SUPPLEMENTARY MATERIAL TO ACCOMPANY:

ION MOBILITY SPECTROMETRY AND TANDEM MASS SPECTROMETRY ANALYSIS OF ESTRADIOL GLUCURONIDE ISOMERS

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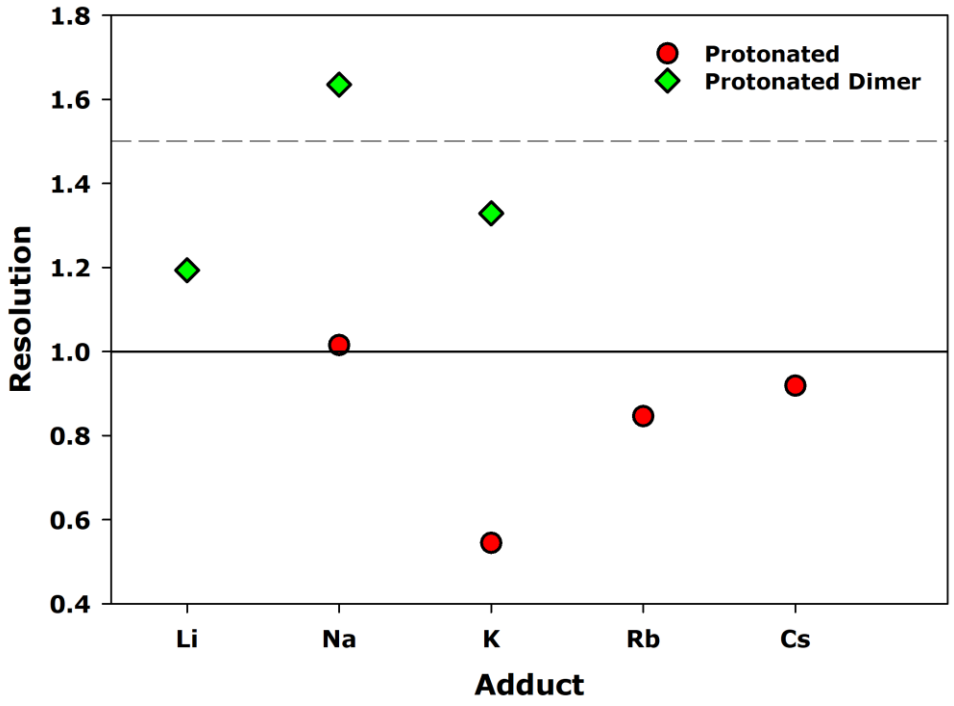

Figure S1. Scatter plot of the resolution values of standards of the neutral estradiol glucuronide with alkali adducts (red circle) and the dimeric neutral estradiol glucuronide with alkali adducts (green diamond).

Table S1. Material sources for chemicals used in this study.

Material	**Source**	**Location**
Polyalanine	Sigma-Aldrich	St. Louis, MO
Estradiol-3-Glucuronide	Cayman Chemical	Ann Arbor, MI
Estradiol-17-Glucuronide	Cayman Chemical	Ann Arbor, MI
HPLC Grade Water	Sigma-Aldrich	St. Louis, MO
Methanol	Fisher Scientific	Pittsburg, PA
Acetonitrile	Fisher Scientific	Pittsburg, PA

Table S2. Resolution values for standards of the neutral estradiol glucuronide with alkali adducts ($[M+H+X]^+$) and the dimeric neutral estradiol glucuronide with alkali adducts ($[2M+2H+X]^+$). N.D. represents not detected.

X	$[M+H+X]^+$	$[2M+2H+X]^+$
Li	N.D.	1.19
Na	1.02	1.64
K	0.54	1.33
Rb	0.85	N.D.
Cs	0.92	N.D.

Table S3. Collision cross sections, standard deviation (n = 4), error, and resolution of the sodiated dimer of the estradiol glucuronide isomers as standards and in a mixture.

Species	Standard CCS (Å²)	Mixture CCS (Å²)	% Error	Resolution
E3G	302.5 ± 3.4	306.7 ± 2.6	1.38	1.23
E17G	310.5 ± 1.9	315.6 ± 2.8	1.64	

Table S4. Collision cross sections (Ω) and standard deviation (n = 4) of metal adducts of estradiol-3-glucuronide (E3G) and estradiol-17-glucuronide (E17G).

	E3G		E17G	
Adduct	**Ω (Å²)**	**Standard Deviation**	**Ω (Å²)**	**Standard Deviation**
[M+Li]⁺	212.3	0.89	214.0	1.06
[M+Na]⁺	216.8	0.92	223.2	1.02
[M+K]⁺	220.5	1.18	224.9	0.93
[M+Rb]⁺	221.0	1.03	225.0	1.03
[M+Cs]⁺	225.7	1.98	227.0	1.03
[M-H+2Na]⁺	230.4	1.04	234.8	1.11
[M-H+2K]⁺	233.8	2.48	231.4	2.04
[M-H+2Rb]⁺	254.1	1.21	254.8	1.26
[M-H+2Cs]⁺	281.5	1.57	281.6	1.51
[2M+H+Li]⁺	305.8	1.54	311.3	1.37
[2M+H+Na]⁺	302.5	1.72	310.5	0.93
[2M+H+K]⁺	303.1	1.84	312.6	0.41

Table S5. Fraction of *m/z* 271 and standard deviation (*n* = 4) of metal adducts of E3G and E17G, where $\text{Abundance}_{271} = \sum \frac{PA_{271}}{PA_{271}+PA_{447}}$.

	E3G		E17G	
Collision Energy (V)	**Abundance$_{271}$ (%)**	**Standard Deviation**	**Abundance$_{271}$ (%)**	**Standard Deviation**
0	0.02	0.007	0.01	0.002
5	0.02	0.003	0.00	0.001
10	0.03	0.004	0.01	0.003
15	0.17	0.016	0.06	0.008
20	0.81	0.050	0.26	0.024
25	2.64	0.038	0.68	0.033
30	11.42	0.177	2.21	0.064
35	54.42	0.448	9.89	0.355
40	92.68	0.191	33.56	0.559
45	98.78	0.107	65.77	0.609