O ¹ H, ¹⁰ B ¹⁸ O ¹ H, ¹³ C ¹⁶ O, ¹² C ¹⁷ O, ...
1	30.0	173	³⁰ Si	¹¹ B ¹⁸ O ¹ H, ¹² C ¹⁸ O, ¹³ C ¹⁷ O, ¹³ C ¹⁶ O ¹ H, ¹² C ¹⁶ O ¹ H ¹ H, ...
1	32.0	85	³² S	¹⁶ O ¹⁶ O, ¹⁴ N ¹⁷ O ¹ H, ¹⁵ N ¹⁷ O, ¹⁴ N ¹⁸ O
1	41.0	53	⁴¹ K	⁴⁰ Ar ¹ H, ²³ Na ¹⁸ O, ²⁵ Mg ¹⁶ O
1	52.0	55	⁵² Cr	¹² C ⁴⁰ Ar, ³⁶ Ar ¹⁶ O, ³⁸ Ar ¹⁴ N, ³⁵ Cl ¹⁶ O ¹ H, ³⁵ Cl ¹⁷ O, ...
1	54.0	916	⁵⁴ Cr, ⁵⁴ Fe	⁴⁰ Ar ¹⁴ N, ³⁶ Ar ¹⁸ O, ³⁸ Ar ¹⁶ O, ⁴² Ca ¹² C, ⁴⁰ Ca ¹⁴ N, ³⁵ Cl ¹⁸ O ¹ H, ...
1	55.0	132	⁵⁵ Mn	⁴¹ K ¹⁴ N, ⁴⁰ Ar ¹⁵ N, ³⁶ Ar ¹⁶ O ¹ H, ³⁸ Ar ¹⁷ O, ⁴⁰ Ar ¹⁴ N ¹ H, ...
1	56.0	10730	⁵⁶ Fe	⁵⁵ Mn ¹ H, ⁴⁰ Ar ¹⁶ O, ⁴⁰ Ar ¹⁵ N ¹ H, ³⁸ Ar ¹⁸ O, ³⁸ Ar ¹⁷ O ¹ H, ...
1	57.0	417	⁵⁷ Fe	⁴⁰ Ar ¹⁶ O ¹ H, ¹¹⁴ Sn ⁺⁺ , ⁴⁵ Sc ¹² C, ¹¹⁴ Cd ⁺⁺ , ³⁸ Ar ¹⁸ O ¹ H, ...
1	58.0	62	⁵⁸ Fe, ⁵⁸ Ni	⁴⁰ Ar ¹⁸ O, ⁴⁰ Ar ¹⁷ O ¹ H, ⁵⁷ Fe ¹ H, ⁴² Ca ¹⁶ O, ²⁴ Mg ³⁴ S, ...
1	62.9	215	⁶³ Cu	⁴⁶ Ca ¹⁷ O, ⁴⁹ Ti ¹⁴ N, ⁴⁸ Ca ¹⁵ N, ⁴⁴ Ca ¹⁸ O ¹ H, ⁴⁶ Ca ¹⁶ O ¹ H, ...
1	64.0	154	⁶⁴ Ni, ⁶⁴ Zn	⁴⁶ Ca ¹⁸ O, ⁵⁰ Ti ¹⁴ N, ²³ Na ²³ Na ¹⁸ O, ⁴⁸ Ca ¹⁶ O, ⁶³ Cu ¹ H, ...
1	64.9	123	⁶⁵ Cu	³⁶ Ar ¹⁴ N ¹⁴ N ¹ H, ¹² C ¹⁶ O ³⁷ Cl, ¹³⁰ Ba ⁺⁺ , ⁴⁸ Ca ¹⁷ O, ...
1	65.9	106	⁶⁶ Zn	²⁴ Mg ⁴⁰ Ar ¹ H, ⁴⁸ Ca ¹⁸ O ¹ H, ³³ S ¹⁶ O ¹⁶ O ¹ H, ¹⁰ B ¹⁶ O ⁴⁰ Ar, ...
1	68.0	74	⁶⁸ Zn	¹¹ B ⁴⁰ Ar ¹⁷ O, ¹⁰ B ⁴⁰ Ar ¹⁸ O, ³⁶ Ar ¹⁸ O ¹⁸ O, ³⁶ Ar ¹⁶ O ¹⁶ O, ...
1	120.9	190	¹²¹ Sb	¹⁰⁴ Ru ¹⁷ O, ⁸¹ Br ⁴⁰ Ar, ¹⁰⁵ Pd ¹⁶ O, ¹⁰⁴ Ru ¹⁶ O ¹ H, ¹²⁰ Sn ¹ H
1	122.9	145	¹²³ Sb, ¹²³ Te	¹⁰⁶ Cd ¹⁷ O, ¹⁰⁷ Ag ¹⁶ O, ¹²² Sn ¹ H, ⁹¹ Zr ¹⁶ O ¹⁶ O, ⁹⁰ Zr ¹⁶ O ¹⁶ O ¹ H
1	137.9	327	¹³⁸ Ba, ¹³⁸ La, ¹³⁸ Ce	⁹⁸ Ru ³⁶ Ar, ¹⁰⁰ Mo ³⁸ Ar, ¹⁰² Ru ³⁶ Ar, ¹²⁰ Sn ¹⁸ O, ¹²¹ Sb ¹⁷ O, ...
2	19.0	320	¹⁹ F	H ₃ O ⁺
2	23.0	407	²³ Na	⁴⁶ Ca ⁺⁺ , ⁷ Li ¹⁶ O, ⁶ Li ¹⁶ O ¹ H, ⁶ Li ¹⁷ O, ⁴⁶ Ti ⁺⁺
2	24.0	122	²⁴ Mg	¹² C ¹² C, ⁴⁸ Ca ⁺⁺ , ⁷ Li ¹⁶ O ¹ H, ⁷ Li ¹⁷ O, ¹⁰ B ¹⁴ N, ⁶ Li ¹⁸ O, ...
2	29.0	814	²⁹ Si	⁵⁸ Fe ⁺⁺ , ¹¹ B ¹⁸ O, ¹¹ B ¹⁷ O ¹ H, ¹⁰ B ¹⁸ O ¹ H, ¹³ C ¹⁶ O, ¹² C ¹⁷ O, ...
2	30.0	177	³⁰ Si	¹¹ B ¹⁸ O ¹ H, ¹² C ¹⁸ O, ¹³ C ¹⁷ O, ¹³ C ¹⁶ O ¹ H, ¹² C ¹⁶ O ¹ H ¹ H, ...
2	32.0	208	³² S	¹⁶ O ¹⁶ O, ¹⁴ N ¹⁷ O ¹ H, ¹⁵ N ¹⁷ O, ¹⁴ N ¹⁸ O
2	64.0	64	⁶⁴ Ni, ⁶⁴ Zn	⁴⁶ Ca ¹⁸ O, ⁵⁰ Ti ¹⁴ N, ²³ Na ²³ Na ¹⁸ O, ⁴⁸ Ca ¹⁶ O, ⁶³ Cu ¹ H, ...
2	101.9	178	¹⁰² Ru, ¹⁰² Pd	²⁰⁴ Hg ⁺⁺ , ⁵² Cr ¹⁶ O ¹⁶ O ¹⁶ O ¹ H ¹ H, ⁵³ Cr ¹⁶ O ¹⁶ O ¹⁶ O ¹ H, ...
2	103.9	2133	¹⁰⁴ Ru, ¹⁰⁴ Pd	⁸⁷ Rb ¹⁶ O ¹ H, ⁵⁴ Cr ¹⁶ O ¹⁶ O ¹⁶ O ¹ H ¹ H, ⁶⁴ Ni ⁴⁰ Ar, ²⁰⁸ Pb ⁺⁺ , ...
2	105.9	4354	¹⁰⁶ Pd, ¹⁰⁶ Cd	¹⁰⁵ Pd ¹ H, ⁸⁸ Sr ¹⁸ O, ⁸⁸ Sr ¹⁷ O ¹ H, ⁸⁹ Y ¹⁷ O, ⁸⁹ Y ¹⁶ O ¹ H, ...
2	107.9	4281	¹⁰⁸ Pd, ¹⁰⁸ Cd	¹⁰⁷ Ag ¹ H, ⁵² Cr ⁴⁰ Ar ¹⁶ O, ⁹² Mo ¹⁶ O, ⁷⁶ Se ¹⁶ O ¹⁶ O, ⁸⁹ Y ¹⁸ O ¹ H, ...
2	109.9	2397	¹¹⁰ Pd, ¹¹⁰ Cd	⁵⁴ Cr ⁴⁰ Ar ¹⁶ O, ¹⁰⁹ Ag ¹ H, ⁷² Ge ³⁸ Ar, ⁷⁰ Ge ⁴⁰ Ar, ⁷⁴ Ge ³⁶ Ar, ...
3	19.0	261	¹⁹ F	H ₃ O ⁺
3	23.0	533	²³ Na	⁴⁶ Ca ⁺⁺ , ⁷ Li ¹⁶ O, ⁶ Li ¹⁶ O ¹ H, ⁶ Li ¹⁷ O, ⁴⁶ Ti ⁺⁺
3	24.0	177	²⁴ Mg	¹² C ¹² C, ⁴⁸ Ca ⁺⁺ , ⁷ Li ¹⁶ O ¹ H, ⁷ Li ¹⁷ O, ¹⁰ B ¹⁴ N, ⁶ Li ¹⁸ O, ...
3	27.0	840	²⁷ Al	⁹ Be ¹⁷ O ¹ H, ⁹ Be ¹⁸ O, ¹⁰ B ¹⁶ O ¹ H, ⁹ B ¹⁸ O, ¹¹ B ¹⁶ O, ¹⁰ B ¹⁷ O, ...
3	28.0	6115	²⁸ Si	⁹ Be ¹⁸ O ¹ H, ⁵⁶ Fe ⁺⁺ , ¹¹ B ¹⁷ O, ¹⁰ B ¹⁸ O, ¹¹ B ¹⁶ O ¹ H, ...

3	29.0	876	²⁹ Si	⁵⁸ Fe ⁺⁺ , ¹¹ B ¹⁸ O, ¹¹ B ¹⁷ O ¹ H, ¹⁰ B ¹⁸ O ¹ H, ¹³ C ¹⁶ O, ¹² C ¹⁷ O, ...
3	30.0	321	³⁰ Si	¹¹ B ¹⁸ O ¹ H, ¹² C ¹⁸ O, ¹³ C ¹⁷ O, ¹³ C ¹⁶ O ¹ H, ¹² C ¹⁶ O ¹ H ¹ H, ...
3	31.0	82	³¹ P	¹⁴ N ¹⁶ O ¹ H, ¹⁵ N ¹⁵ N ¹ H, ¹³ C ¹⁸ O, ¹² C ¹⁸ O ¹ H, ¹³ C ¹⁷ O ¹ H, ...
3	32.0	341	³² S	¹⁶ O ¹⁶ O, ¹⁴ N ¹⁷ O ¹ H, ¹⁵ N ¹⁷ O, ¹⁴ N ¹⁸ O
3	64.0	73	⁶⁴ Ni, ⁶⁴ Zn	⁴⁶ Ca ¹⁸ O, ⁵⁰ Ti ¹⁴ N, ²³ Na ²³ Na ¹⁸ O, ⁴⁸ Ca ¹⁶ O, ⁶³ Cu ¹ H, ...
3	65.9	65	⁶⁶ Zn	²⁴ Mg ⁴⁰ Ar ¹ H, ⁴⁸ Ca ¹⁸ O ¹ H, ³³ S ¹⁶ O ¹⁶ O ¹ H, ¹⁰ B ¹⁶ O ⁴⁰ Ar, ...
3	137.9	58	¹³⁸ Ba, ¹³⁸ La, ¹³⁸ Ce	⁹⁸ Ru ³⁶ Ar, ¹⁰⁰ Mo ³⁸ Ar, ¹⁰² Ru ³⁶ Ar, ¹²⁰ Sn ¹⁸ O, ¹²¹ Sb ¹⁷ O, ...
3	208.0	51	²⁰⁸ Pb	¹⁶⁸ Er ⁴⁰ Ar, ¹⁶⁸ Yb ⁴⁰ Ar, ¹⁹² Os ¹⁶ O, ²⁰⁷ Pb ¹ H, ¹⁷¹ Yb ³⁷ Cl, ...
4	19.0	193	¹⁹ F	H ₃ O ⁺
4	23.0	497	²³ Na	⁴⁶ Ca ⁺⁺ , ⁷ Li ¹⁶ O, ⁶ Li ¹⁶ O ¹ H, ⁶ Li ¹⁷ O, ⁴⁶ Ti ⁺⁺
4	24.0	149	²⁴ Mg	¹² C ¹² C, ⁴⁸ Ca ⁺⁺ , ⁷ Li ¹⁶ O ¹ H, ⁷ Li ¹⁷ O, ¹⁰ B ¹⁴ N, ⁶ Li ¹⁸ O, ...
4	27.0	76	²⁷ Al	⁹ Be ¹⁷ O ¹ H, ⁹ Be ¹⁸ O, ¹⁰ B ¹⁶ O ¹ H, ⁹ B ¹⁸ O, ¹¹ B ¹⁶ O, ¹⁰ B ¹⁷ O, ...
4	29.0	912	²⁹ Si	⁵⁸ Fe ⁺⁺ , ¹¹ B ¹⁸ O, ¹¹ B ¹⁷ O ¹ H, ¹⁰ B ¹⁸ O ¹ H, ¹³ C ¹⁶ O, ¹² C ¹⁷ O, ...
4	30.0	279	³⁰ Si	¹¹ B ¹⁸ O ¹ H, ¹² C ¹⁸ O, ¹³ C ¹⁷ O, ¹³ C ¹⁶ O ¹ H, ¹² C ¹⁶ O ¹ H ¹ H, ...
4	31.0	4798	³¹ P	¹⁴ N ¹⁶ O ¹ H, ¹⁵ N ¹⁵ N ¹ H, ¹³ C ¹⁸ O, ¹² C ¹⁸ O ¹ H, ¹³ C ¹⁷ O ¹ H, ...
4	32.0	1427	³² S	¹⁶ O ¹⁶ O, ¹⁴ N ¹⁷ O ¹ H, ¹⁵ N ¹⁷ O, ¹⁴ N ¹⁸ O
4	34.0	102	³⁴ S	¹⁵ N ¹⁸ O ¹ H, ¹⁶ O ¹⁷ O ¹ H, ¹³ C ¹⁸ O ¹ H ¹ H, ¹⁷ O ¹⁷ O, ¹⁶ O ¹⁸ O, ³³ S ¹ H
4	47.0	127	⁴⁷ Ti	³⁰ Si ¹⁷ O, ²⁹ Si ¹⁸ O, ¹² C ³⁵ Cl, ³³ S ¹⁴ N, ⁴⁶ Ca ¹ H, ⁷ Li ⁴⁰ Ar, ...
4	48.0	65	⁴⁸ Ca, ⁴⁸ Ti	³⁰ Si ¹⁸ O, ¹² C ¹² C ¹² C ¹² C, ¹² C ³⁶ Ar, ¹⁴ N ¹⁶ O ¹⁸ O, ...
4	56.0	360	⁵⁶ Fe	⁵⁵ Mn ¹ H, ⁴⁰ Ar ¹⁶ O, ⁴⁰ Ar ¹⁵ N ¹ H, ³⁸ Ar ¹⁸ O, ³⁸ Ar ¹⁷ O ¹ H, ...
4	63.0	137	⁶³ Cu	⁴⁶ Ca ¹⁷ O, ⁴⁹ Ti ¹⁴ N, ⁴⁸ Ca ¹⁵ N, ⁴⁴ Ca ¹⁸ O ¹ H, ⁴⁶ Ca ¹⁶ O ¹ H, ...
4	64.0	191	⁶⁴ Ni, ⁶⁴ Zn	⁴⁶ Ca ¹⁸ O, ⁵⁰ Ti ¹⁴ N, ²³ Na ²³ Na ¹⁸ O, ⁴⁸ Ca ¹⁶ O, ⁶³ Cu ¹ H, ...
4	64.9	68	⁶⁵ Cu	³⁶ Ar ¹⁴ N ¹⁴ N ¹ H, ¹² C ¹⁶ O ³⁷ Cl, ¹³⁰ Ba ⁺⁺ , ⁴⁸ Ca ¹⁷ O, ...
4	65.9	127	⁶⁶ Zn	²⁴ Mg ⁴⁰ Ar ¹ H, ⁴⁸ Ca ¹⁸ O ¹ H, ³³ S ¹⁶ O ¹⁶ O ¹ H, ¹⁰ B ¹⁶ O ⁴⁰ Ar, ...
4	67.9	70	⁶⁸ Zn	¹¹ B ⁴⁰ Ar ¹⁷ O, ¹⁰ B ⁴⁰ Ar ¹⁸ O, ³⁶ Ar ¹⁸ O ¹⁸ O, ³⁶ Ar ¹⁶ O ¹⁶ O, ...
4	103.9	219	¹⁰⁴ Ru, ¹⁰⁴ Pd	⁸⁷ Rb ¹⁶ O ¹ H, ⁵⁴ Cr ¹⁶ O ¹⁶ O ¹⁶ O ¹ H ¹ H, ⁶⁴ Ni ⁴⁰ Ar, ²⁰⁸ Pb ⁺⁺ , ...
4	105.9	577	¹⁰⁶ Pd, ¹⁰⁶ Cd	¹⁰⁵ Pd ¹ H, ⁸⁸ Sr ¹⁸ O, ⁸⁸ Sr ¹⁷ O ¹ H, ⁸⁹ Y ¹⁷ O, ⁸⁹ Y ¹⁶ O ¹ H, ...
4	107.9	581	¹⁰⁸ Pd, ¹⁰⁸ Cd	¹⁰⁷ Ag ¹ H, ⁵² Cr ⁴⁰ Ar ¹⁶ O, ⁹² Mo ¹⁶ O, ⁷⁶ Se ¹⁶ O ¹⁶ O, ⁸⁹ Y ¹⁸ O ¹ H, ...
4	109.9	252	¹¹⁰ Pd, ¹¹⁰ Cd	⁵⁴ Cr ⁴⁰ Ar ¹⁶ O, ¹⁰⁹ Ag ¹ H, ⁷² Ge ³⁸ Ar, ⁷⁰ Ge ⁴⁰ Ar, ⁷⁴ Ge ³⁶ Ar, ...

^a All interferences are positively charged ions unless otherwise noted.