Electronic Supporting Information

A TIMS-TOF mass spectrometry study of either the positive or the negative ions of disaccharides from in-situ derivatization ESI with 3-pyridinylboronate

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Figure S1. Mobilograms of the sodium ion adducts of 9 disaccharides

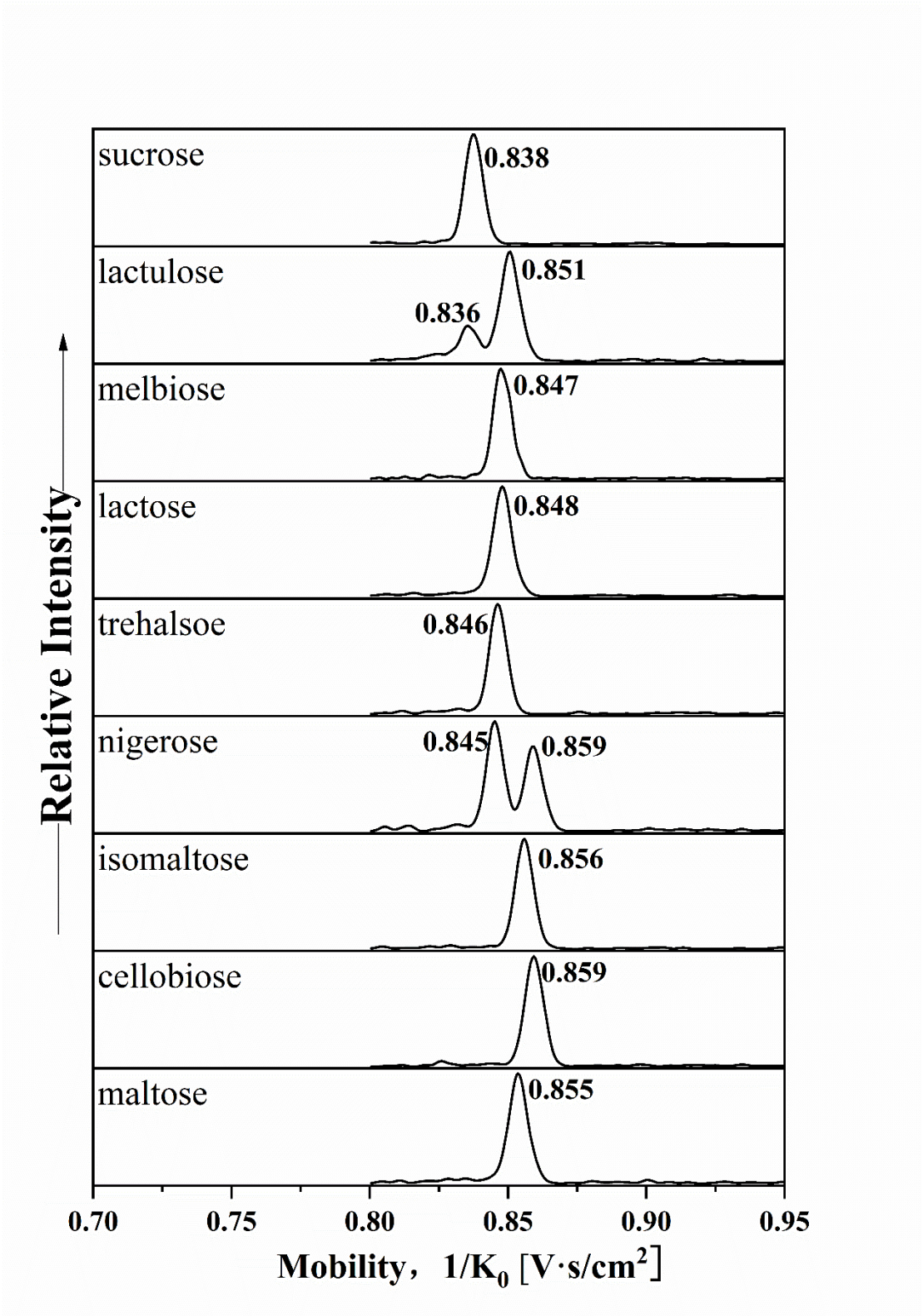

Figure S2. Mobilograms of the PBA double-tagged ions of 9 disaccharides (m/z 517) in cation mode

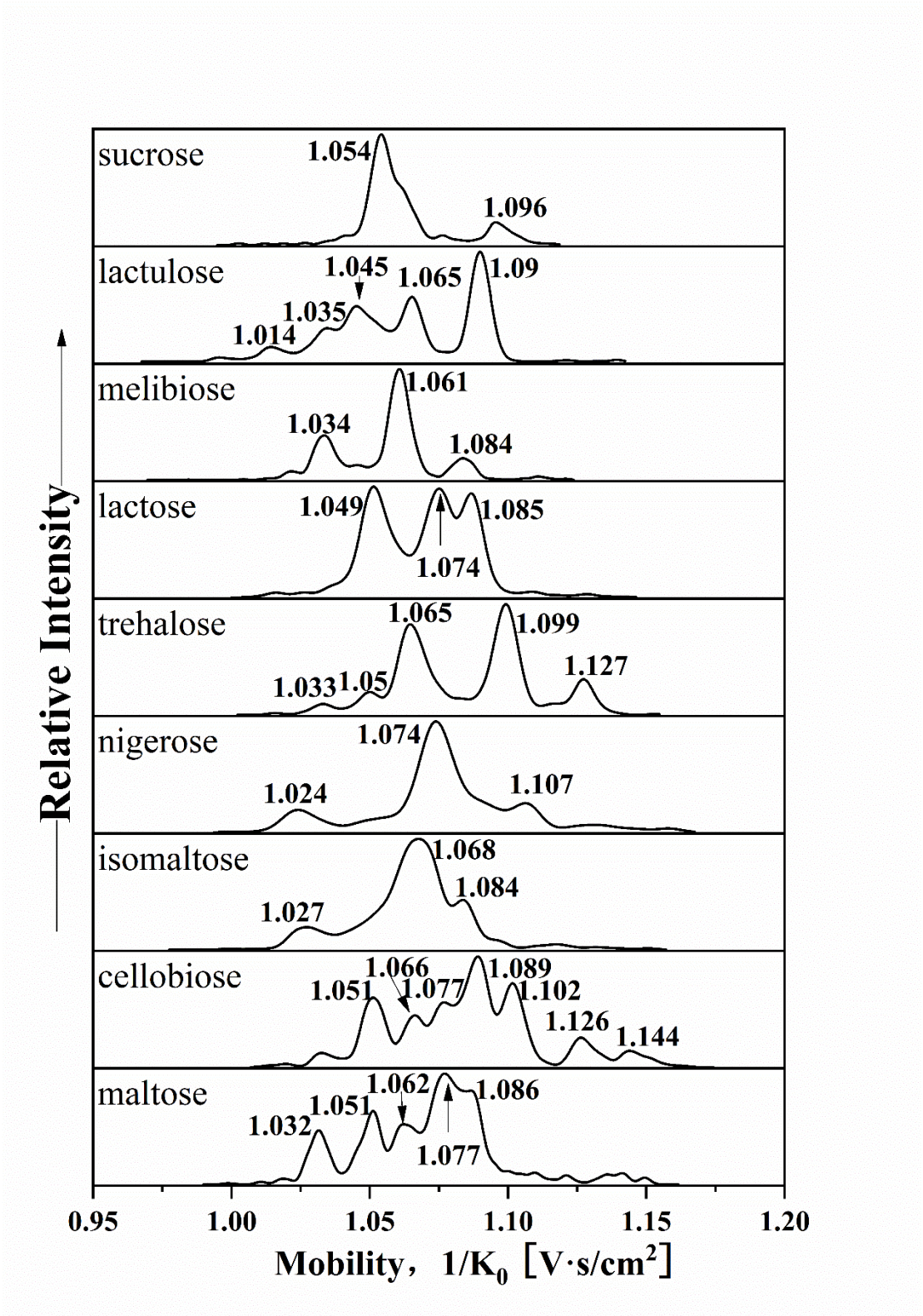

Figure S3. Mobilograms of the PBA double-tagged ions of 9 disaccharides (m/z 535) in cation mode

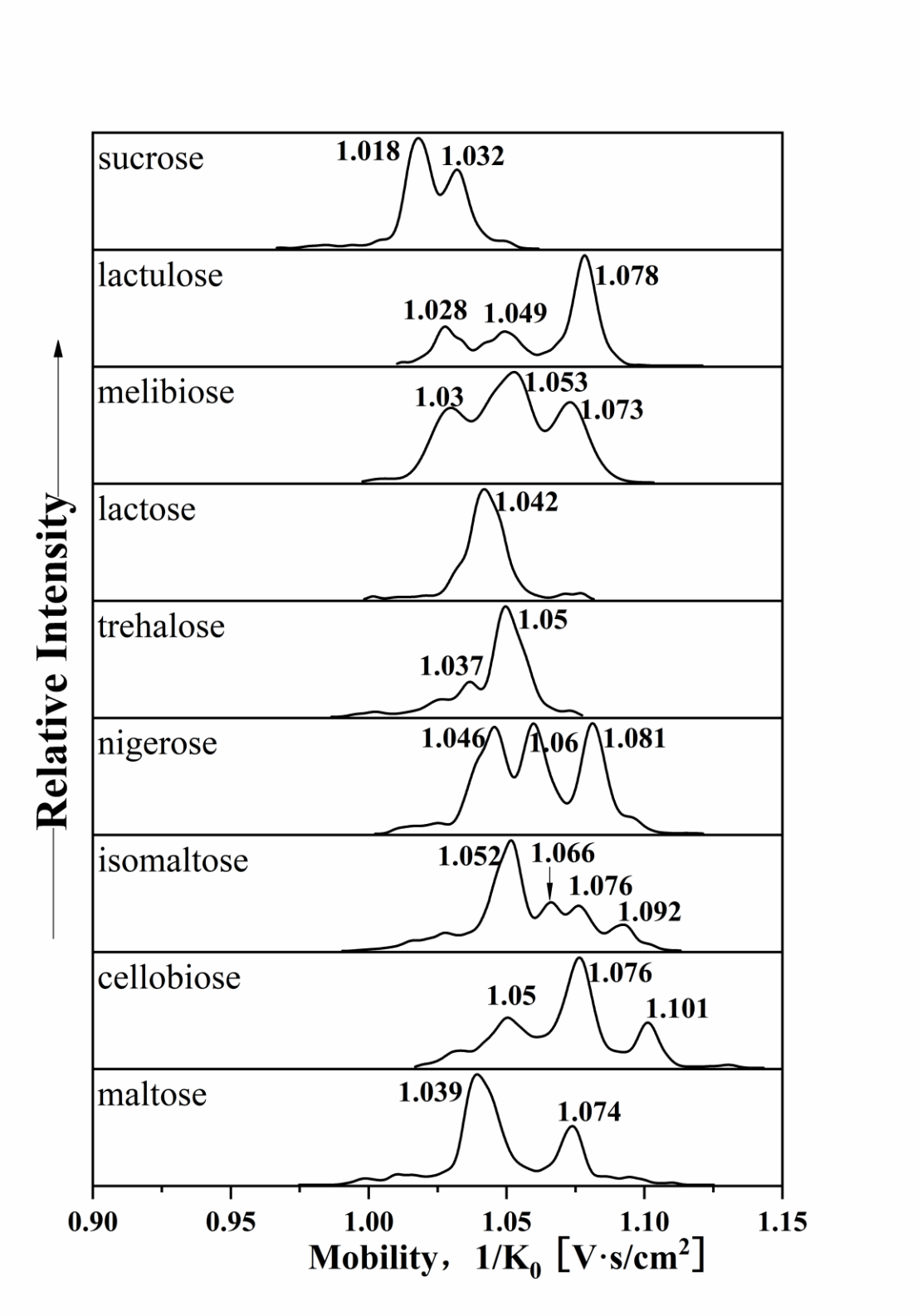

Figure S4. Mobilograms of the PBA double-tagged ions of 9 disaccharides (m/z 515) in anion mode

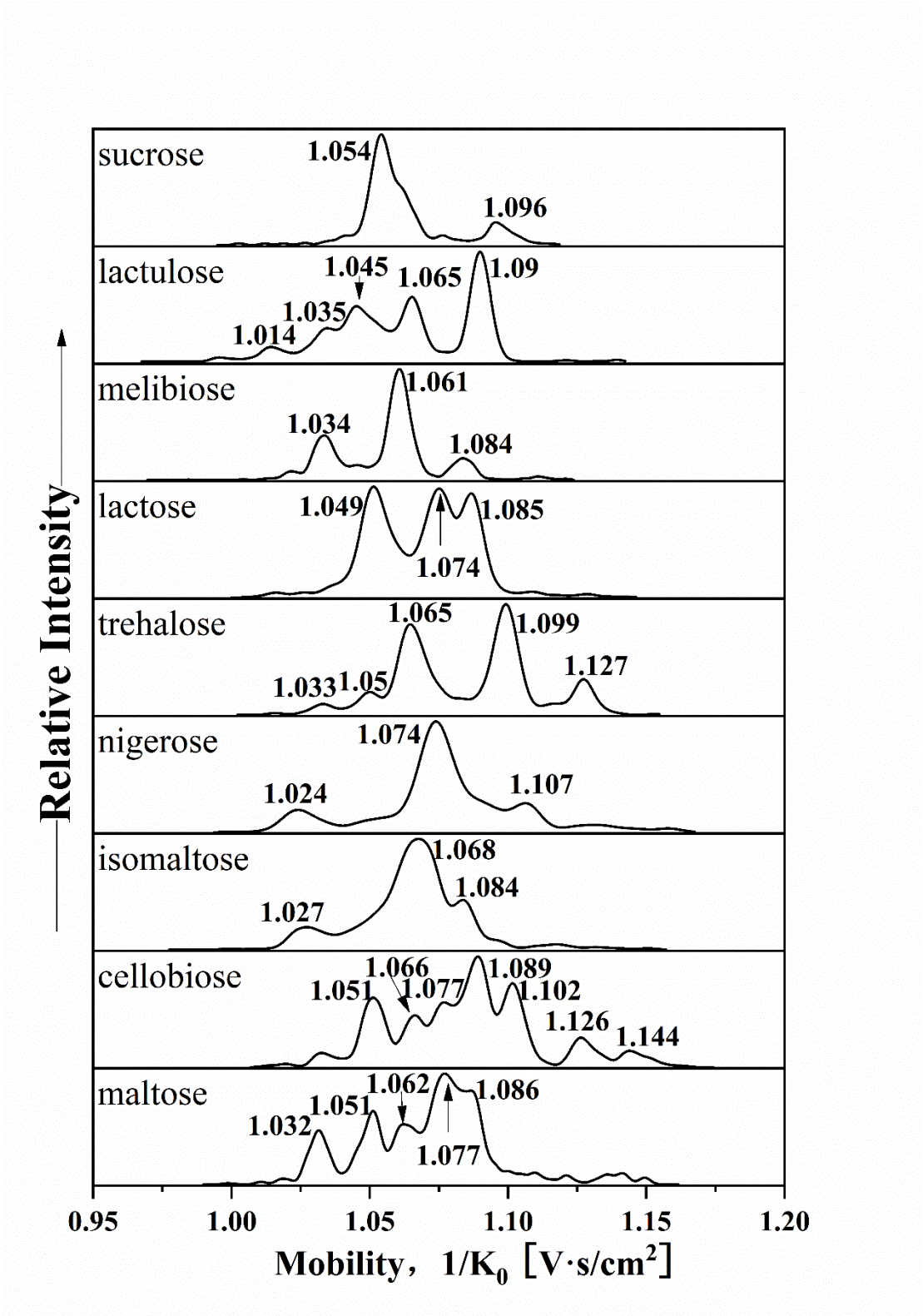

Figure S5. Energy-resolved fragment ion yields for PBA tagged disaccharide ions ($[PBA+M-2H_2O+H]^+$ m/z 430)

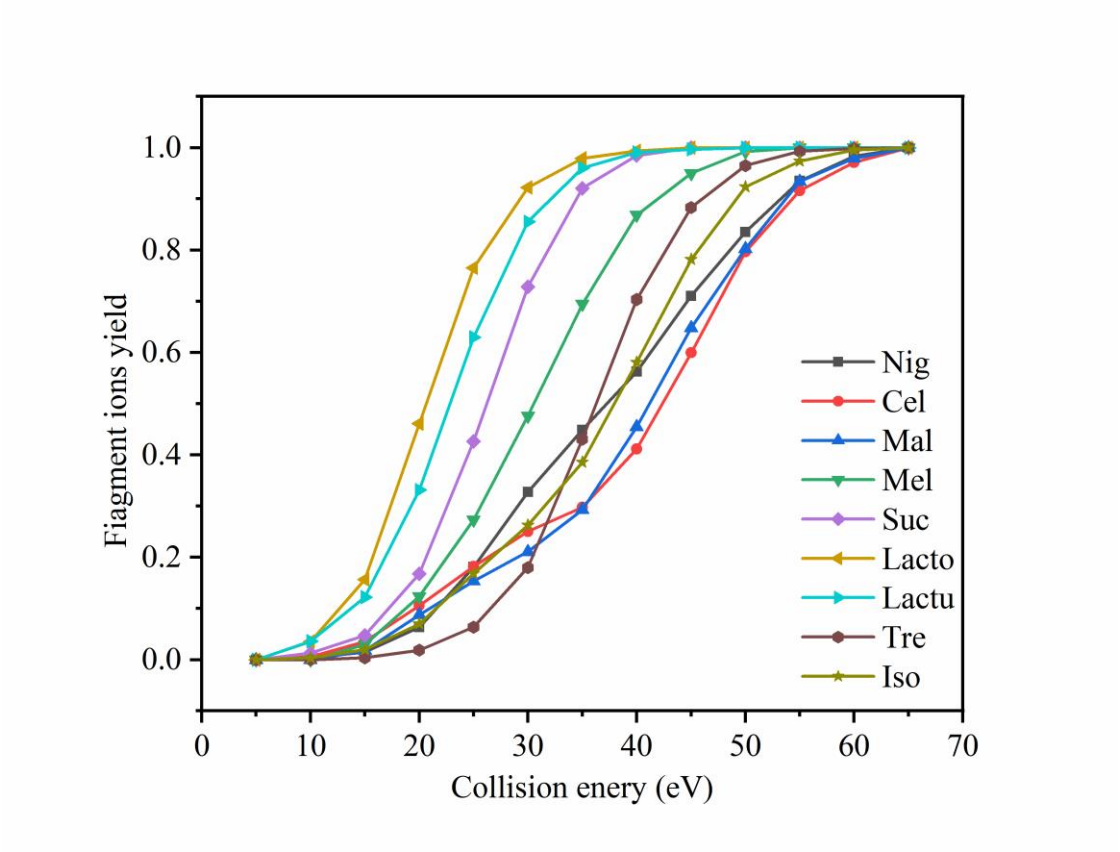

Table S1. CCS values of sodium ion adducts in this report in comparison with that in the literature

	CCS (literature[1]) [Å^2]	CCS (this work) [Å^2]	CCS differences (%)
[Sucrose+Na]$^+$	173.9	174.0	0.057
[Lactose+Na]$^+$	178.8	176.2	1.45
[Maltose+Na]$^+$	179.2	177.6	0.89
[Melibiose+Na]$^+$	181.1	176.2	2.71
[Cellobiose+Na]$^+$	178.7	178.6	0.056
[Isomaltose+Na]$^+$	178.0	177.8	0.11
[Lactulose+Na]$^+$	180.1	176.8	1.83
[Trehalose+Na]$^+$	177.8	175.9	1.07
[Nigerose+Na]$^+$	——	175.6	——

Table S2. The CCS values of the sodium ion adducts and those of the PBA tagged ions of the 9 disaccharides in cation mode (all the experiments were performed using N_2 as buffer gas in trapped ion mobility, major peaks were in bold)

	CCS [Å^2]			
	$[M+Na]^+$	$[M+PBA-2H_2O+H]^+$	$[M+2PBA-4H_2O+H]^+$	$[M+2PBA-3H_2O+H]^+$
Sucrose	174.0	**203.2**	**204.1**/209.4	**209.1**/212
Lactose	176.2	**188.1**/194.3	204.4/**208.9**/214.5	**214**
Maltose	177.6	**204.8**	**204.4**/209.2/211.8	**213.5**/220.6
Melibiose	176.2	188.3/**207.2**	204.4/**209.7**/213/223.1	211.6/**216.3**/220.4
Cellobiose	178.6	**206.4**	**215.1**/221	215.8/**221.1**/226.2
Isomaltose	177.8	**206.4**	206.5/210.2/**212.5**/217.9	**216**
Lactulose	176.8	**190.1**/192.2	204.1/**207.8**/212.3	211.1/215.6/**221.5**
Trehalose	175.9	197.5/**206.8**	**206.8**/214.1	**215.6**
Nigerose	175.6	**190.6**/**206.6**	**212.4**	214.8/**217.7**/**222.1**

Table S3. The CCS values of the sodium ion adducts and those of the PBA tagged ions of the 9 disaccharides in anion mode (all the experiments were performed using N_2 as buffer gas in trapped ion mobility, major peaks were in bold)

	CCS [Å^2]	
	$[M+PBA-2H_2O-H]^-$	$[M+2PBA-4H_2O-H]^-$
Sucrose	**190**/193/195.4/198.6/202.5	**216.8**/225.3
Lactose	188.4/**192.7**/197.1	**216**/221.1/223.3
Maltose	190.3/**192.9**	212.1/215.8/218.6/**221.5**
Melibiose	185.2/**191.5**	212.6/**218.5**
Cellobiose	**192.9**/196.9	216.2/219.3/221.4/**223.9**/226.5
Isomaltose	185.8/**192**	**219.6**/222.8
Lactulose	188.4/192.8/**196.8**	215.1/219.1/**224.1**
Trehalose	191.4/194.6/**197.9**/204.3	218.9/**226**/231.6
Nigerose	187.2/192.5/**199.3**	**221**

Table S4. Magnifications of the IMS R_{P-P} values of the main peaks for PBA tagged disaccharides in comparison with those of the sodium ion adducts

Disaccharide Pair	Magnification				
	m/z 430	m/z 517	m/z 535	m/z 428	m/z 515
sucrose-lactose	7.15	2.34	2.19	1.06	0.40
sucrose-maltose	0.42	0.06	0.81	0.61	0.92
sucrose-melibiose	1.80	2.00	1.65	0.70	0.59
sucrose-cellobiose	0.68	2.02	1.84	0.56	1.07
sucrose-isomaltose	0.84	1.92	1.26	0.52	0.42
sucrose-lactulose	4.09	1.24	3.54	2.55	2.35
sucrose-trehalose	2.00	1.51	2.76	4.73	4.47
sucrose-nigerose	8.27	4.84	2.39/3.86/6.90	5.18	1.92
lactose-maltose	9.69	2.88	0.02	0.16	1.92
lactose-melibiose	82.03	2.84	0.46	3.51	9.05
lactose-cellobiose	6.64	2.07	1.70	0.11	1.98
lactose-isomaltose	9.38	1.74	0.67	0.15	0.77
lactose-lactulose	2.14	1.21	6.14	3.86	7.31
lactose-trehalose	81.78	10.00	5.07	19.04	36.16
lactose-nigerose	5.53	7.27	1.06/5.13/12.87	9.93	6.53
maltose-melibiose	1.73	3.27	1.00	0.78	1.90
maltose-cellobiose	1.69	10.55	5.34	——	1.62
maltose-isomaltose	3.47	16.47	3.67	1.20	2.00
maltose-lactulose	18.95	5.05	8.32	4.05	2.91
maltose-trehalose	1.05	1.41	0.81	1.90	1.75
maltose-nigerose	6.53	3.30	0.37/1.16/2.70	1.73	0.16
melibiose-cellobiose	0.33	1.61	0.93	0.49	1.80
melibiose-isomaltose	0.47	1.25	0.06	0.33	0.51
melibiose-lactulose	22.67	2.19	4.00	7.67	9.00
melibiose-trehalose	0.86	5.36	0.68	13.71	16.79
melibiose-nigerose	25.19	3.05	0.95/1.00/4.48	9.24	3.14
cellobiose-isomaltose	——	3.05	4.91	0.95	3.23
cellobiose-lactulose	8.29	3.47	0.17	1.80	0.08
cellobiose-trehalose	0.14	2.60	1.28	1.41	0.49
cellobiose-nigerose	5.17	0.71	1.18/0.68/0.25	1.42	0.59
isomaltose-lactulose	14.76	3.84	3.59	3.84	2.41
isomaltose-trehalose	0.18	2.51	0.13	2.37	1.66
isomaltose-nigerose	6.98	0.07	0.30/0.42/1.83	2.21	0.26
lactulose-trehalose	13.54	0.95	4.05	0.89	1.51
lactulose-nigerose	0.30	3.09	3.30/2.00/0.41	1.45	1.86
trehalose-nigerose	74.79	24.11	2.33/6.16/22.88	5.07	16.71

References

1. Zheng, X.; Aly, N. A.; Zhou, Y.; Dupuis, K. T.; Bilbao, A.; Paurus, V. L.; Orton, D. J.; Wilson, R.; Payne, S. H.; Smith, R. D.; Baker, E. S. A structural examination and collision cross section database for over 500 metabolites and xenobiotics using drift tube ion mobility spectrometry. *Chem. Sci.* **2017,** *8* (11), 7724-7736.