Electronic Supplementary Material (ESI) for Analyst.

Supplemental Information for:

Collision-energy Resolved Ion Mobility Characterization of Isomeric Mixtures

Michael Pettit[1], Brett Harper[2], Matthew Brantley[1], and Touradj Solouki*[1]
[1]Department of Chemistry and Biochemistry, Baylor University, Waco, TX 76798, USA
[2]Institute of Biomedical Studies, Baylor University, Waco, TX 76798, USA

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*Please address reprint requests to: Professor Touradj Solouki, Department of Chemistry and Biochemistry, Baylor University Sciences Building, One Bear Place #97348, Waco, TX 76798 Telephone number: 254-710-2678, E-mail: Touradj_Solouki@baylor.edu

Table S1

Table S1. Experimental parameters used in this study

Instrument parameter	Ternary Mixture	Quaternary Mixture
ESI flow rate (uL/min)	0.5	0.5
ESI voltage (kV)	3.5	2.25
Source temperature (C)	100	100
Sampling cone voltage (V)	0	35
Source offset voltage (V)	0	35
Trap DC bias (V)	45.8	30.8
Trap cell pressure (bar)*	1.99×10^{-5}	1.55×10^{-5}
Transfer cell pressure (bar)*	2.25×10^{-5}	$1. \times 10^{-5}$
Helium cell pressure (bar)*	1.36×10^{3}	1.36×10^{3}
IM cell pressure (bar)*	3.79×10^{-3}	3.88×10^{-3}
IM wave velocity (m/s)	652	2000
IM wave height (V)	40	40

* Indicate instrument pressure readings and do not include any pressure corrections

Table S2

Table S2. Calculated *R* Values for (a) $[M_T + Li]^+$ and (b) $[M_P + 2H]^{2+}$ at each measured collision-energy. *R* values greater than 0.75 qualified as an acceptable match when comparing an isomer's deconvoluted mass spectrum to its pure counterpart

(a)

Collision-energy (V)	***R* Value**		
	$[\text{Raffinose} + \text{Li}]^+$	**$[\text{Isomaltotriose} + \text{Li}]^+$**	**$[\text{Cellotriose} + \text{Li}]^+$**
20	––	––	––
25	––	––	––
30	0.7598	––	––
35	0.9976	––	––
40	0.9601	0.9175	––
45	0.9869	0.8198	0.9136
50	0.9629	0.8831	0.9362
55	0.8925	––	0.955
60	0.7804	––	––
65	––	0.8510	––
70	––	0.9186	––
75	0.7980	––	––
80	0.7578	––	––

(b)

Collision-energy (V)	***R* Value**			
	$[\text{MGRYGF} + 2H]^{2+}$	**$[\text{MFRYGG} + 2H]^{2+}$**	**$[\text{MFGRYG} + 2H]^{2+}$**	**$[\text{FRMYGG} + 2H]^{2+}$**
20	––	0.9278	––	––
22	––	0.8938	––	––
24	0.8335	0.9594	––	––
26	0.8260	0.9287	0.7889	0.7983
28	0.8383	––	––	––

Figure S1

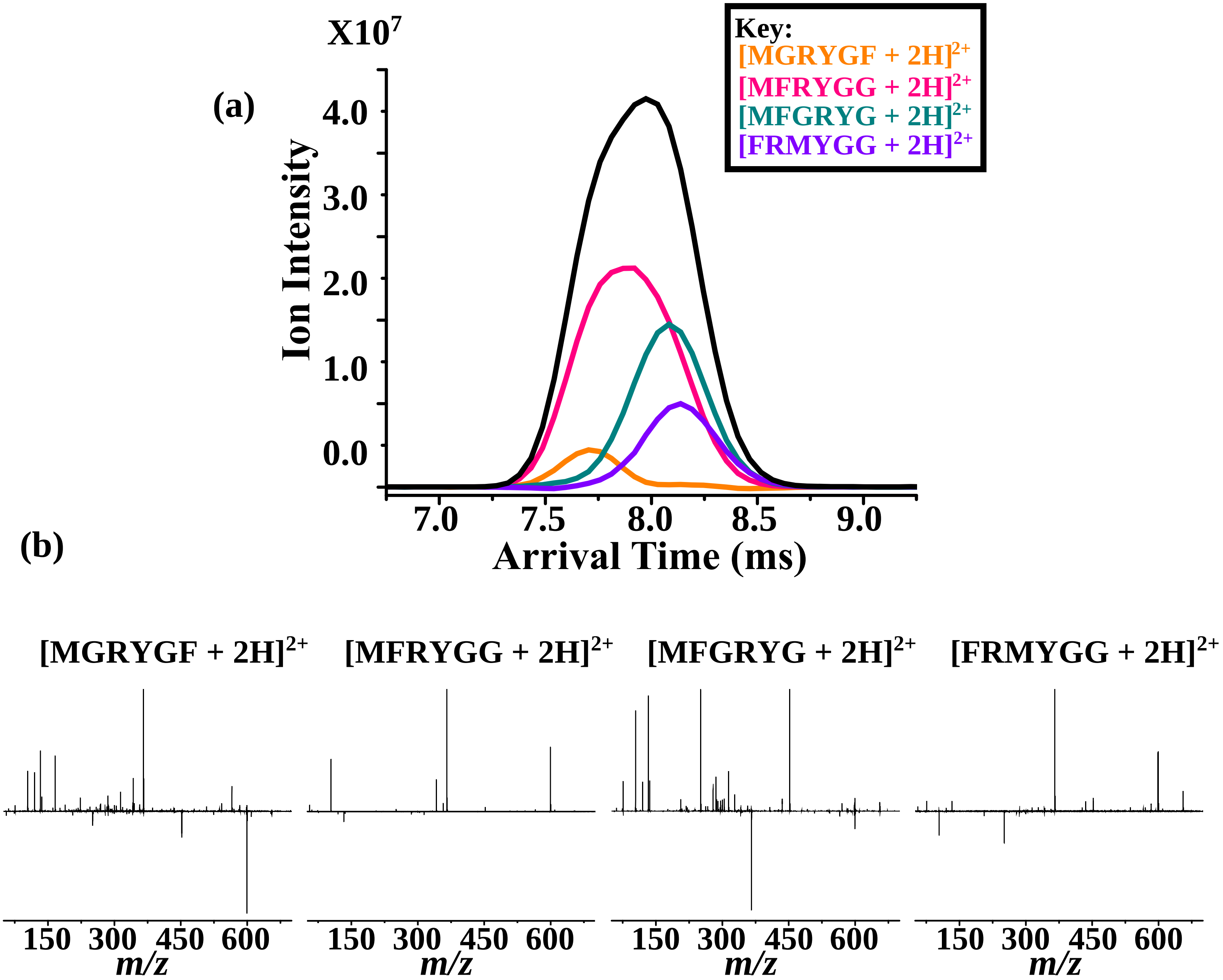

Figure S1. Suboptimal IM-MS deconvolution at a 20 V collision-energy. (a) IM distribution for the quaternary mixture of hexapeptide isomers shown before (black profile) and after (colored profiles) deconvolution. While deconvoluted arrival times match corresponding pure samples when individually measured under similar conditions, deconvoluted CID mass spectra (b) for [MGRYGF + 2H]$^{2+}$, [MFGRYG + 2H]$^{2+}$, and [FRMYGG + 2H]$^{2+}$ have negative intensity values that are greater than 15% of the respective base peak intensities. According to the criteria described in the experimental section of the main text, deconvolution results for [MGRYGF + 2H]$^{2+}$, [MFGRYG + 2H]$^{2+}$, and [FRMYGG + 2H]$^{2+}$ were classified as unsuccessful.