Electronic Supplementary Material (ESI) for Analyst.

Supplementary Information

Figure S1. (a) Representative CsI spectrum, acquired using an IM wave height of 25 V and wave velocity of 500 m/s (inset shows a zoomed-in view of the 600 – 2300 *m/z* region; intensity of the $(CsI)_3Cs^+$ peak is 3.95% of that of the Cs^+ peak). (b) Survival yield of the four $(CsI)_nCs^+$ clusters focused on in this study as a function of He cell DC voltage (normalized to the highest value observed for each cluster across these experiments), showing a typical sigmoidal curve.

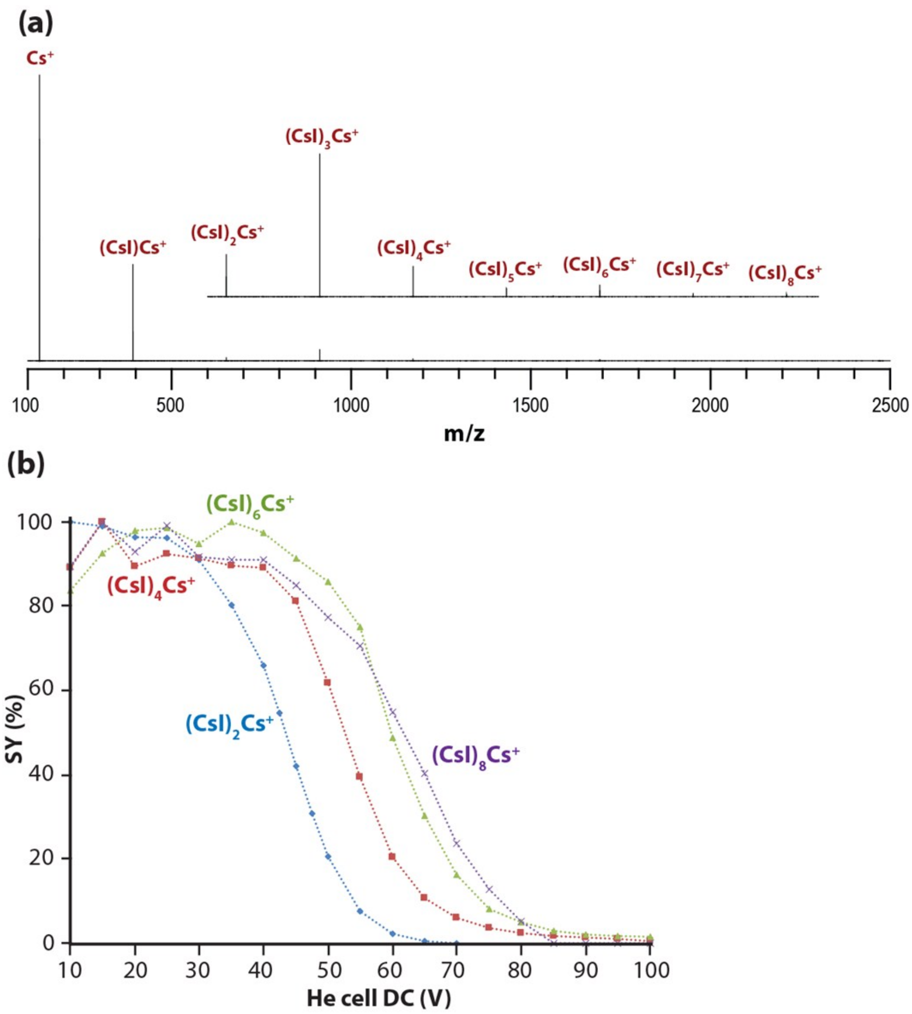
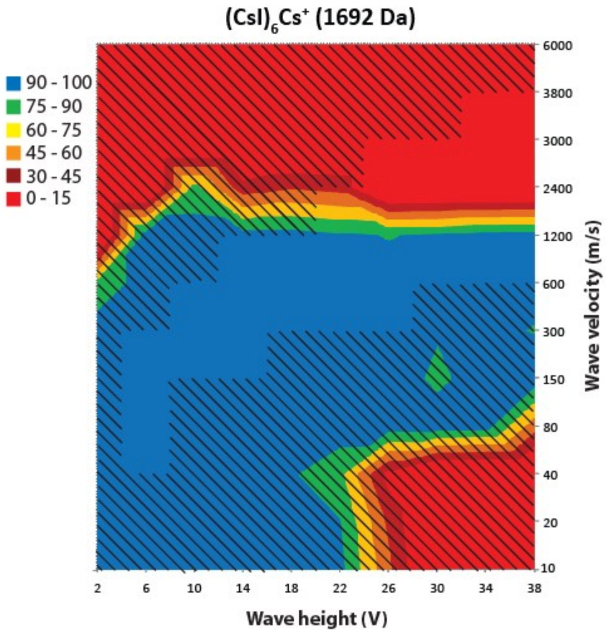


Figure S2. Contour map showing survival yields of $(CsI)_6Cs^+$ (1692 Da) and $(CsI)_8Cs^+$ (2212 Da) across a wide range of different IM T-wave conditions. Hatching indicates the range where no ion mobility separation is typically observed, *i.e.* T-wave wave velocity either too high or too low.



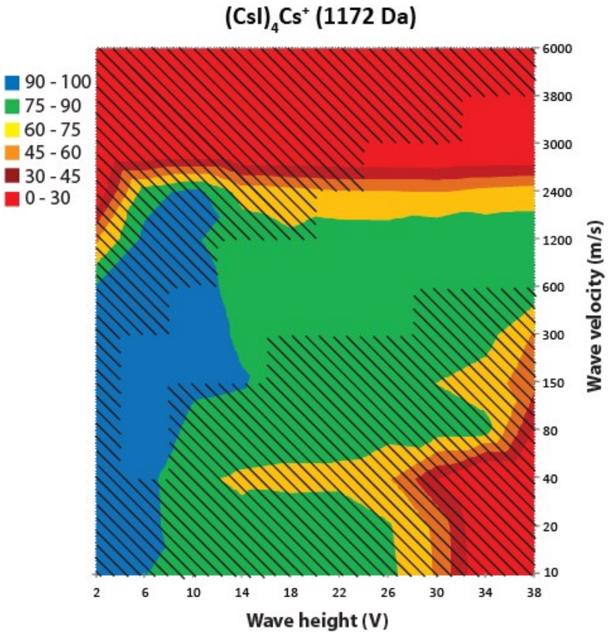
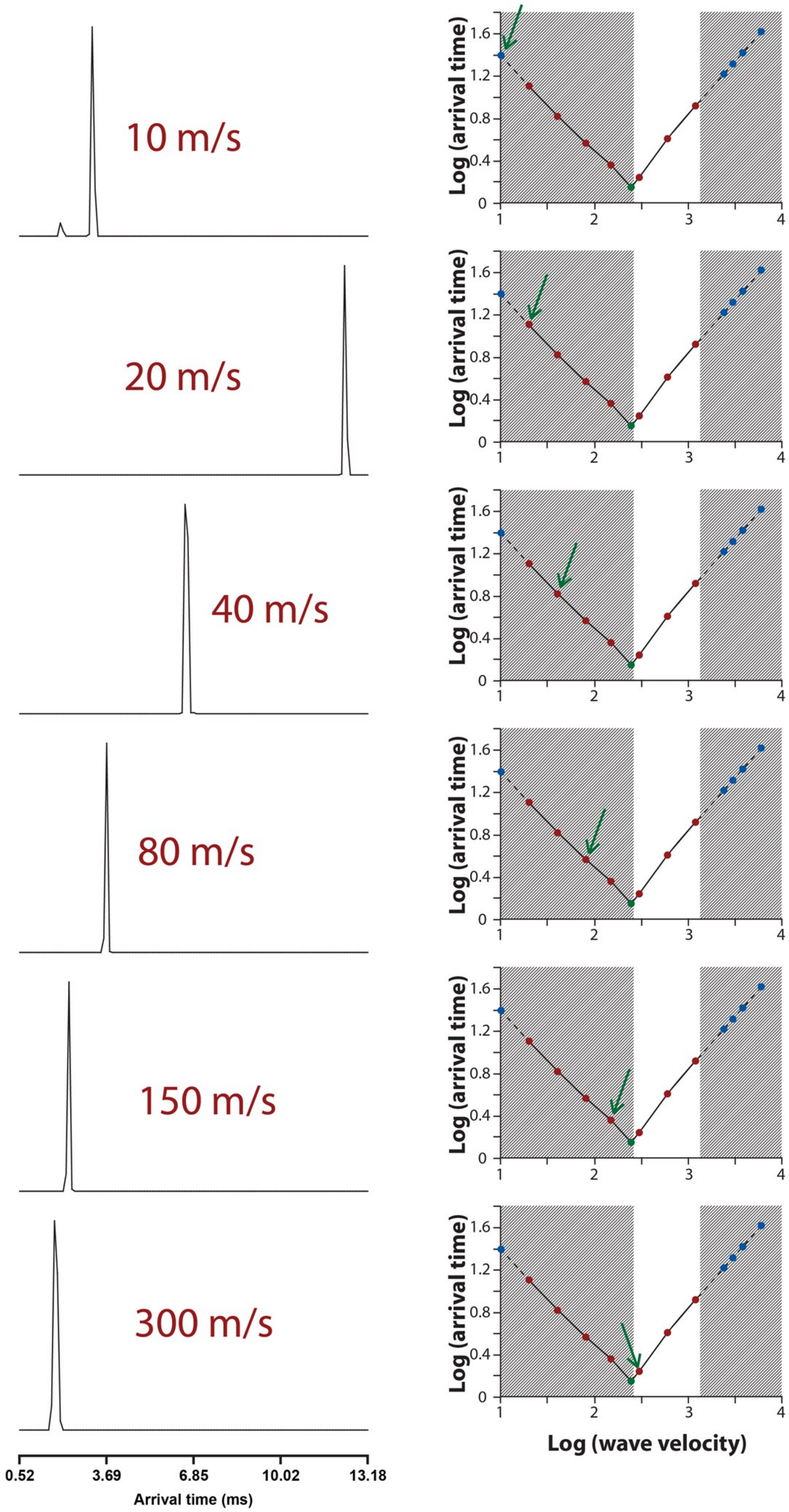
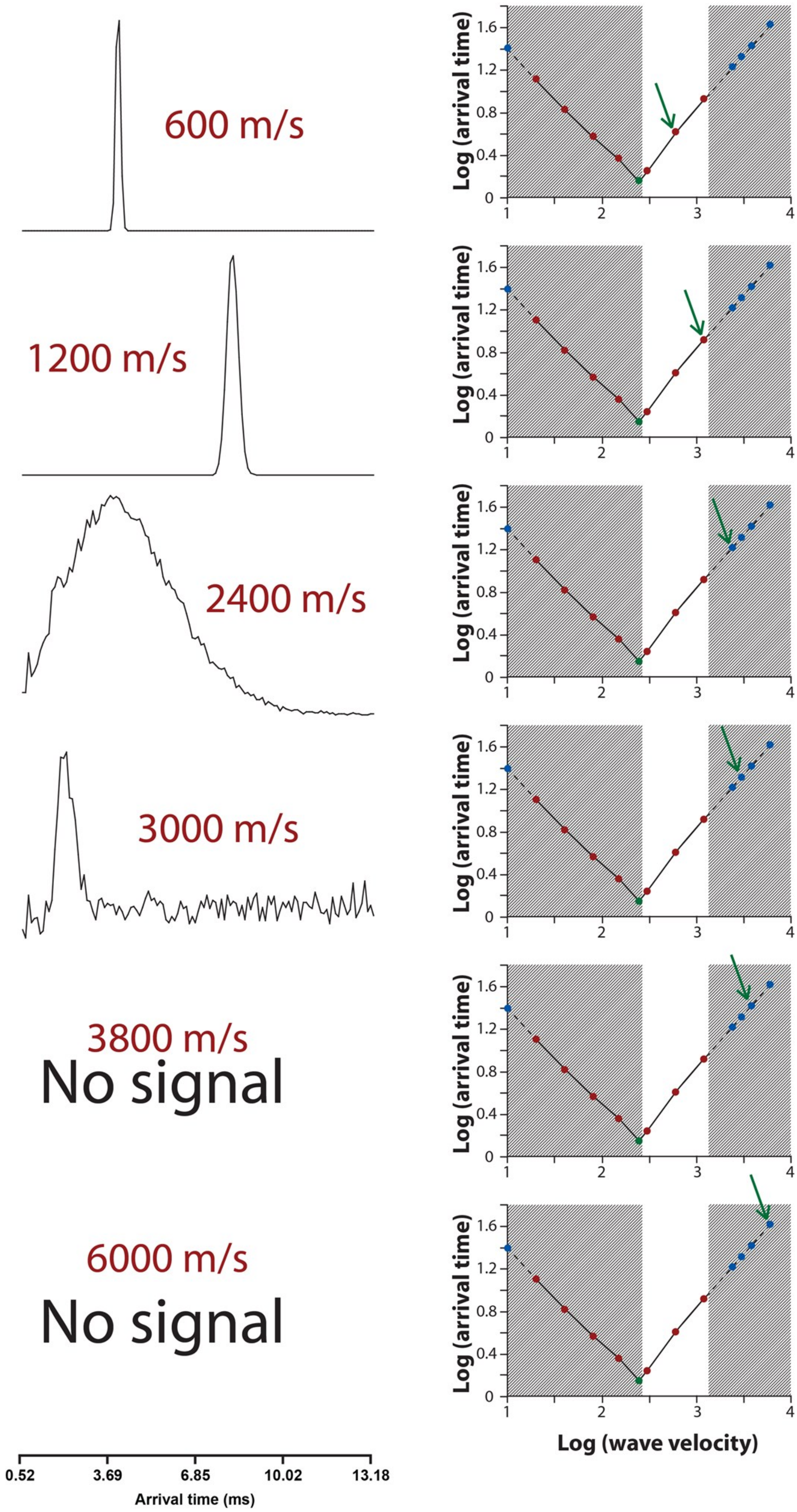


Figure S3: (left) arrival time distributions (Mobility mode) for $(CsI)_2Cs^+$ (652 Da) at an IM wave height of 22 V and various wave velocities; (right) plots of log (arrival time) versus log (wave velocity). The green arrow in each of these plots indicates the data point corresponding to the spectrum shown on the left. Arrival times could be reliably measured for data points shown in red (connected be a solid black line); those in blue (connected by a dashed black line) were calculated based on the observed data. Clear linear (in this log-log plot) trends (both with R^2 values of 0.998) in the observed data are visible in the ranges between (20 – 150 m/s) and (300 – 1200 m/s). The experiment corresponding to the data point in green (245 m/s; 1.43 ms) was not performed; rather, this is the theoretical minimum transit time calculated based on the aforementioned linear trends. As in Figures 1 and S1, hatched areas are not useful for ion mobility, either because (hatched area on the left-hand side) ions are swept through the cell by a single traveling wave (*i.e.* no mobility separation), or (hatched area on the right-hand side) arrival times could not be reliably measured (apparent 'peaks' – with very poor shape – at low arrival time for wave velocities of 2400 and 3000 m/s are due to roll-over).



10 m/s
20 m/s
40 m/s
80 m/s
150 m/s
300 m/s
0.52
3.69
6.85
10.02
13.18
Arrival time (ms)
Log (arrival time)
1.6
1.2
0.8
0.4
0
1
2
3
4
Log (wave velocity)



600 m/s
1200 m/s
2400 m/s
3000 m/s
3800 m/s
No signal
6000 m/s
No signal
0.52
3.69
6.85
10.02
13.18
Arrival time (ms)
Log (arrival time)
Log (wave velocity)

S4. Survival yields (SY), drift times (DT) and estimated effective temperature increases (based on Equations 1 and 3 in the main text) due to field heating induced by the traveling wave (ΔT_{IM}) for the four CsI clusters studied, for some of the IM wave height/velocity combinations in Figures 1 and S2. The last columns in Tables (b), (c) and (d) show the drift time(s) observed for some of the smaller clusters released by field heating (N/A: no IM separation under these conditions and thus no discernible peak; no signal: ion absent or too low in abundance to determine DT). Measured drift time (marked with an asterisk) for (wave height = 22 V/wave velocity = 10 m/s) was not reliably measured due to roll-over; as a result, this value was entered manually (highlighted in bold), assuming (based on accurately measured v_d at slightly higher wave velocities and wave height = 22 V) that $v_d = s$ under these conditions.

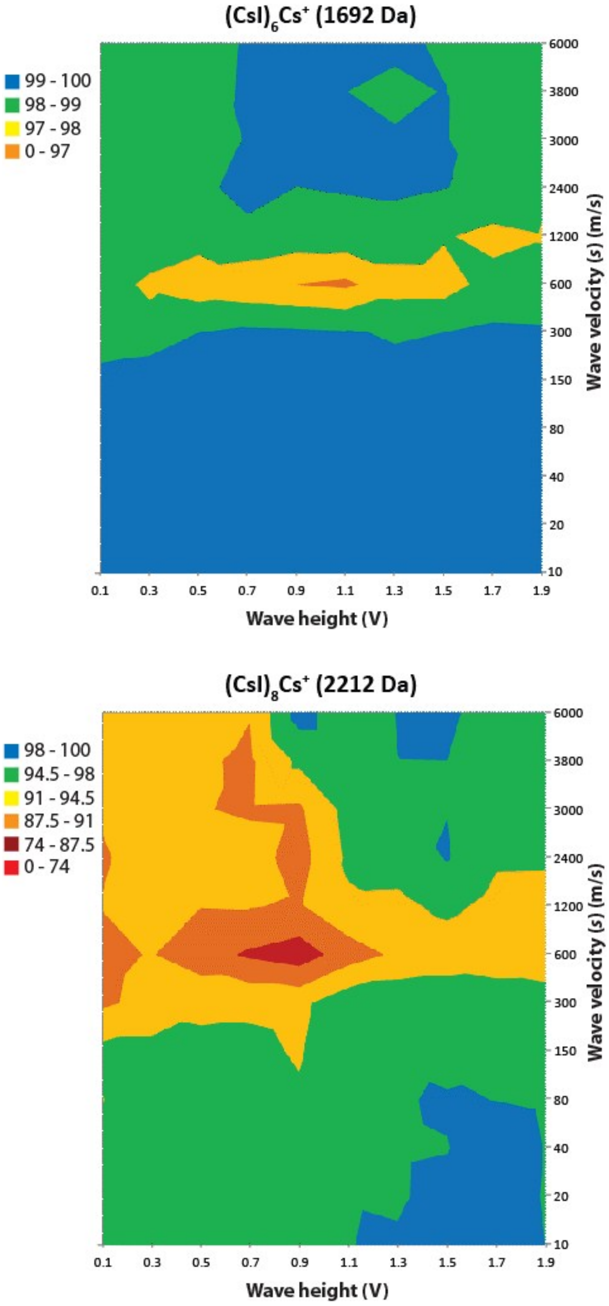
$(CsI)_2Cs^+$ (652 Da)						
WH (V)	**WV (m/s)**	**SY (%)**	**DT (ms)**	**v_d (m/s)**	**v^2 (m^2/s^2)**	**ΔT_{IM} (K)**
2	600	98.8	N/A	N/A	N/A	N/A
6	600	99.6	N/A	N/A	N/A	N/A
10	600	99.2	17.20	14.5	8721	228
14	600	98.9	9.15	27.3	16393	429
18	600	98.9	5.73	43.6	26178	684
22	10	33.2	3.20*	**10.0**	100	3
22	20	35.8	12.79	19.5	1486	39
22	40	24.7	6.73	37.1	5333	139
22	80	63.0	3.75	66.7	16164	423
22	150	85.9	2.32	107.8	42614	1114
22	300	98.3	1.76	142.0	36765	961
22	600	98.4	4.08	61.3	35800	936
22	1200	98.4	8.38	29.8	8721	228
22	2400	97.8	N/A	N/A	N/A	N/A
22	3000	91.1	N/A	N/A	N/A	N/A
22	3800	0.0	No signal	N/A	N/A	N/A
22	6000	0.0	No signal	N/A	N/A	N/A
26	600	91.2	3.09	80.9	48544	1269
30	600	91.6	2.43	102.9	61728	1614
34	600	68.5	1.98	126.3	75758	1980
38	600	30.7	1.76	142.0	85227	2228

$(CsI)_4Cs^+$ (1172 Da)							
WH (V)	**WV (m/s)**	**SY (%)**	**DT (ms)**	**v_d (m/s)**	**v^2 (m^2/s^2)**	**ΔT_{IM} (K)**	**DT652 (ms)**
2	600	91.9	N/A	N/A	N/A	N/A	N/A
6	600	92.9	N/A	N/A	N/A	N/A	N/A
10	600	94.1	N/A	N/A	N/A	N/A	N/A
14	600	86.1	9.04	27.7	16593	780	9.04
18	600	84.6	5.73	43.6	26178	1230	5.73
22	10	86.6	3.31*	**10.0**	100	5	3.20
22	20	84.8	12.90	19.4	388	18	12.79
22	40	71.5	6.84	36.5	1462	69	6.84
22	80	80.6	3.75	66.7	5333	251	3.75
22	150	77.5	2.32	107.8	16164	759	2.32
22	300	83.0	3.31	75.5	22659	1065	1.76/3.31
22	600	82.5	6.84	36.5	21930	1030	4.08
22	1200	84.1	15.32	16.3	19582	920	8.38/15.44
22	2400	62.1	N/A	N/A	N/A	N/A	N/A
22	3000	0.0	No signal	N/A	N/A	N/A	N/A
22	3800	0.0	No signal	N/A	N/A	N/A	No signal
22	6000	0.0	No signal	N/A	N/A	N/A	No signal
26	600	82.8	5.07	49.3	29586	1390	3.09
30	600	84.2	3.97	63.0	37783	1775	2.43
34	600	84.1	3.20	78.1	46875	2202	1.98
38	600	84.8	2.65	94.3	56604	2660	1.76/2.65

(CsI)$_6$Cs$^+$ (1692 Da)								
WH (V)	**WV (m/s)**	**SY (%)**	**DT (ms)**	**v_d (m/s)**	**v^2 (m^2/s^2)**	**ΔT_{IM} (K)**	**DT652 (ms)**	**DT1172 (m/s)**
2	600	79.7	N/A	N/A	N/A	N/A	N/A	N/A
6	600	97.0	N/A	N/A	N/A	N/A	N/A	N/A
10	600	98.7	N/A	N/A	N/A	N/A	7.17/17.53	N/A
14	600	98.6	20.73	12.1	7236	491	9.26/15.66	14-21
18	600	98.6	12.90	19.4	11628	789	5.84	9.81/13.01
22	10	94.1	3.31*	**10.0**	100	7	3.20	3.31
22	20	90.9	12.90	19.4	388	26	12.79	12.90
22	40	78.8	6.84	36.5	1462	99	6.84	6.84
22	80	98.5	3.75	66.7	5333	362	N/A	3.75
22	150	99.3	2.32	107.8	16164	1096	2.32	2.32
22	300	98.3	4.30	58.1	17442	1183	1.87	3.31/4.19
22	600	97.1	8.82	28.3	17007	1154	4.08/5.40	6.95/8.93
22	1200	92.5	21.72	11.5	13812	937	8.49	15.32/21.72
22	2400	39.9	N/A	N/A	N/A	N/A	3.31/4.74	N/A
22	3000	0.0	No signal	N/A	N/A	N/A	2.65/3.09	No signal
22	3800	0.0	No signal	N/A	N/A	N/A	No signal	No signal
22	6000	0.0	No signal	N/A	N/A	N/A	No signal	No signal
26	600	94.7	6.50	38.5	23077	1565	2.98	5.07/6.50
30	600	96.9	5.07	49.3	29586	2007	2.43	3.97/5.07
34	600	97.9	3.97	63.0	37783	2563	2.76	3.20/4.08
38	600	93.4	3.31	75.5	45317	3074	2.09	2.20/2.65/3.31

(CsI)$_8$Cs$^+$ (2212 Da)									
WH (V)	**WV (m/s)**	**SY (%)**	**DT (ms)**	**v_d (m/s)**	**v^2 (m^2/s^2)**	**ΔT_{IM} (K)**	**DT652 (ms)**	**DT1172 (ms)**	**DT1692 (ms)**
2	600	0.0	N/A	N/A	N/A	N/A	N/A	N/A	N/A
6	600	93.8	N/A	N/A	N/A	N/A	N/A	N/A	N/A
10	600	94.5	N/A	N/A	N/A	N/A	N/A	N/A	N/A
14	600	95.4	18.08	13.8	8296	736	9.48	15.55	5.3/13.34/20.84
18	600	95.8	17.31	14.4	8666	768	5.62	9.70	8.49/12.90/17.31
22	10	62.9	3.31*	**10.0**	100	9	2.02/3.20	N/A	3.31
22	20	69.0	12.90	19.4	388	34	12.90	12.90	12.90
22	40	50.3	6.84	36.5	1462	130	6.84	6.84	6.84
22	80	98.8	3.75	66.7	5333	473	3.64	3.75	3.75
22	150	99.4	2.32	107.8	16164	1433	2.32	2.32	2.32
22	300	96.7	5.62	44.5	13345	1183	1.76	3.53	2.54/4.19/5.62
22	600	94.1	11.91	21.0	12594	1117	4.08	6.95	5.73/8.82/12.13
22	1200	91.2	N/A	N/A	N/A	N/A	8.49	15.44	15.99/21.45
22	2400	0.0	No signal	N/A	N/A	N/A	7.39	No signal	No signal
22	3000	0.0	No signal	N/A	N/A	N/A	2.65/3.09	No signal	No signal
22	3800	0.0	No signal	N/A	N/A	N/A	No signal	No signal	No signal
22	6000	0.0	No signal	N/A	N/A	N/A	No signal	No signal	No signal
26	600	95.4	8.71	28.7	17222	1527	2.98	5.18/8.71	4.30/6.50/8.71
30	600	97.1	6.61	37.8	22693	2012	2.43	3.97	3.31/5.07/6.73
34	600	95.9	5.92	42.2	25338	2247	No signal	No signal	2.65/3.97/5.40
38	600	97.7	4.41	56.7	34014	3016	1.76/2.32	2.54	2.32/3.31/4.41

Figure S5. Contour map showing survival yields of $(CsI)_6Cs^+$ (1692 Da) and $(CsI)_8Cs^+$ (2212 Da) across a wide range of different Trap T-wave conditions.



S6. Survival yields (SY) for the four CsI clusters studied, for some of the Trap wave height/velocity combinations in Figures 2 and S4.

		SY			
WH (V)	**WV (m/s)**	**$(CsI)_2Cs^+$ (652 Da)**	**$(CsI)_4Cs^+$ (1172 Da)**	**$(CsI)_6Cs^+$ (1692 Da)**	**$(CsI)_8Cs^+$ (2212 Da)**
0.1	600	86.9	91.9	98.6	90.3
0.3	600	80.1	86.6	97.8	91.2
0.5	600	90.1	86.0	97.4	89.0
0.7	600	86.9	83.3	97.2	86.9
0.9	10	99.5	99.9	100.0	95.6
0.9	20	99.5	100.0	99.8	95.7
0.9	40	99.3	99.6	99.8	95.2
0.9	80	98.9	99.4	99.6	94.9
0.9	150	98.8	98.5	99.5	94.2
0.9	300	95.0	97.2	99.2	93.6
0.9	600	86.5	81.2	97.0	85.7
0.9	1200	57.3	84.9	98.5	90.7
0.9	2400	86.2	89.8	99.0	89.7
0.9	3000	85.7	90.7	99.2	90.5
0.9	3800	82.1	95.9	99.1	95.2
0.9	6000	85.4	94.8	99.3	99.5
1.1	600	85.6	88.6	96.8	89.3
1.3	600	84.8	84.8	97.6	91.7
1.5	600	83.4	88.3	97.6	92.4
1.7	600	83.0	90.3	98.4	91.2
1.9	600	83.5	91.1	98.3	91.3

S7. ETD spectra of 9+ ubiquitin, acquired using a Trap T-wave height of 0.3 V and velocities of 150, 300, and 1200 m/s (no supplemental activation applied). Note that non-dissociative charge reduction dominates in the top spectrum (indicating a very short reaction time), whereas the bottom spectrum shows only one (extensively) charge-reduced state and almost exclusively singly charged fragments (both indicating a very long reaction time) and possesses a fairly low signal-to-noise ratio. Intermediate wave velocities (middle spectrum) are optimal for efficient detection of fragments at a high S/N ratio.