

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Combined hydrophilic interaction liquid chromatography-scanning field asymmetric waveform ion mobility spectrometry-time-of-flight mass spectrometry for untargeted metabolomics

Katarzyna M. Szykuła, Joris Meurs, Matthew A. Turner, Colin S. Creaser,
James C. Reynolds

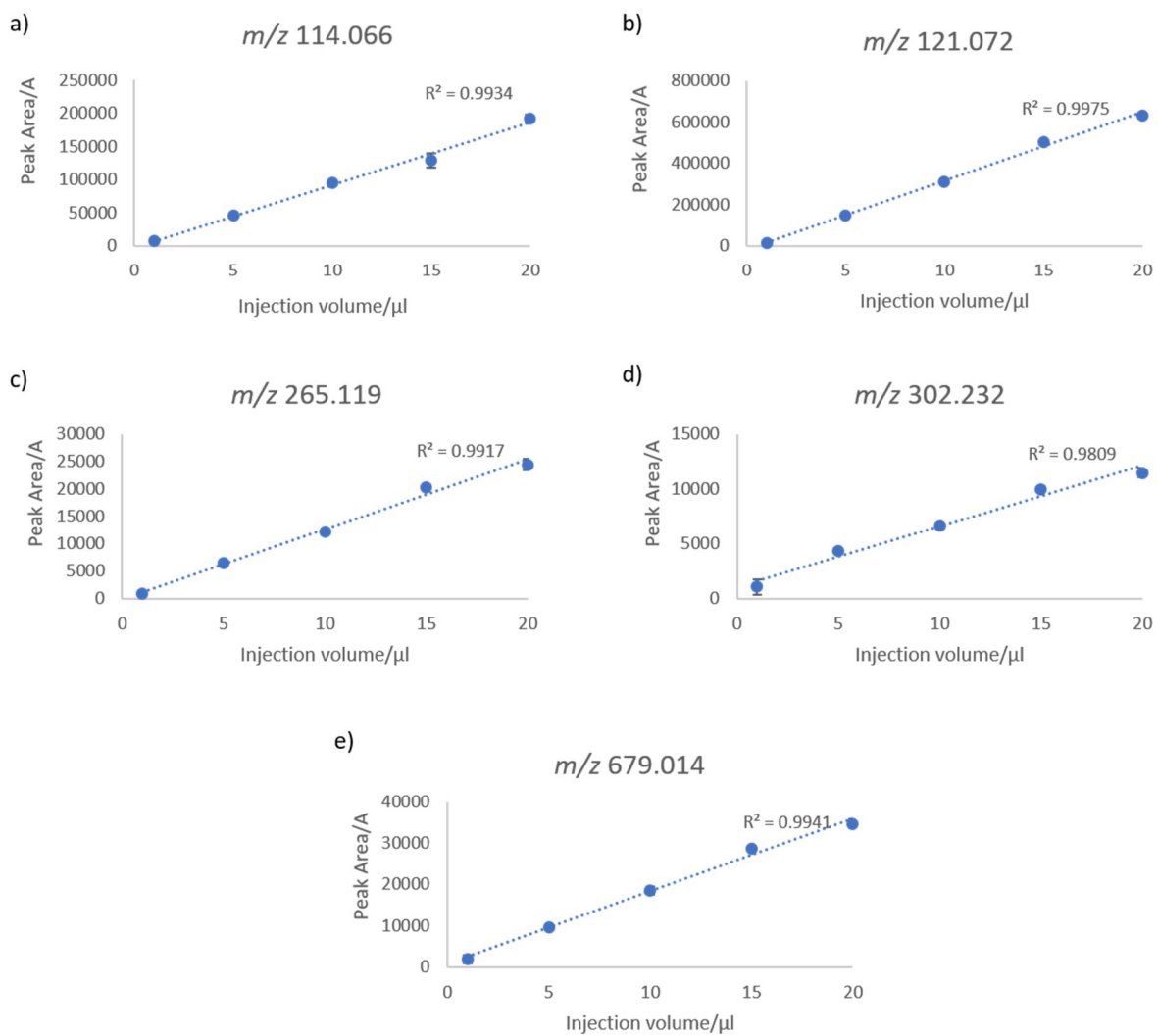


Fig. S1 Calibration graphs for selected ions for pooled urine sample. Injection volume range 1 – 20 μl in triplicates

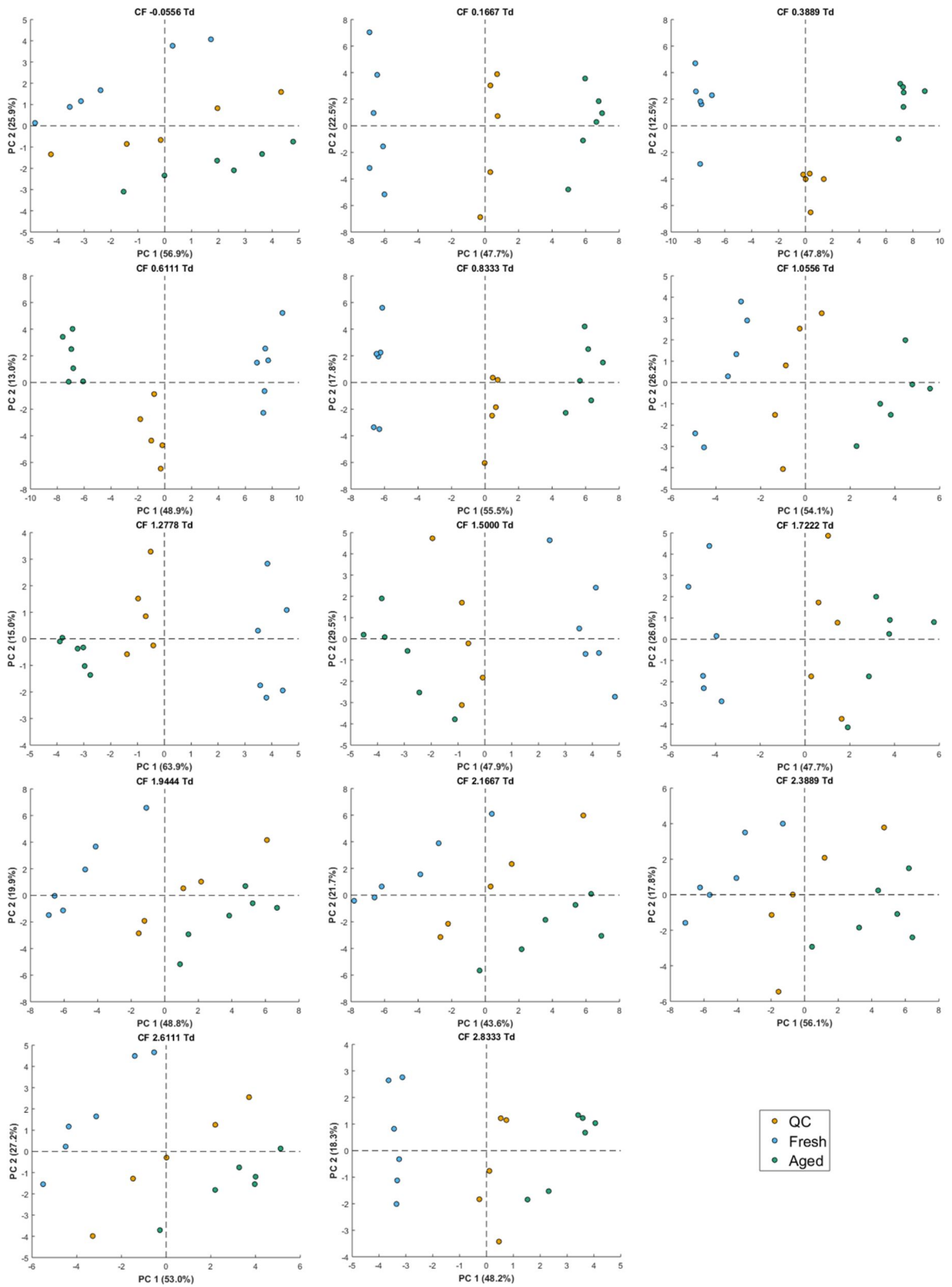


Fig. S2 PCA plots of urine samples containing fresh (blue), aged (green) and quality control samples (orange) at selected CF values

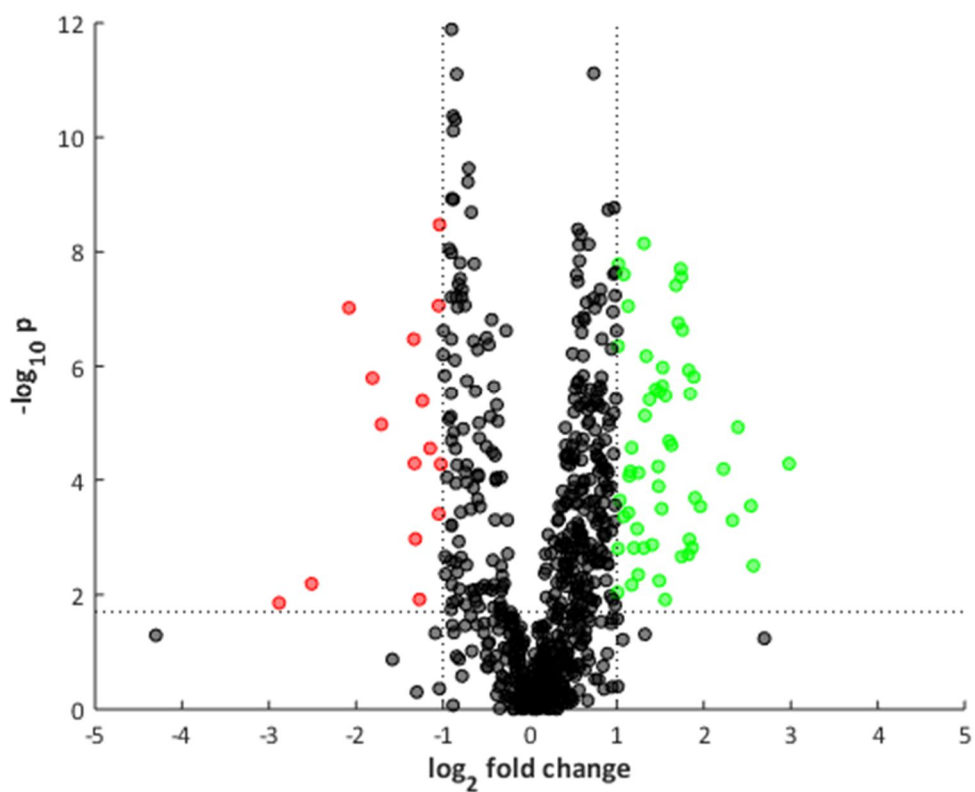


Fig. S3 Volcano plot of urine samples presenting ions with significant change in abundance between fresh and aged urine samples

Table S1 Ions with significant and at least two-fold change in abundance between fresh and aged urine samples

Mass measured	Retention time [min]	Median Fold change	p-value	0.011	CF (Td)
104.1943	9.02	3.04	2.08E-05	0.014	0.39
108.081	8.02	3.57	1.1E-03	0.018	-0.28
110.055	6.54	2.29	1.5E-03	0.038	-0.06
114.0664	3.41	2.80	5.7E-03	0.007	0.83
116.1074	5.16	2.05	2.2E-04	0.029	-0.28
121.0718	1.55	3.54	2.0E-03	0.005	0.83
121.1644	1.55	3.59	3.11E-06	0.009	-0.28
124.0723	5.28	3.09	2.47E-05	0.007	-0.06
131.1174	8.32	5.25	1.21E-05	0.020	-0.06
136.0395	1.94	2.01	9.1E-03	0.036	0.17
151.1444	8.75	2.37	4.5E-03	0.008	0.83
156.0777	8.10	0.42	4.13E-06	0.009	0.39
157.0611	8.40	0.31	1.07E-05	0.004	0.39
160.0967	7.65	0.48	8.79E-08	0.021	0.17
162.1119	8.18	0.41	1.2E-02	0.017	1.94
166.0723	2.95	2.23	7.11E-05	0.001	1.50
167.0571	1.25	2.12	2.48 E-08	0.006	1.94
181.0722	0.99	2.59	3.93E-06	0.008	2.17
185.1281	2.41	2.94	3.70E-06	0.014	2.61
191.1773	8.67	2.38	7.47E-05	0.019	0.83
196.0962	1.54	3.35	2.2E-03	0.011	-0.06
203.1468	7.94	0.49	5.31E-05	0.002	-0.06
207.1095	2.41	3.69	1.54E-06	0.023	2.17
212.0928	5.97	0.17	6.4E-03	0.022	-0.06
218.0213	3.38	0.13	1.4E-02	0.015	0.17
227.1264	3.41	2.19	8.94E-08	0.002	1.06
227.1789	7.96	2.48	7.12E-09	0.018	-0.28
229.1628	7.44	0.40	5.15E-05	0.010	2.61
229.2843	7.41	0.45	2.82E-05	0.004	0.17
231.2002	8.61	2.02	4.47E-07	0.014	0.61
241.1547	7.58	0.48	3.9E-04	0.003	0.39
247.0956	1.54	2.03	1.65E-08	0.003	0.17
247.1461	5.26	2.53	6.66E-07	0.007	-0.06
248.1454	7.84	0.40	3.37E-07	0.002	0.17
257.1155	2.41	2.88	1.06E-06	0.001	1.94
262.1305	8.45	0.49	3.36E-09	0.013	0.17
269.1204	1.43	2.35	7.15E-04	0.010	1.94
283.1050	2.19	2.19	3.74E-04	0.018	1.72
286.1029	1.99	0.40	1.07E-03	0.012	0.39
286.2034	5.62	2.21	8.50E-05	0.018	2.17

287.1024	4.04	2.02	1.58E-03	0.005	1.94
290.1623	8.50	0.24	9.53 E-08	0.008	0.17
298.1145	2.62	7.89	5.20E-05	0.019	1.94
300.2018	2.62	2.65	1.35E-03	0.004	2.39
300.2176	5.32	2.81	2.87E-06	0.011	2.39
302.2028	5.36	2.78	5.86E-05	0.015	2.39
302.2331	4.99	2.86	3.19E-04	0.010	2.17
310.2031	5.41	3.73	2.05E-04	0.001	1.94
312.1335	2.85	3.20	3.85E-08	0.013	2.17
312.2202	5.51	4.68	6.43E-05	0.028	2.39
330.2343	5.91	2.94	1.22E-02	0.011	0.61
344.2331	2.99	2.50	7.50E-06	0.018	2.83
358.2600	5.44	5.03	5.08E-04	0.009	2.17
378.1819	4.03	2.25	2.75E-05	0.022	2.39
388.2567	3.25	3.89	2.90E-04	0.002	2.83
391.2341	2.40	3.35	2.73E-08	0.009	2.39
441.2404	2.40	2.79	1.29E-04	0.004	1.94
451.1645	2.723	2.73	2.55E-06	0.006	1.94
476.3110	3.72	3.33	1.98E-08	0.007	2.83
515.2209	2.79	2.87	2.24E-06	0.023	1.50
529.2289	4.01	5.94	3.14E-03	0.003	2.17
550.2043	2.20	3.55	1.17E-06	0.002	1.94
565.2099	2.20	3.27	1.76E-07	0.016	1.72
576.1310	3.37	2.48	1.55E-03	0.021	1.94
576.1669	3.42	2.25	6.76E-03	0.013	1.72
586.1524	4.02	3.64	1.51E-03	0.016	1.72
597.0168	6.10	2.11	4.35E-04	0.009	2.17
850.2716	4.01	5.82	2.83E-04	0.006	1.72
909.5473	4.37	3.37	2.32E-07	0.022	1.50
1194.1103	1.11	0.28	1.61E-06	0.011	1.06