Supplementary information

Instrument parameters

The analytical instrument used in this work was the TIMS-time-of-flight mass spectrometry (TIMS-TOF MS) from Bruker Daltonik (Bremen, Germany), which equipped with an electrospray ionization (ESI) source. All samples were analyzed by direct injection with a glass syringe of 500 mL from Hamilton (Giarmata, Romania). The sample solutions were directly injected into the ESI emitter through a syringe pump at a rate of 3 μL/min. The parameters of the TIMS-TOF MS are set as follows: the end plate offset voltage was set at 500V, the capillary voltage was set at 4.5 kV, the range of $1/K_0$ was set to 0.5-2.09 V·s cm^{-2}, the dry gas flow rate was set at 4 L min^{-1} at 200 ℃, and the nebulizer gas pressure was set at 0.3 bar; With these parameter settings, the mass and ion mobility was calibrated using the Agilent ESI Low Concentration Tuning Mix before the experiment.

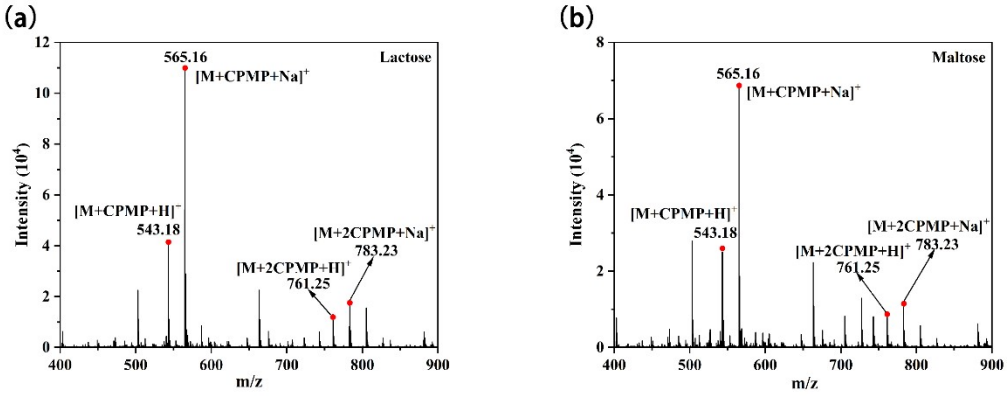

Fig. S1 Positive ion mass spectra of CPMP labeled lactose (a) and maltose (b).

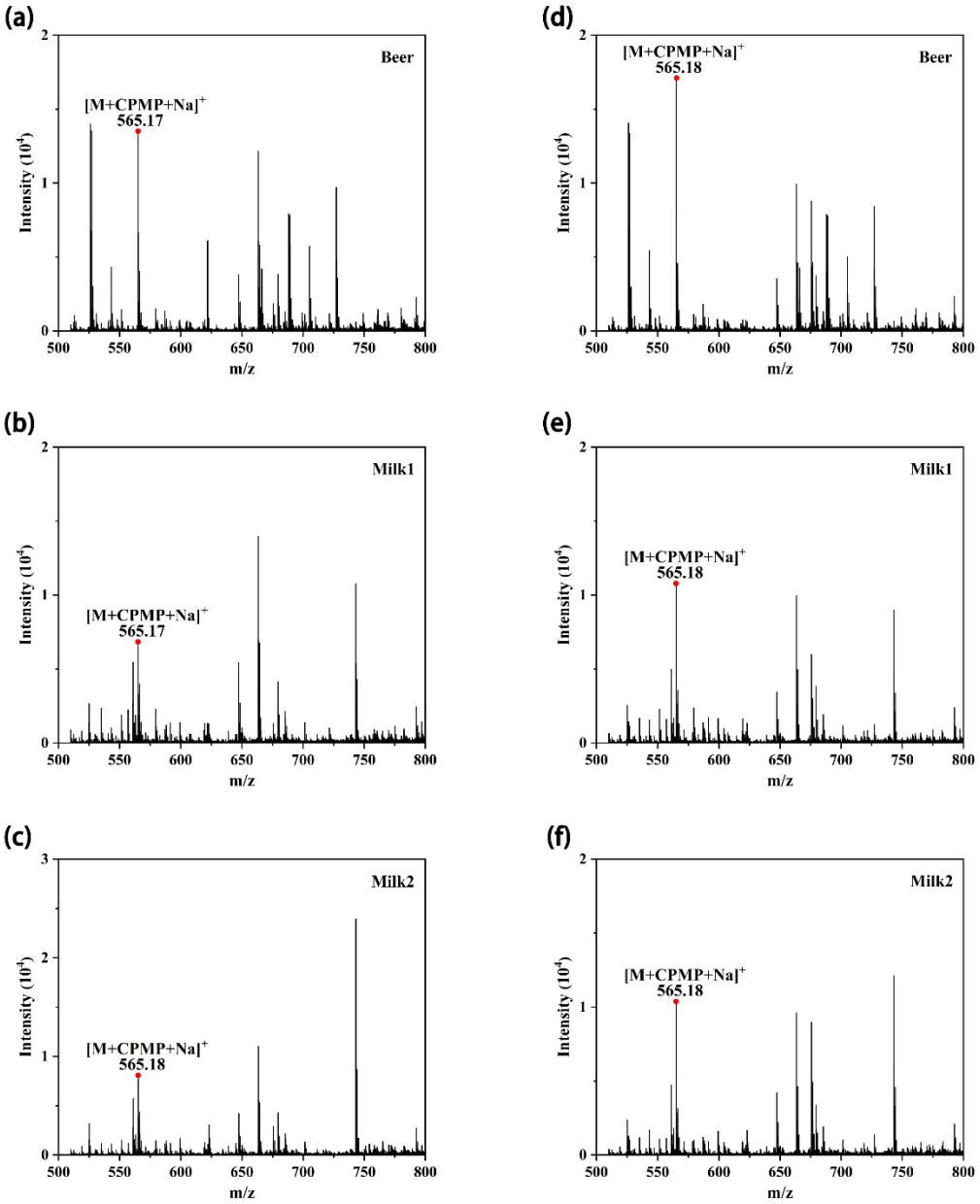

Fig. S2 Mass spectra of beer and milk after derivatization. (a) (b) (c) unspiked and (d) (e) (f) spiked with lactose and maltose (1mg/mL).

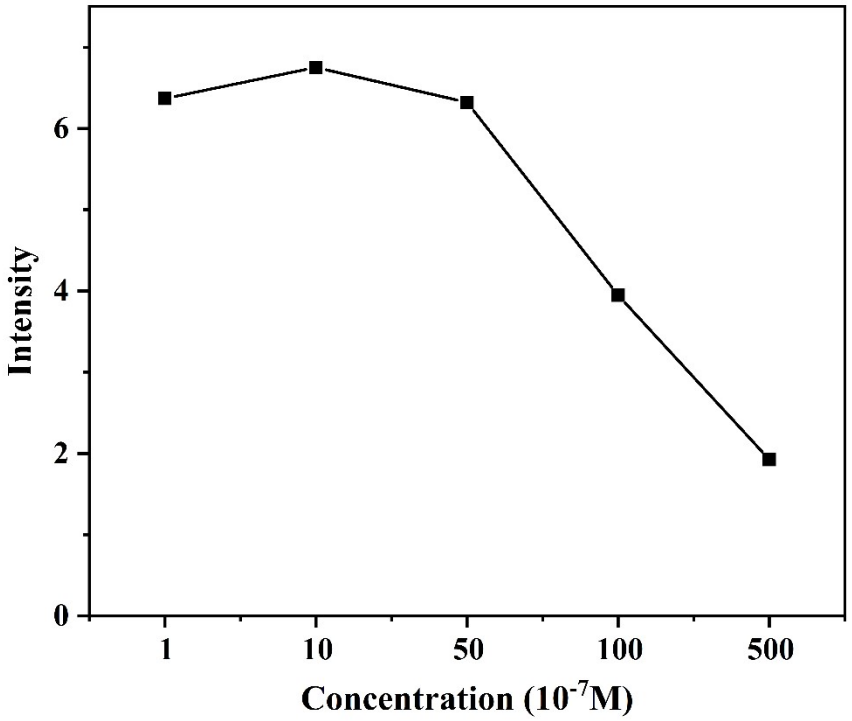

Fig. S3 Signal intensity of $[M + CPMP + Na]^+$ at different Na^+ concentrations.

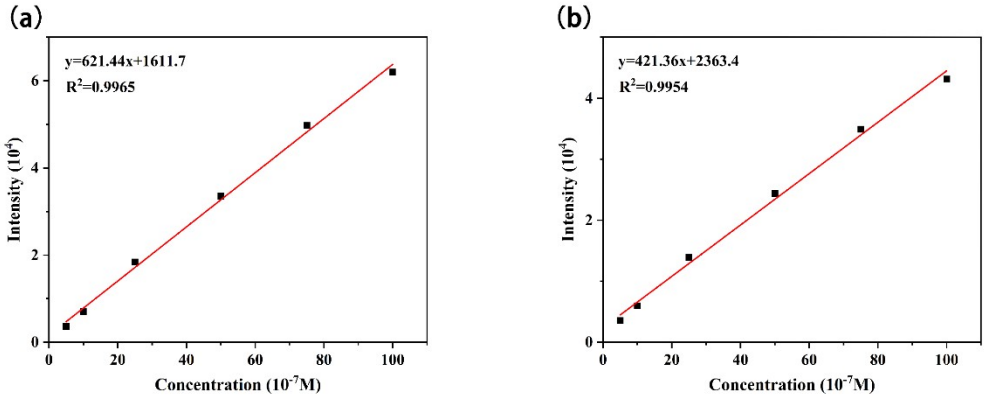

Fig. S4 The linear curves for absolute quantification of lactose (a) and maltose (b).

Table S1 Analytical results after derivatization of the isomers lactose and maltose.

Ions	m/z	$1/K_0$		W_{FWHM}		CCS		R_{P-P}
Analyte		Lactose	Maltose	Lactose	Maltose	Lactose	Maltose	
$[M + Na]^+$	365.12	0.837	0.850	0.013	0.012	173.9	176.6	0.763
$[M + K]^+$	381.09	0.852	0.865	0.009	0.010	176.7	179.5	0.803
$[M + CPMP + H]^+$	543.18	1.102	1.117	0.011	0.011	226.2	229.4	0.801
$[M + CPMP + Na]^+$	565.16	1.116	1.137	0.012	0.012	229.0	233.2	1.028
$[M + 2CPMP + H]^+$	761.25	1.328	1.352	0.010	0.009	270.7	275.7	1.484
$[M + 2CPMP + Na]^+$	783.23	1.352	1.342	0.010	0.011	275.6	273.4	0.559

Table S2 Analysis of $[M + CPMP + Na]^+$ after disaccharide derivatization.

$[M + CPMP + Na]^+$	$1/K_0$ (V·s/cm^2)	CCS (Å^2)
Isomaltose	1.128	231.3
Melibiose	1.130	231.7
Cellobiose	1.132	232.1
Gentiobiose	1.125	230.7

Table S3 Analysis of $[M + 2CPMP + H]^+$ after disaccharide derivatization.

$[M + 2CPMP + H]^+$	$1/K_0$ (V·s/cm^2)	CCS (Å^2)
Isomaltose	1.324	269.9
Melibiose	1.326	270.4
Cellobiose	1.332	271.7
Gentiobiose	1.325	270.1

Table S4 Quantitative results of spiked lactose and maltose isomers in real samples.

Real samples	Spiked (mol/L)		Detected (mol/L)		Recovery rate (%)
	Lactose	Maltose	Lactose	Maltose	
Beer	5.85×10^{-7} M	/	4.67×10^{-7} M	/	79.8
Milk1	/	5.56×10^{-7} M	/	4.77×10^{-7} M	85.8
Milk2	/	5.56×10^{-7} M	/	5.86×10^{-7} M	105.4

Table S5 Comparison with previous methods used to identify and quantify disaccharides.

Method	Sample pre-treatment	Analysis time (min)	Sensitivity	recovery rate (%)	Reference
CZE	Complex	22	μg/L	94.0-102.5%	1
HPLC-ELSD	Complex	50	mg/L	80.4-99.4%	2
HPLC	Complex	16	mg/L	96.0-107.0%	3
IMS	Simple	3	μg/L	79.8-105.4%	This work

Reference

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2. Y.Q. Zhang, W.H. Zhang, J.B. Hou, J.M. He, K. Li, Y. Li, D.M. Xu, Determination of sugars and sugar alcohols in infant formula by high performance liquid chromatography with evaporative light-scattering detector, *J. Chromatogr. B*, 2023, **1217**, 123621. DOI: 10.1016/j.jchromb.2023.123621.
3. E. Akyüz, K.S. Baskan, E. Tütem, R. Apak, High performance liquid chromatographic method with post-column detection for quantification of reducing sugars in foods, *J. Chromatogr. A*, 2021, **1660**, 462664. DOI: 10.1016/j.chroma.2021.462664.