

Supporting Information

Detection of firearm discharge residue from skin swabs using Trapped Ion Mobility Spectrometry coupled to Mass Spectrometry

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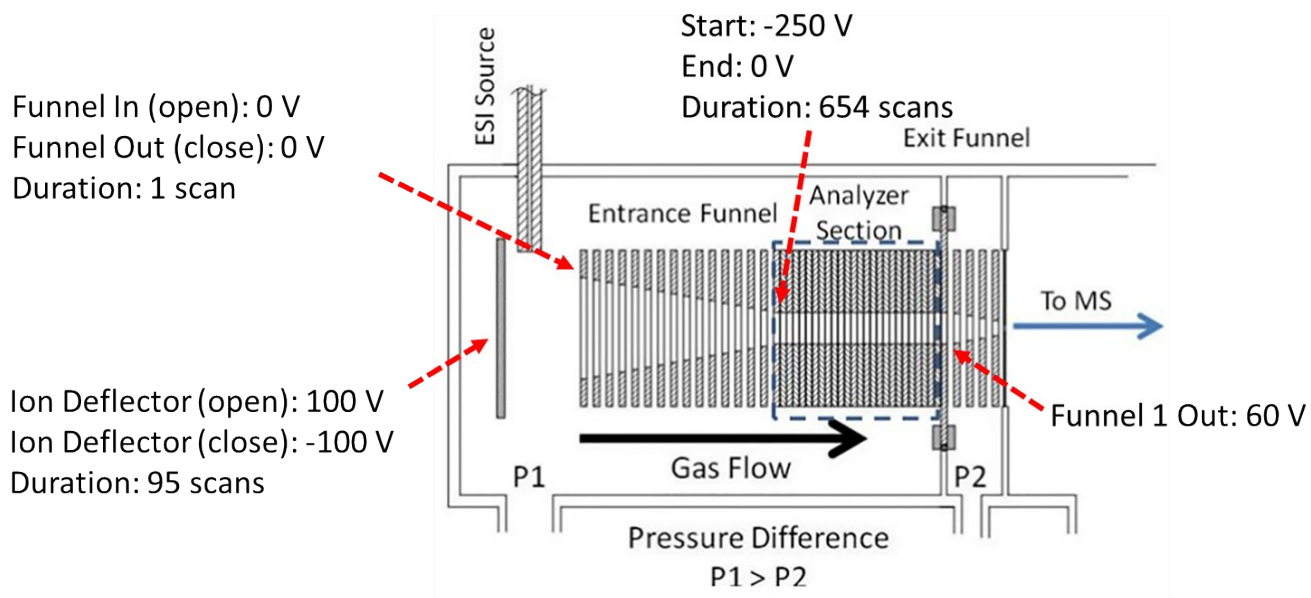


Figure S1. Scheme of the TIMS cell.

Table S1. Geometry coordinates of 15-5 Crown Ether and Copper optimized structure

Element	x	y	z
O	-0.363222	2.149494	0.410556
O	-2.238633	0.406092	-0.545466
O	2.026119	1.055537	-0.324598
O	-1.012784	-1.984866	-0.112281
O	1.631153	-1.566010	0.273230
C	-1.691006	2.606300	0.119546
C	0.677642	3.006118	-0.076736
C	-2.641909	1.448604	0.349619
C	2.004392	2.360136	0.266211
C	-3.017522	-0.797764	-0.532114
C	3.139948	0.247480	0.075722
C	-2.365725	-1.864943	0.337669
C	2.859702	-1.180331	-0.349581
C	-0.234267	-3.006144	0.520676
C	1.175885	-2.888228	-0.026312
H	-1.746218	2.931366	-0.927943
H	-1.948273	3.449580	0.773903
H	0.613110	3.992302	0.402132
H	0.571395	3.128127	-1.163435
H	-2.593568	1.106494	1.392781
H	-3.669064	1.764827	0.124710
H	2.828198	2.969887	-0.128549
H	2.116143	2.270758	1.355529
H	-3.055110	-1.139032	-1.570634
H	-4.040058	-0.596899	-0.190080
H	3.254473	0.298760	1.166965
H	4.060687	0.610950	-0.399578

H	-2.377445	-1.594361	1.403731
H	-2.895578	-2.819295	0.212027
H	2.762098	-1.255647	-1.441733
H	3.679363	-1.832279	-0.018587
H	-0.648007	-3.995993	0.287278
H	-0.242769	-2.860779	1.609868
H	1.829349	-3.632955	0.447508
H	1.180084	-3.047352	-1.113575
Cu	0.018527	0.006283	-0.135932

Table S2. Geometry coordinates of 15-5 Crown Ether and Potassium optimized structure

Element	x	y	z
O	0.068157	-2.071720	-0.371500
O	-2.351370	-0.876620	0.443570
O	2.421956	-0.704988	0.207586
O	-1.494283	1.846721	0.046693
O	1.269991	1.757224	-0.298354
C	-1.144963	-2.818096	-0.284232
C	1.270821	-2.799544	-0.127861
C	-2.295464	-1.873100	-0.583179
C	2.443284	-1.924787	-0.539724
C	-3.253803	0.210551	0.205863
C	3.186229	0.355841	-0.374632
C	-2.643878	1.331231	-0.628316
C	2.638167	1.694204	0.094974
C	-0.795818	2.857487	-0.687145
C	0.607274	3.006681	-0.123416
H	-1.258338	-3.257281	0.719236
H	-1.146783	-3.635027	-1.020518
H	1.295288	-3.722584	-0.725267
H	1.337885	-3.082850	0.935110
H	-2.137499	-1.408361	-1.565491
H	-3.238514	-2.437565	-0.606385
H	3.384022	-2.467159	-0.366201
H	2.361368	-1.697383	-1.611031
H	-3.526550	0.590948	1.195429
H	-4.169704	-0.149599	-0.282449
H	3.108206	0.305185	-1.468580
H	4.245037	0.266866	-0.092780

H	-2.349973	0.971290	-1.625352
H	-3.398373	2.121621	-0.761224
H	2.731139	1.802401	1.188724
H	3.219792	2.502111	-0.372548
H	-1.330155	3.815700	-0.617303
H	-0.729682	2.567345	-1.744831
H	1.131790	3.806270	-0.666650
H	0.575482	3.284528	0.943031
K	0.026782	-0.001275	1.400376

Table S3. Geometry coordinates of 15-5 Crown Ether, Potassium, and 15-5 Crown Ether optimized structure

Element	x	y	z
O	1.697400	-1.136800	-2.248700
O	1.538100	-2.517300	0.292900
O	2.067800	1.547700	-1.560400
O	2.442600	-0.321400	1.815700
O	1.836400	2.304400	1.095700
C	2.398000	-2.355200	-2.015200
C	2.412600	-0.232100	-3.087100
C	1.657000	-3.175400	-0.968200
C	1.861100	1.170000	-2.911300
C	2.688900	-2.581900	1.130500
C	1.752600	2.897900	-1.240400
C	2.477700	-1.653800	2.310900
C	2.363700	3.199400	0.116600
C	2.367400	0.690900	2.807900
C	2.733200	2.016300	2.165400
H	3.424000	-2.129900	-1.688100
H	2.465800	-2.946800	-2.942900
H	2.328400	-0.537200	-4.141700
H	3.476600	-0.231800	-2.810100
H	0.629500	-3.355600	-1.294600
H	2.162100	-4.146500	-0.850900
H	2.395100	1.849600	-3.594600
H	0.790800	1.207000	-3.167400
H	3.590600	-2.269900	0.586500
H	2.836400	-3.612300	1.490200
H	0.663100	3.045800	-1.238700

H	2.192700	3.586800	-1.979200
H	1.538700	-1.899600	2.830900
H	3.310400	-1.778100	3.020900
H	3.452100	3.070700	0.048900
H	2.156200	4.244200	0.395400
H	3.082200	0.494500	3.622600
H	1.358500	0.723100	3.247900
H	2.704000	2.813500	2.924900
H	3.758500	1.946200	1.777100
K	-0.000800	-0.066700	0.000400
O	-2.447100	-0.286200	-1.817100
O	-1.574900	-2.496200	-0.296300
O	-1.804000	2.328100	-1.092200
O	-1.712200	-1.118400	2.248300
O	-2.044600	1.571300	1.563300
C	-2.502000	-1.617300	-2.313600
C	-2.354800	0.725600	-2.808300
C	-2.726400	-2.543600	-1.134200
C	-2.701700	2.055900	-2.165400
C	-1.703400	-3.154700	0.963600
C	-2.321400	3.227800	-0.112200
C	-2.431600	-2.325300	2.012200
C	-1.713600	2.918000	1.244400
C	-2.413200	-0.204500	3.088800
C	-1.841900	1.189700	2.913800
H	-1.567000	-1.876400	-2.834400
H	-3.336800	-1.728600	-3.023400
H	-3.071000	0.540600	-3.624600
H	-1.344700	0.742800	-3.246500

H	-3.623700	-2.219600	-0.589900
H	-2.888400	-3.571400	-1.495100
H	-2.657000	2.853600	-2.923700
H	-3.729300	2.002000	-1.780900
H	-0.678700	-3.351100	1.289600
H	-2.223200	-4.117800	0.844800
H	-3.411100	3.110900	-0.044600
H	-2.102400	4.270600	-0.389700
H	-3.454000	-2.083200	1.685500
H	-2.508700	-2.917600	2.938700
H	-0.622400	3.053300	1.242700
H	-2.145600	3.611200	1.983800
H	-2.331800	-0.512200	4.143000
H	-3.477500	-0.188600	2.813500
H	-2.365700	1.876200	3.598000
H	-0.771000	1.211500	3.169000

Table S4. Geometry coordinates of 15-5 Crown Ether, Barium, and Nitrate optimized structure

Element	x	y	z
O	0.498710	2.444829	0.346501
O	2.407321	0.858152	-1.140559
O	-0.890977	0.657103	1.973853
O	2.019017	-1.606939	0.015291
O	-0.375139	-1.964382	1.259420
C	1.917142	2.467986	0.602132
C	-0.327340	2.882057	1.449914
C	2.618387	2.196782	-0.669072
C	-1.451449	1.947458	1.651787
C	3.495584	-0.048198	-0.875126
C	-1.883751	-0.375084	2.173128
C	2.997155	-1.426425	-1.021232
C	-1.163596	-1.637487	2.421066
C	1.511918	-2.932950	0.253816
C	0.733785	-2.840962	1.502208
H	2.101027	1.725985	1.365939
H	2.133483	3.487576	0.878765
H	-0.726770	3.828934	1.132979
H	0.286457	2.892626	2.335192
H	2.179576	2.828258	-1.427432
H	3.672546	2.371745	-0.548610
H	-1.952810	2.273089	2.545506
H	-2.146668	1.840544	0.808689
H	3.818907	0.106994	0.139489
H	4.205240	0.148445	-1.661553
H	-2.565061	-0.382047	1.310526
H	-2.373920	-0.122190	3.096163

H	2.529225	-1.553577	-1.987172
H	3.814045	-2.094988	-0.825221
H	-0.486508	-1.498412	3.246825
H	-1.888307	-2.425077	2.516978
H	2.353909	-3.573238	0.441703
H	0.876331	-3.240029	-0.564719
H	0.330431	-3.800285	1.770431
H	1.357404	-2.347829	2.231188
Ba	-0.082254	0.001057	-0.503341
N	-3.027298	-0.168336	-1.739530
O	-2.006943	-0.660832	-2.327976
O	-4.150380	-0.234346	-2.200832
O	-2.802638	0.413108	-0.597394

Table S5. Geometry coordinates of 15-5 Crown Ether, Barium, and 15-5 Crown Ether optimized structure

Element	x	y	z
O	-2.051510	-2.137849	0.479903
O	-1.439204	-1.290299	-2.175914
O	-1.850529	0.019578	2.118204
O	-1.906771	1.382239	-1.688447
O	-1.688792	2.399636	0.856937
C	-2.728500	-2.722875	-0.640780
C	-2.874203	-2.074052	1.654756
C	-1.820058	-2.642778	-1.858029
C	-2.165808	-1.246217	2.713018
C	-2.395883	-0.565201	-2.968199
C	-1.791952	1.193440	2.939839
C	-1.974731	0.890787	-3.033583
C	-2.362805	2.341600	2.123306
C	-1.894495	2.809028	-1.518102
C	-2.438601	3.117494	-0.135369
H	-3.677149	-2.193718	-0.808486
H	-2.960702	-3.777943	-0.436061
H	-3.066451	-3.085901	2.037850
H	-3.834322	-1.606188	1.397802
H	-0.884375	-3.171869	-1.660208
H	-2.310669	-3.110804	-2.720759
H	-2.835958	-1.113519	3.571288
H	-1.244607	-1.735549	3.053326
H	-3.392849	-0.638616	-2.517028
H	-2.432531	-0.987633	-3.981154
H	-0.752066	1.384161	3.238831

H	-2.393162	1.064383	3.847856
H	-1.000525	1.001393	-3.531413
H	-2.723352	1.452277	-3.607436
H	-3.432864	2.165816	1.952963
H	-2.245000	3.290145	2.665408
H	-2.543997	3.286231	-2.262950
H	-0.874044	3.191074	-1.643494
H	-2.382666	4.199008	0.050947
H	-3.490582	2.807863	-0.081631
Ba	-0.086228	0.004943	-0.027553
O	1.224231	-1.658205	1.908551
O	1.471168	-2.324724	-0.814225
O	2.051950	1.011242	1.799478
O	2.221479	0.147009	-1.972156
O	1.374016	2.420419	-0.569469
C	1.556152	-2.989789	1.476818
C	1.974536	-1.072627	2.984891
C	2.303489	-2.978917	0.154358
C	2.862928	0.059136	2.499662
C	2.026494	-2.233757	-2.136813
C	2.766947	2.204821	1.452205
C	2.955566	-1.042351	-2.289970
C	1.858882	3.084684	0.608629
C	3.032764	1.325051	-2.024717
C	2.146812	2.534159	-1.775029
H	0.606851	-3.522760	1.361445
H	2.152467	-3.504712	2.238683
H	2.587051	-1.830293	3.487047
H	1.247088	-0.689879	3.709556

H	3.265344	-2.457104	0.249972
H	2.499849	-4.012994	-0.162521
H	3.341453	0.534897	3.367658
H	3.653597	-0.310178	1.830269
H	1.170751	-2.126966	-2.809539
H	2.557226	-3.159758	-2.392506
H	3.686525	1.938975	0.912794
H	3.053055	2.749456	2.363483
H	3.829489	-1.121469	-1.627224
H	3.319602	-0.997227	-3.326179
H	0.964185	3.354053	1.178002
H	2.385026	4.008156	0.336882
H	3.495616	1.423759	-3.017420
H	3.838567	1.248151	-1.281222
H	2.757203	3.445166	-1.755431
H	1.422186	2.631086	-2.590673

Table S6. Geometry coordinates of 15-5 Crown Ether, Lead, and Nitrate optimized structure

Element	x	y	z
O	-1.740927	0.362579	1.030866
O	-0.506503	2.417277	-0.437231
O	-0.304171	-1.903387	0.644663
O	1.974784	1.067106	-0.630733
O	1.849713	-1.709853	-0.993388
C	-1.754671	1.704244	1.549764
C	-1.733569	-0.652172	2.054151
C	-1.657072	2.682893	0.387555
C	-1.516165	-2.009634	1.410558
C	0.734722	3.001905	-0.000928
C	0.256246	-3.120583	0.119293
C	1.859332	2.471185	-0.869725
C	1.729977	-2.854959	-0.144454
C	2.954034	0.390109	-1.425269
C	3.102863	-1.024933	-0.896060
H	-0.919098	1.820853	2.253645
H	-2.694332	1.877235	2.090764
H	-2.693373	-0.639436	2.585718
H	-0.923605	-0.433672	2.762408
H	-2.520434	2.581254	-0.274212
H	-1.620709	3.710721	0.768209
H	-1.393912	-2.762171	2.199844
H	-2.350595	-2.291810	0.759577
H	0.926948	2.750739	1.049611
H	0.669386	4.092494	-0.104437
H	-0.282739	-3.418994	-0.789879
H	0.160537	-3.925509	0.858307

H	1.650984	2.667468	-1.932272
H	2.794613	2.981713	-0.600183
H	2.237439	-2.657085	0.808959
H	2.190491	-3.735062	-0.614398
H	3.924768	0.899428	-1.347983
H	2.649642	0.390928	-2.482994
H	3.872303	-1.552930	-1.476542
H	3.418568	-0.986564	0.155096
N	-3.473836	-0.522741	-1.805649
O	-4.654112	-0.704187	-1.988944
O	-2.925166	0.640793	-1.908323
O	-2.672325	-1.492759	-1.483111
Pb	-0.620027	-0.112469	-1.282288

Table S7. Geometry coordinates of 15-5 Crown Ether, Lead, and 15-5 Crown Ether optimized structure

Element	x	y	z
O	-2.346863	0.137746	1.855981
O	-1.701538	-2.220601	0.450292
O	-1.333020	2.421410	0.598369
O	-0.902348	-1.526949	-2.174737
O	-1.834595	1.127711	-1.896931
C	-3.211482	-0.996776	1.955801
C	-3.014971	1.383018	2.065381
C	-2.377114	-2.242699	1.718744
C	-2.000273	2.496734	1.865764
C	-2.477192	-2.668953	-0.667706
C	-1.928920	3.095610	-0.520960
C	-1.547586	-2.776376	-1.864059
C	-2.710312	2.165197	-1.435328
C	-1.402755	-0.768257	-3.288544
C	-2.432654	0.269386	-2.875337
H	-4.028653	-0.904304	1.224927
H	-3.659234	-1.048653	2.958809
H	-3.412946	1.434548	3.089235
H	-3.860389	1.473942	1.368546
H	-1.585246	-2.303266	2.468878
H	-3.005784	-3.138817	1.794822
H	-2.485509	3.473566	1.984734
H	-1.207652	2.414139	2.615820
H	-3.307530	-1.977174	-0.863290
H	-2.897229	-3.661801	-0.453817
H	-1.099199	3.539355	-1.077968
H	-2.587046	3.901040	-0.172478

H -0.745309 -3.484979 -1.637649
H -2.102171 -3.141600 -2.736330
H -3.573296 1.715162 -0.925327
H -3.081708 2.745065 -2.292210
H -1.830079 -1.439209 -4.043056
H -0.530665 -0.272903 -3.726335
H -2.727394 0.855727 -3.757416
H -3.336171 -0.198277 -2.458196
Pb 0.008779 -0.009602 -0.014542
O 0.884506 -1.340308 2.262698
O 1.695215 -2.271681 -0.268069
O 1.794974 1.293675 1.800880
O 2.385655 -0.026947 -1.822828
O 1.346881 2.365555 -0.804526
C 1.513653 -2.623458 2.082084
C 1.355736 -0.495162 3.325631
C 2.453969 -2.640180 0.889750
C 2.383738 0.517665 2.851684
C 2.384696 -2.392989 -1.523271
C 2.666451 2.308610 1.283141
C 3.237223 -1.176300 -1.836242
C 1.899792 3.143021 0.269461
C 3.072559 1.193169 -2.111486
C 2.062175 2.325932 -2.047527
H 0.703947 -3.340585 1.916730
H 2.055678 -2.910181 2.990475
H 1.774982 -1.102115 4.136650
H 0.471174 0.023434 3.708357
H 3.298789 -1.953386 1.033986

H	2.852486	-3.656730	0.763895
H	2.658473	1.172136	3.691153
H	3.297533	0.028474	2.484970
H	1.600507	-2.497626	-2.276932
H	3.003087	-3.299373	-1.527706
H	3.555171	1.836691	0.841939
H	2.996987	2.964566	2.101013
H	4.048516	-1.043620	-1.105318
H	3.692969	-1.300895	-2.828973
H	1.046314	3.618718	0.760198
H	2.556328	3.926694	-0.128132
H	3.508690	1.154157	-3.120245
H	3.892028	1.336514	-1.392840
H	2.560768	3.285390	-2.231968
H	1.297571	2.183479	-2.817450