Electronic Supplementary Material (ESI) for Analyst.

Ion Mobility Mass Spectrometry of Peptide, Protein, and Protein Complex Ions using a Radio-Frequency Confining Drift Cell

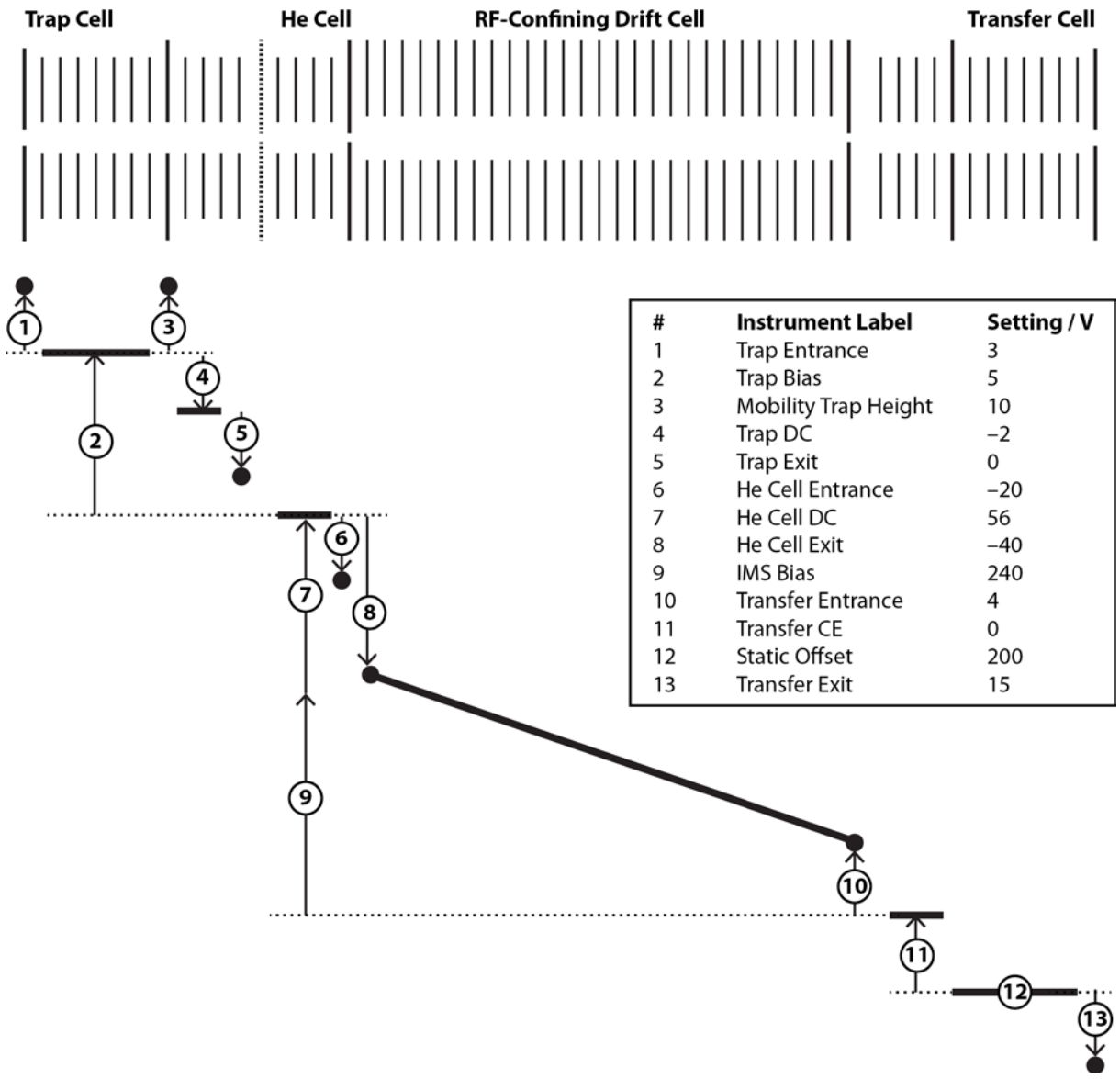
Electronic Supplementary Information

Samuel J. Allen,[a] Kevin Giles,[b] Tony Gilbert,[b] and Matthew F. Bush[a]*

a University of Washington, Department of Chemistry, Box 351700 Seattle, WA 98195-1700, United States of America

b Waters Corporation, Stamford Avenue, Altrincham Road, Wilmslow, SK9 4AX, United Kingdom

* Address correspondence to mattbush@uw.edu



#	Instrument Label	Setting / V
1	Trap Entrance	3
2	Trap Bias	5
3	Mobility Trap Height	10
4	Trap DC	–2
5	Trap Exit	0
6	He Cell Entrance	–20
7	He Cell DC	56
8	He Cell Exit	–40
9	IMS Bias	240
10	Transfer Entrance	4
11	Transfer CE	0
12	Static Offset	200
13	Transfer Exit	15

Fig. S1 Diagram of the RF-confining drift cell integrated into the Waters Synapt G2 HDMS. The RF-confining drift cell replaced the original traveling-wave ion mobility cell, but contains the same physical dimensions and electrical inputs. Below, a potential energy diagram of the Trap Cell, RF-Confining Drift Cell, and Transfer Cell is shown. Typical voltages used in these experiments are provided. Ion injection into the drift cell is controlled using optics 2 to 6, and 8. The drift voltage is controlled by optics 7 to 10. The method used to calculate the drift voltage is shown in ESI Fig. S2. All voltages are relative to the transfer cell voltage, which is controlled by the Static Offset (optic 12) and referenced to ground. The dashed line represents the location of the helium cell entrance plate of the original traveling-wave ion mobility cell, which was removed for these experiments.

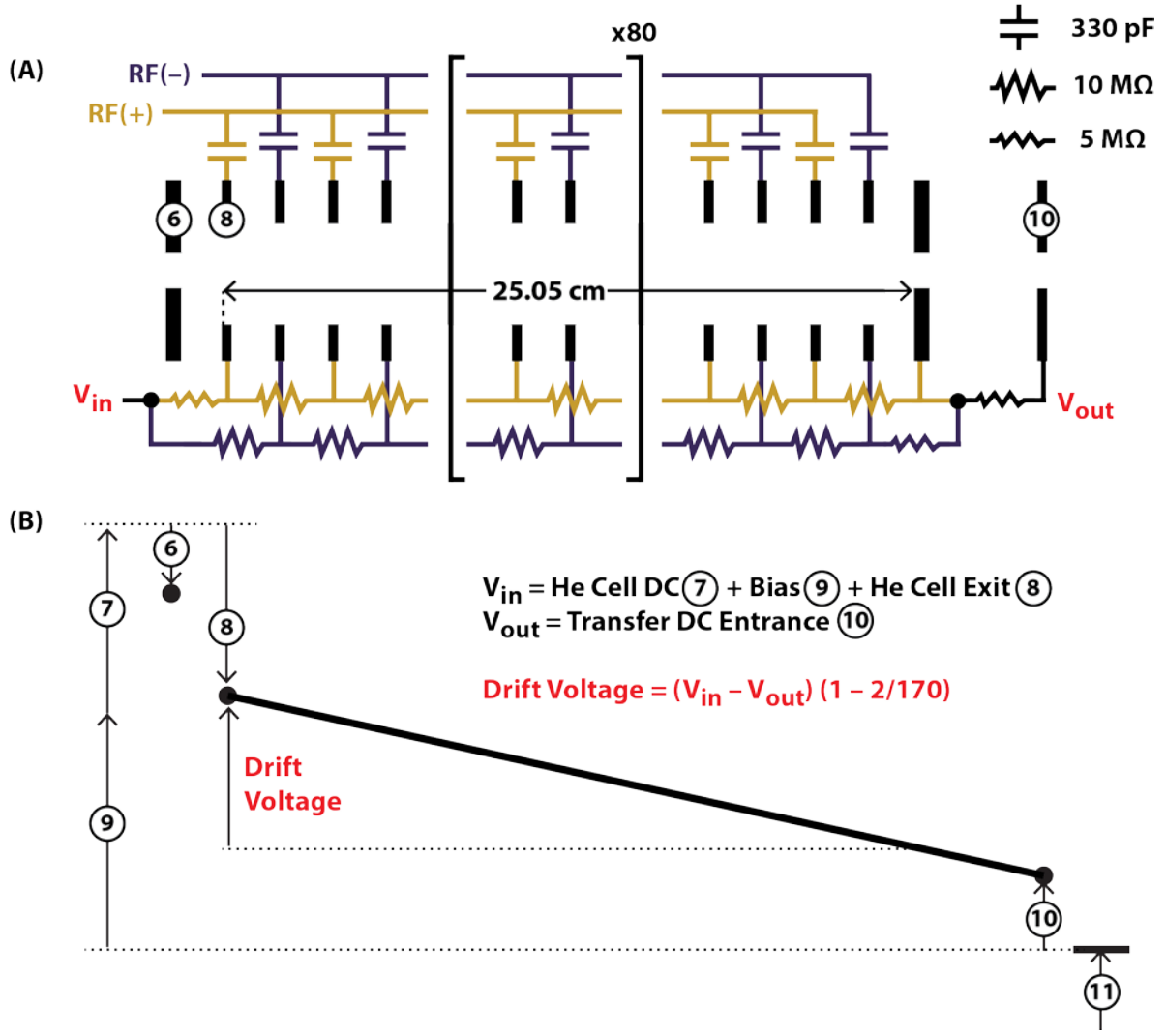


Fig. S2 (A) Schematic of RF-confining drift cell containing two resistor series that are connected in parallel to establish a uniform DC voltage drop. The RF voltage is applied through two series of 330 pF capacitors. (B) Note, the nomenclature is the same of that in ESI Fig. S1. The drift voltage is established using connections from the He Cell DC (7), He Cell Exit (8, a negative voltage), Bias (9), and Transfer DC Entrance (10). The electrical inputs were adjusted such that the first electrode of the RF-confining drift cell is controlled using (8). The He Cell Entrance (6) controls the helium cell exit plate and does not affect the drift voltage but is set so that it is half the value of (8), generating a uniform voltage drop into the drift region. The drift voltage equation is used to calculate the actual drift voltage by summing the voltages before the drift region (V_{in}) and subtracting voltages after (V_{out}). A factor of (1 – 2/170) is used to correct for two resistors, one before V_{in} and one between the RF-confining drift cell exit plate and (10). This equation represents the drift voltage from the first electrode to the exit plate of the RF-confining drift cell, resulting in an actual drift cell length of 25.05 cm. Most experiments use drift voltages ranging from 104 to 354 V.

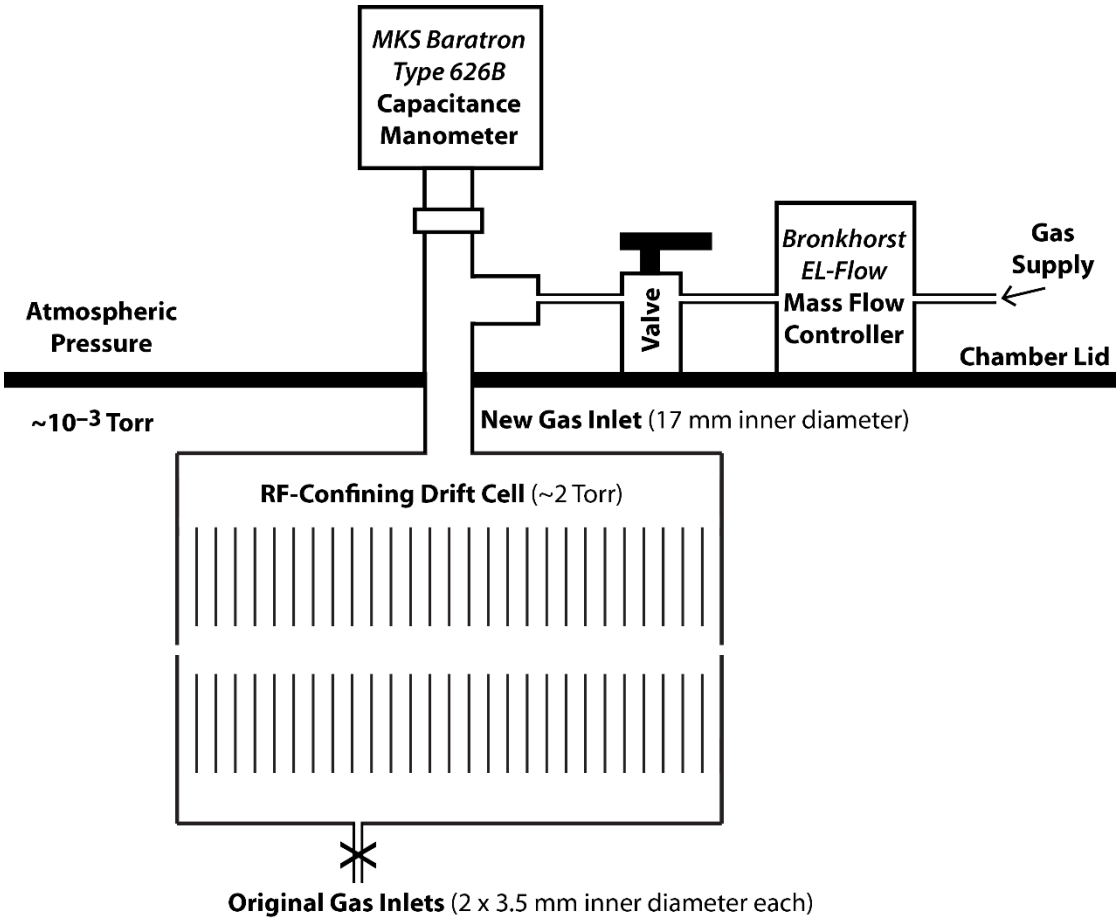


Fig. S3 The gas inlet system is regulated by a Bronkhorst EL-Flow mass flow controller (rated up to 500 mL min^{-1}) that is controlled using the original Helium Cell gas flow electrical cabling. The mass flow controller delivers mobility gas through 1/8” Swagelok stainless steel tubing to a KF16 Tee attached to a 17 mm hole in the top plate of the cell. The KF16 tee also connects to a capacitance manometer (MKS Baratron Type 626B) that directly measures the absolute pressure inside the drift cell.

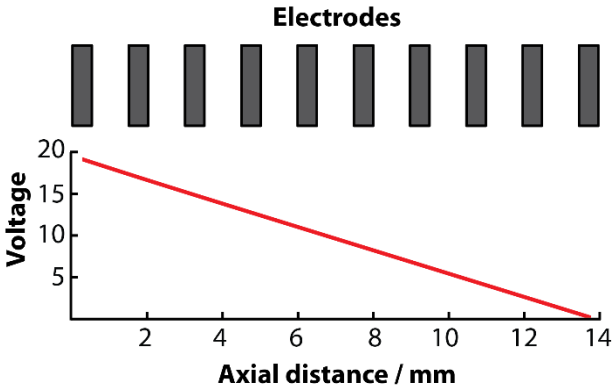


Fig. S4 The DC voltage profile along the axis of transmission (red line) in an RF-confining drift cell with an applied field strength of 14 V cm^{-1} obtained using SIMION. The line consists of data points collected every 50 ns. The voltage profile is linear, indicating that any effect of using discrete electrodes is negligible.

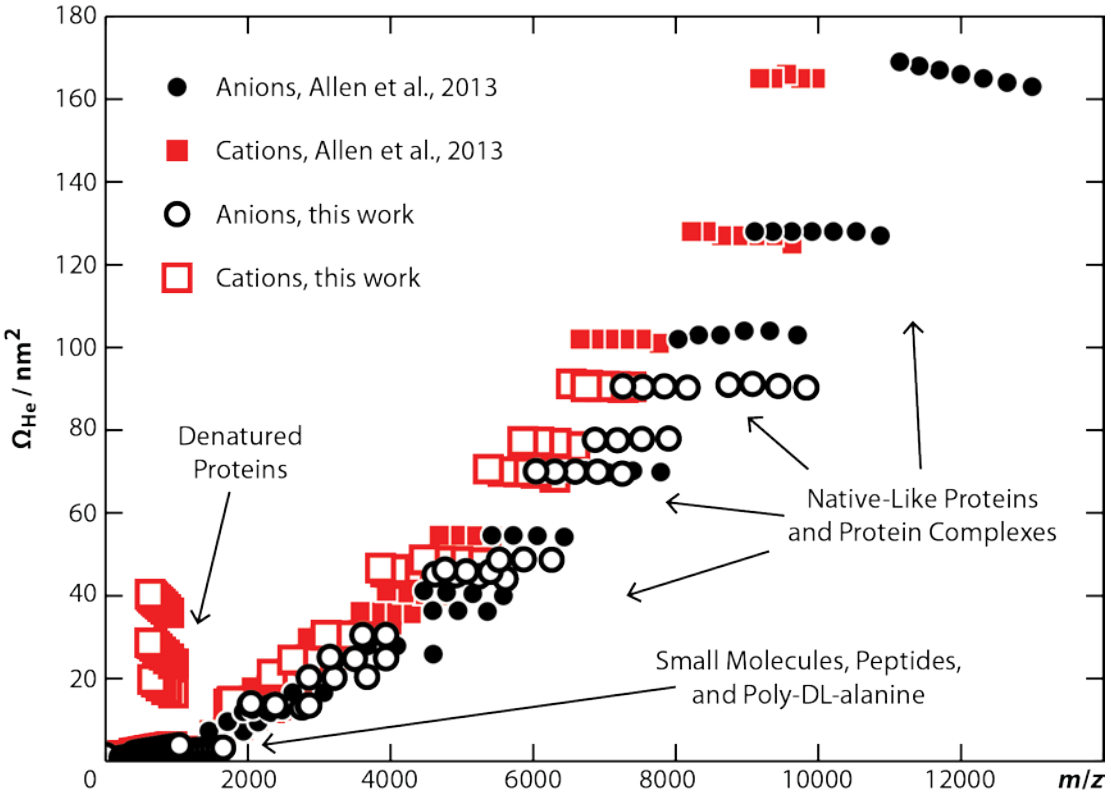


Fig. S5 Collision cross sections measured in helium gas (Ω_{He}) of all cations (*red squares*) and anions (*black circles*) from ESI Table S2 and S3. Values measured using this new RF-confining drift cell include those reported previously (*closed symbols*, Allen et al. *Anal. Chem.* **2013**, *85*, 12055 – 12061.) and new values measured in this work (*open symbols*).

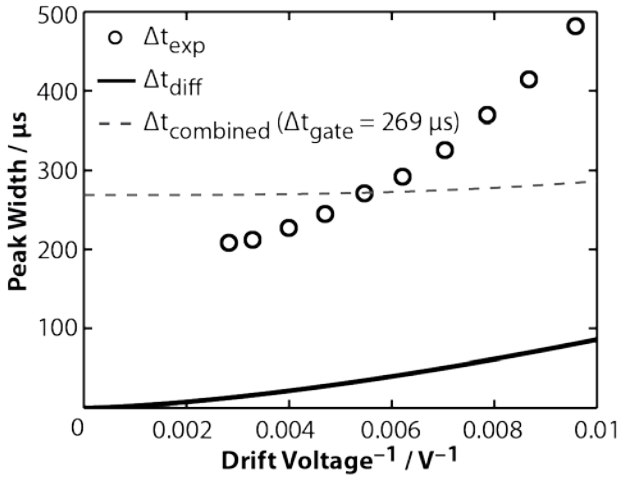


Fig. S6 Analysis of full width at half maximum (peak width, Δt) as a function of reciprocal drift voltage. Experimental peaks widths (Δt_{exp}, black circles) of the 25+ charge state of glyceraldehyde-3-phosphate dehydrogenase are greater than those expected using diffusion-limited theory from eqn 1 of main text (Δt_{diff}, solid line). Using eqn 5 of main text, a least-squares fitting of the combined peak width ($\Delta t_{combined}$, dashed line) to Δt_{exp} results in a Δt_{gate} of 269 µs.

Table S1 Selected Analytes, Sources, and Solution Conditions

Name	Supplier	Item #	Positive Ion Mode Solution	Negative Ion Mode Solution
poly-DL-alanine	Sigma	P9003	Solution A	Solution B
N-ethylaniline	Sigma	426385	Solution C	Solution D
acetaminophen	Sigma	A5000	Solution C	Solution D
alprenolol	MP	190092	Solution C	Solution D
ondansetron	Sigma	O3639	Solution C	Solution D
clozapine N-oxide	Sigma	C0832	Solution C	Solution D
betamethasone	MP	154853	Solution C	Solution D
dexamethasone	Sigma	D1756	Solution C	Solution D
colchicine	Sigma	C9754	Solution C	Solution D
verapamil	Sigma	V4629	Solution C	Solution D
reserpine	Sigma	R0875	Solution C	Solution D
GRGDS	Waters	700005089	Solution A	Solution E
SDGRG	Waters	700005089	Solution A	Solution E
bradykinin	Sigma	B3259	Solution A	-
leucine enkephalin	Sigma	L9133	Solution B	
denatured ubiquitin	Sigma	U6253	Solution A	-
denatured cytochrome *c*	Sigma	C2506	Solution A	-
denatured myoglobin	Sigma	M1882	Solution A	-
insulin monomer/dimer	Sigma	I2643	Solution F	
ubiquitin	Sigma	U6253	Buffer	
cytochrome *c*	Sigma	C2506	Buffer	
ribonuclease A	Sigma	R6513	Buffer, BS	
α-lactalbumin	Sigma	L6010	Buffer	
lysozyme	Sigma	L6876	Buffer, BS	
α-chymotrypsinogen A	Sigma	C4879	Buffer, BS	
carbonic anhydrase	Sigma	C2624	Buffer, BS	
insulin hexamer	Sigma	I2643	Solution G	
β-lactoglobulin	Sigma	L7880	Buffer, BS	
ovalbumin	Sigma	A7641	Buffer, BS	
avidin	Sigma	A9275	Buffer	
albumin	Sigma	A2153	Buffer, BS	
holotransferrin	Sigma	T1408	Buffer, BS	
lactoferrin	Sigma	L0520	Buffer	
enolase	Sigma	E6126	Buffer, BS	
concanavalin A	Sigma	C2010	Buffer	
glyceraldehyde-3-phosphaste dehydrogenase	Sigma	G2267	Buffer	
alcohol dehydrogenase	Sigma	A7011	Buffer, BS	
aldolase	Sigma	A2714	Buffer, BS	

phosphorylase b	Sigma	P6635	Buffer, BS
pyruvate kinase	Sigma	P9136	Buffer, BS
catalase	Sigma	C40	Buffer, BS
glutamate dehydrogenase	Sigma	G7882	Buffer, BS
β-galactosidase	Sigma	G5635	Buffer, BS

Solution A = 0.01 mg/mL sample prepared in 49.5/49.5/1 water/acetonitrile/formic acid.

Solution B = 0.01 mg/mL sample prepared in water.

Solution C = 0.1 µM sample prepared in water with 0.1 % formic acid.

Solution D = 0.1 µM sample prepared in water with 1 % ammonium hydroxide.

Solution E = 0.01 mg/mL sample prepared in water with 1 % ammonium hydroxide.

Solution F = 10 µM sample prepared in 100 mM aqueous ammonium acetate at pH 7.0.

Solution G = 5 µM sample prepared in 2.5 µM zinc chloride, 1.67 µM ammonium chloride, and 5 mM phenol in 300 mM aqueous ammonium acetate at pH 7.0.

Buffer = 10 µM sample prepared in 200 mM aqueous ammonium acetate at pH 7.0.

BS = On the same day as measurements, sample buffer was exchanged using a Micro Bio-Spin 6 column (Bio-Rad, Hercules, CA) that was equilibrated with 200 mM aqueous ammonium acetate at pH 7.0.

Table S2 Collision cross sections with helium and nitrogen gas (Ω_{He} and Ω_{N2}, respectively) of poly-DL-alanine anions $(Ala_n - zH)^{z-}$ and Ω_{He} of poly-DL-alanine cations $(Ala_n - zH)^{z+}$. The monoisotopic mass of oligomers (*n*) are provided. Mobility measurements were conducted in 2.0 Torr helium or 1.5 Torr nitrogen gas. Note, improved transmission of lower-mobility ions was observed when the pressure of nitrogen gas from dropped from 2.0 to 1.5 Torr. Ω values were determined by measuring drift times for 10 different drift voltages ranging from 104 to 354 V.

	z	1+	1–	1–	2+	2–	2–
n	**mass**	**Ω_{He} / Å²**	**Ω_{He} / Å²**	**Ω_{N2} / Å²**	**Ω_{He} / Å²**	**Ω_{He} / Å²**	**Ω_{N2} / Å²**
3	231.1	88	89	150			
4	302.2	99	104	165			
5	373.2	113	117	179			
6	444.2	126	131	195			
7	515.3	139	143	209			
8	586.3	156	155	223			
9	657.3	169	167	238			
10	728.4	181	179	253			
11	799.4	192	190	267	196	202	297
12	870.5	204	200	279	205	215	309
13	941.5	215	213	294	215	226	322
14	1012.5	226	226	308	226	237	333
15	1083.6	238	237	322	239	248	344
16	1154.6	249	248	335	250	257	355
17	1225.6		260	348	262	267	366
18	1296.7		271	361	272	277	377
19	1367.7		283	374	287	286	387
20	1438.8		294	387	294	296	399
21	1509.8		305		310	306	410
22	1580.8		317		315	316	422
23	1651.9		329		330	327	434
24	1722.9				335	337	445
25	1793.9				349	347	457
26	1865.0				356	358	469
27	1936.0					367	481
28	2007.0					378	492
29	2078.1					389	

Table S3 Collision cross section values of small molecule, peptide, denatured protein, and native-like protein and protein complex cations (Ω+) and anions (Ω–) measured in 2.0 Torr helium gas. Oligomeric states (*n*), charge (*z*), and mass are provided. † symbol represents values previously reported in Allen et al. *Anal. Chem.* **2013**, *85*, 12055 – 12061. Solution conditions are reported in Table S1.

	Sample	***n***	**mass (Da)**	***z***	**Ω+ / nm^2**	**Ω– / nm^2**
Small Molecules	N-ethylaniline	1	121.1	1	0.63	-
	acetominophen	1	151.1	1	0.67	0.67
	alprenolol	1	149.2	1	0.97	-
	ondanestron	1	293.2	1	1.05	1.06
	clozapine N-oxide	1	342.2	1	1.12	1.13
	betamethasone	1	392.2	1	1.15	1.15
	dexamethasone	1	392.2	1	1.16	1.15
	colchicine	1	399.2	1	1.30	1.29
	verapamil	1	454.3	1	1.42	-
	reserpine	1	609.2	1	1.77	-
Peptides	GRGDS	1	490	1	1.32	1.26
				2	1.41	1.44
	SDGRG	1	490	1	1.30	1.26
				2	1.44	1.42
	leucine enkephalin	1	555.6	1	1.57	1.52
	bradykinin	1	1060	2	2.41	-
Denatured Proteins	denatured ubiquitin	1	8.57k	9	16.5	-
	bovine erythrocytes			10	17.3	-
				11	18.2	-
				12	19.1	-
				13	19.8	-
	denatured cytochrome *c*	1	12.4k	13	23.6	-
	equine heart			14	24.8	-
				15	25.7	-
				16	26.4	-
				17	27.2	-
				18	27.8	-
				19	28.4	-
				20	28.7	-

	Sample	*n*	mass	*z*	Ω+ / nm^2	Ω– / nm^2
Denatured Proteins	denatured myoglobin	1	16.9k	19	35.9	-
	equine heart			20	36.7	-
				21	37.4	-
				22	38.0	-
				23	38.5	-
				24	39.0	-
				25	39.4	-
				26	39.9	-
				27	40.4	-
Native-like Proteins and Protein Complexes	insulin†	1	5.81k	3	7.43	7.28
	recombinant human			4	7.68	7.32
	ubiquitin†	1	8.57k	4	9.72	9.50
	bovine erythrocytes			5	9.82	9.60
	insulin†	2	11.6k	5	12.3	11.8
	recombinant human			6	12.9	12.0
	cytochrome *c*†	1	12.4k	5	-	12.4
	equine heart			6	12.4	12.5
				7	13.0	-
	ribonuclease A	1	13.8k	5	-	13.0
	bovine pancreas			6	12.9	13.0
				7	13.4	-
				8	13.9	-
	α-lactalbumin	1	14.2k	5	-	13.5
	bovine milk			6	13.6	13.5
				7	13.8	13.8
				8	14.4	-
	lysozyme	1	14.3k	5	-	13.5
	chicken egg white			6	13.6	13.6
				7	13.7	14.0
				8	14.6	-
	β-lactoglobulin†	1	18.4k	6	-	16.6
	bovine milk			7	16.7	16.6
				8	17.1	-
				9	18.0	-
	α-chymotrypsinogen A	1	25.7k	7	-	20.4
	bovine pancreas			8	-	20.2
				9	20.2	20.3
				10	20.3	-
				11	21.1	-

Sample	***n***	**mass**	***z***	**Ω+ / nm²**	**Ω– / nm²**
carbonic anhydrase	1	31.5k	8	-	24.9
bovine erythrocytes			9	-	24.8
			10	24.3	25.2
			11	24.3	-
			12	24.5	-
insulin†	6	35.3k	10	24.0	23.7
recombinant human			11	24.1	23.7
β-lactoglobulin†	2	36.8k	8	-	25.9
bovine milk			9	-	27.9
			10	-	27.9
			11	28.4	-
			12	29.0	-
			13	29.9	-
ovalbumin	1	43.3k	11	30.1	30.5
egg white			12	30.1	30.5
			13	30.4	-
			14	30.5	-
avidin†	4	64.3k	12	-	36.2
egg white			13	-	36.4
			14	-	36.4
			15	35.7	-
			16	35.9	-
			17	36.1	-
			18	36.2	-
albumin†	1	67.0k	12	-	40.0
bovine serum			13	-	40.5
			14	40.1	40.8
			15	40.3	41.2
			16	40.7	-
			17	41.1	-
holotransferrin	1	78.6k	14	-	44.1
bovine			15	-	44.7
			16	-	45.0
			17	44.2	45.2
			18	45.0	-
			19	45.4	-
			20	45.7	-

Sample	***n***	**mass**	***z***	**Ω+ / nm²**	**Ω– / nm²**
lactoferrin	1	81.0k	15	-	45.8
human milk			16	-	45.9
			17	-	46.3
			18	45.9	-
			19	46.4	-
			20	46.3	-
			21	46.7	-
enolase	2	93.9k	15	-	48.7
saccharomyces cerevisiae			16	-	48.8
			17	-	48.7
			18	48.0	-
			19	48.3	-
			20	48.4	-
			21	48.7	-
concanavalin A[†]	4	103k	16	-	54.2
jack bean			17	-	54.5
			18	-	54.6
			19	54.4	54.6
			20	54.5	-
			21	54.6	-
			22	54.6	-
glyceraldehyde-3-phosphate	4	145k	20	-	69.5
dehydrogenase			21	-	70.0
rabbit muscle			22	-	70.0
			23	68.6	70.0
			24	69.6	70.1
			25	69.9	-
			26	70.0	-
			27	70.6	-
alcohol dehydrogenase[†]	4	148k	19	-	69.9
saccharomyces cerevisiae			20	-	70.2
			21	-	69.8
			22	-	70.3
			23	69.9	70.1
			24	70.2	-
			25	70.2	-
			26	70.2	-
			27	70.2	-

Sample	***n***	**mass**	***z***	**Ω+ / nm^2**	**Ω– / nm^2**
aldolase	4	158k	20	-	78.0
rabbit muscle			21	-	77.9
			22	-	77.6
			23	-	77.7
			24	76.1	-
			25	76.9	-
			26	77.2	-
			27	77.3	-
phosphorylase b	2	196k	24	-	90.3
rabbit muscle			25	-	90.6
			26	-	90.4
			27	90.3	90.6
			28	90.7	-
			29	90.9	-
			30	91.2	-
pyruvate kinase[†]	4	233k	24	-	103
rabbit muscle			25	-	104
			26	-	104
			27	-	103
			28	-	103
			29	-	102
			30	101	-
			31	102	-
			32	102	-
			33	102	-
			34	102	-
			35	102	-
catalase	4	236k	24	-	90.3
bovine liver			25	-	90.7
			26	-	91.2
			27	-	91.0
			32	90.5	-
			33	90.6	-
			34	90.5	-
			35	90.9	-
			35	90.5	-

Native-like Proteins and Protein Complexes

Sample	***n***	**mass**	***z***	**Ω+ / nm^2**	**Ω– / nm^2**
glutamate dehydrogenase[†]	6	337k	31	-	127
bovine liver			32	-	128
			33	-	128
			34	-	128
			35	125	128
			36	127	128
			37	127	128
			38	127	-
			39	127	-
			40	128	-
			41	128	-
β-galactosidase[†]	4	468k	36	-	163
Escherichia coli			37	-	164
			38	-	165
			39	-	166
			40	-	167
			41	-	168
			42	-	169
			47	165	-
			48	165	-
			49	166	-
			50	165	-
			51	165	-

Table S4 Collision cross sections with helium gas (Ω_{He}) of peptides and denatured proteins from Table S3. Ω_{He} are compared to literature values measured using traditional DC-only drift tubes (Ω_{Lit}).

Analyte	Charge State (Chain Length)	*m*/*z*	Ω_{He} / Å^2	$\Omega_{Lit.}$ / Å^2	(Ω_{He} / $\Omega_{Lit.}$)–1
GRGDS	1+	491.5	132	135.2[a]	–2.37%
	2+	246.3	141	145.6[a]	–3.16%
SDGRG	1+	491.5	130	133.9[a]	–2.91%
	2+	246.3	144	149.7[a]	–3.81%
bradykinin	2+	531.1	241	240[b]	0.42%
poly-DL-alanine	1+ (3)	232.1	88	89[c]	–1.12%
	1+ (4)	303.2	99	102.9[c]	–3.79%
	1+ (5)	374.2	113	115.0[c]	–1.74%
	1+ (6)	445.2	126	127.0[c]	–0.79%
	1+ (7)	516.3	139	140.5[c]	–1.07%
	1+ (8)	587.3	156	155.5[c]	0.32%
	1+ (9)	658.3	169	167.9[c]	0.66%
	1+ (10)	729.4	181	176.3[c]	2.67%
	1+ (11)	780.4	192	192.2[c]	–0.10%
	1+ (12)	871.5	204	202.4[c]	0.79%
	1+ (13)	942.5	215	214.9[c]	0.05%
	1+ (14)	1014	226	224.9[c]	0.49%
ubiquitin	9+	952.6	1650	1649[d]	0.06%
	10+	857.5	1730	1732[d]	–0.12%
	11+	779.6	1820	1802[d]	1.00%
cytochrome *c*	13+	953.6	2360	2391[e]	–1.30%
	14+	885.6	2480	2473[e]	0.28%
	15+	826.6	2570	2579[e]	–0.35%
	16+	775.0	2640	2679[e]	–1.46%
	17+	729.5	2720	2723[e]	–0.11%
	18+	689.0	2780	2766[e]	0.51%
	19+	652.8	2840	2800[e]	1.43%
	20+	620.2	2870	2889[e]	–0.66%
myoglobin	19+	893.2	3590	3570[f]	0.56%
	20+	848.6	3670	3682[f]	–0.33%
	21+	808.2	3740	3792[f]	–1.37%
	22+	771.5	3800	3815[f]	–0.39%
			Average		–0.55%
			Standard Deviation		1.48%

[a]Kemper, P. R.; Dupuis, N. F.; Bowers, M. T. *Int. J. Mass Spectrom.* **2009**, *287*, 46–57.
[b]Counterman, A. E.; Valentine, S. J.; Srebalus, C. A.; Henderson, S. C.; Hoaglund, C. S.; Clemmer, D. E. *J. Am. Soc. Mass Spectrom.* **1998**, *9*, 743–759.
[c]Henderson, S. C.; Li, J.; Counterman, A. E.; Clemmer, D. E. *J. Phys. Chem. B* **1999**, *103*, 8780–8785.

[d]Valentine, S. J.; Counterman, A. E.; Clemmer, D. E. *J. Am. Soc. Mass Spectrom.* **1997**, *8*, 954–961.
[e]Shelimov, K. B.; Clemmer, D. E.; Hudgins, R. R.; Jarrold, M. F. *J. Am. Chem. Soc.* **1997**, *119*, 2240–2248.
[f]Liu, Y.; Valentine, S. J.; Clemmer, D. E. *Unpublished Results*
http://www.indiana.edu/~clemmer/Research/Cross%20Section%20Database/cs_database.php.

Example Waters Synapt G2 HDMS Parameters File

Parameters for C:\MassLynx\BlueWater\tuneexp.exp
Created by Masslynx v4.1

Temperature Correction:

Temperature Correction	Disabled

Instrument Configuration:

Lteff	1800.0
Veff	7246.00
Resolution	10000
Min Points in Peak	2
Acquisition Device	WatersADC
ADC Trigger Threshold (V)	1.50
ADC Input Offset (V)	-1.59
Average Single Ion Intensity	21
ADC Amplitude Threshold	4
ADC Centroid Threshold	-1
ADC Ion Area Threshold	4
ADC Ion Area Offset	10
ADC Pushes Per IMS Increment	1
EDC Delay Coefficient	1.5700
EDC Delay Offset	1.8100
Tof Emulation Transfer Pulse Height (V)	0.1

Experimental Instrument Parameters

Polarity	ES+
Analyser	Sensitivity Mode
Capillary (kV)	0.8700
Source Temperature (°C)	20
Sampling Cone	25.0000
Extraction Cone	2.0000
Source Gas Flow (mL/min)	0.00
Desolvation Temperature (°C)	150
Cone Gas Flow (L/Hr)	0.0
Nanoflow Gas Pressure (Bar)	0.0
Purge Gas Flow (mL/h)	500.0
Desolvation Gas Flow (L/Hr)	500.0
LM Resolution	12.0
HM Resolution	15.0
Aperture 1	0.0
Pre-filter	2.0
Ion Energy	1.8
Manual Trap Collision Energy	TRUE
Trap Collision Energy	10.0
Manual Transfer Collision Energy	FALSE
Transfer Collision Energy	0.0
Manual Gas Control	TRUE
Trap Gas Flow (mL/min)	4.00
HeliumCellGasFlow	0.00
IMS Gas Flow (mL/min)	145.00
Detector	3000
DetectorCache	2300
Sample Infusion Flow Rate (µL/min)	5
Sample Flow State	Waste

Sample Fill Volume (µL)	250
Sample Reservoir	Wash
LockSpray Infusion Flow Rate (µL/min)	10
LockSpray Flow State	Infusion
LockSpray Reservoir	B
LockSpray Capillary (kV)	3.00
Use Manual LockSpray Collision Energy	FALSE
Collision Energy	4.0
Acceleration1	70.0
Acceleration2	200.0
Aperture2	40.0
Transport1	70.0
Transport2	70.0
Steering	0.0
Tube Lens	75
Pusher	1900.0
Pusher Offset	-0.25
Puller	1370.0
Collector	50
Collector Pulse	10.0
Stopper	10
Stopper Pulse	20.0
Entrance	62
Static Offset	200
Puller Offset	0.00
Reflectron Grid (kV)	1.481
Flight Tube (kV)	10.00
Reflectron (kV)	3.780
Use Manual Trap DC	TRUE
Trap DC Entrance	3.0
Trap DC Bias	5.0
Trap DC	-2.0
Trap DC Exit	0.0
Use Manual IMS DC	TRUE
IMS DC Entrance	-20.0
Helium Cell DC	56.0
Helium Exit	-40.0
IMSBias	240.0
IMS DC Exit	0.0
USe Manual Transfer DC	TRUE
Transfer DC Entrance	4.0
Transfer DC Exit	0.0
Source Manual Control	OFF
Source Wave Velocity (m/s)	200
Source Wave Height (V)	0.2
Trap Manual Control	OFF
Trap Wave Velocity (m/s)	311
Trap Wave Height (V)	6.0
IMS Manual Control	ON
IMS Wave Velocity (m/s)	250
IMS Wave Height (V)	0.0
Transfer Manual Control	ON
Transfer Wave Velocity (m/s)	65
Transfer Wave Height (V)	2.0
Target Enhancement Enabled	FALSE
Target Enhancement Mode	EDC
Target Enhancement Mass	556.0

Target Enhancement Trap Height (V)	20.0
Target Enhancement Extract Height (V)	15.0
Mobility Trapping Manual Release Enabled	FALSE
Mobility Trapping Release Time (µs)	200
Mobility Trap Height (V)	15.0
Mobility Extract Height (V)	0.0
Trag Gate LUT table enabled	FALSE
TriWave Trap Gate LookUp Table	
Using Drift Time Trimming	FALSE
Drift Time Bins	0
Using Mobility Delay after Trap Release	TRUE
IMS Wave Delay (µs)	450
Variable Wave Height Enabled	FALSE
Wave Height Ramp Type	Linear
Wave Height Start (V)	8.0
Wave Height End (V)	20.0
Wave Height Using Full IMS	TRUE
Wave Height Ramp (%)	100.0
Wave Height Look Up Table	
Variable Wave Velocity Enabled	FALSE
Wave Velocity Ramp Type	Linear
Wave Velocity Start (m/s)	300.0
Wave Velocity End (m/s)	600.0
Wave Velocity Using Full IMS	TRUE
Wave Velocity Ramp (%)	100.0
Wave Velocity Look Up Table	
Backing	4.31e0
Source	2.16e-3
Sample Plate	1.00e-6
Trap	3.95e-2
Helium Cell	8.76e-2
IMS	1.39e3
Transfer	4.17e-2
TOF	1.39e-6
SourceRFOffset	350
IMSRFOffset	350
IMSMobilityRFOffset	100
TrapRFOffset	300
TransferRFOffset	350
MS Profile Type	Auto P
MSProfileMass1	100
MSProfileDwellTime1	20
MSProfileRampTime1	20
MSProfileMass2	300
MSProfileDwellTime2	20
MSProfileRampTime2	40
MSProfileMass3	500
LockMassValidSigma	5
Acquisition mass range	
Start mass	2000.000
End mass	14000.000
Calibration mass range	
Start mass	0.000
End mass	0.000

Experiment Reference Compound Name: N/A

Function Parameters - Function 1 - TOF MS FUNCTION	
Scan Time (sec)	1.000
Interscan Time (sec)	0.024
Start Mass	2000.0
End Mass	14000.0
Start Time (mins)	0.00
End Time (mins)	1.50
Data Format	Continuum
ADC Sample Frequency (GHz)	3.0
Use Tune Page Cone Voltage	YES
Using Auto Trap Collision Energy (eV)	4.000000
Use Auto Transfer Collision Energy	NO
Transfer Collision Energy 1 (eV)	30.0
Sensitivity	Normal
Dynamic Range	Normal
Save Collapsed Retention Time Data	No
Use Rule File Filtering	No
FragmentationMode	CID
Calibration	Dynamic 2