

SUPPORTING INFORMATION

Liquid Chromatography-Mass Spectrometry Approach for Characterizing Sucrose Isomers in Complex Mono-Floral Honey

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1. Study of Voltage Effect on Sugar-Chloride Adduct Formation using cESI Platform

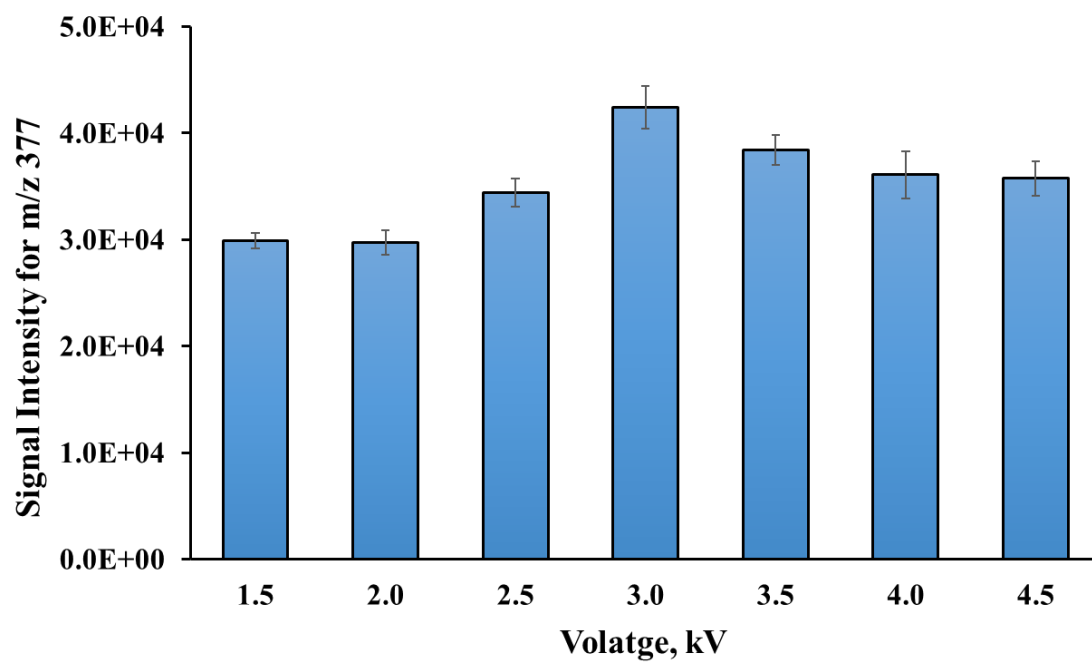


Figure S1. Effect of voltage on chloride adduction of sucrose (100 μ M). Error bars represent standard deviation of five replicates.

2. Optimization of Reagent Flow Rate for Chloride-Sucrose Adduction

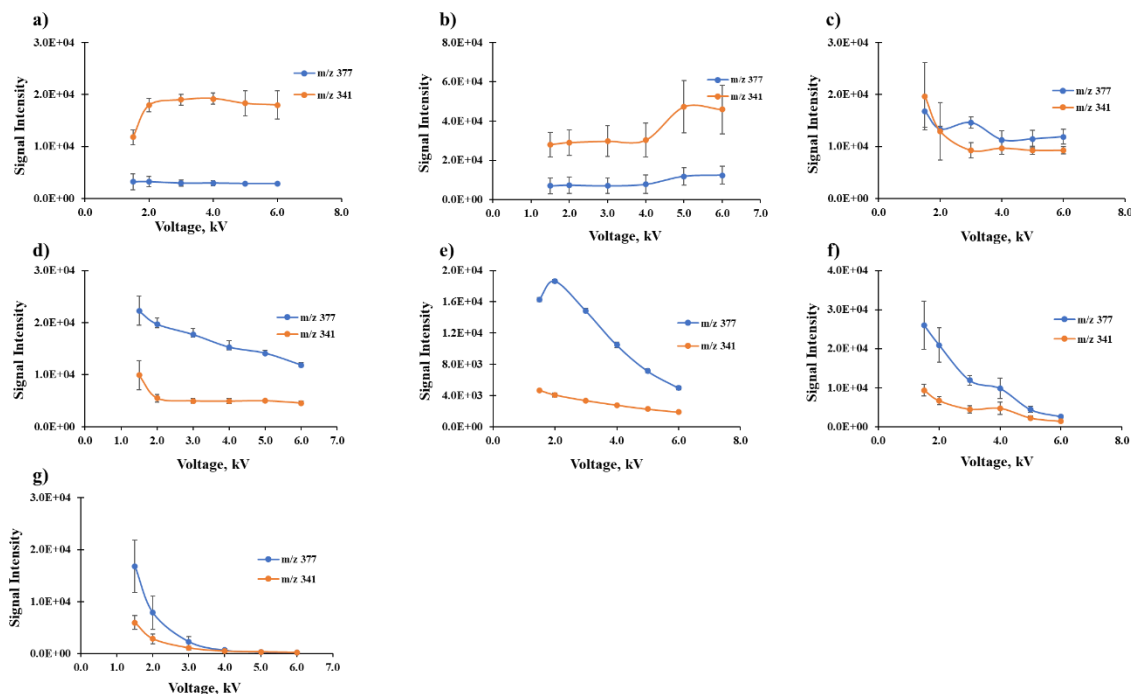


Figure S2. Effect of reagent flow rate on chloride adduction relative to deprotonated sucrose at **a)** 5 **b)** 10 **c)** 20 **d)** 30 **e)** 40 **f)** 50 and **g)** 60 $\mu\text{L}/\text{min}$. Error bars represent standard deviation of three replicates.

3. Effect of Chloride concentration in Adduction of Sucrose

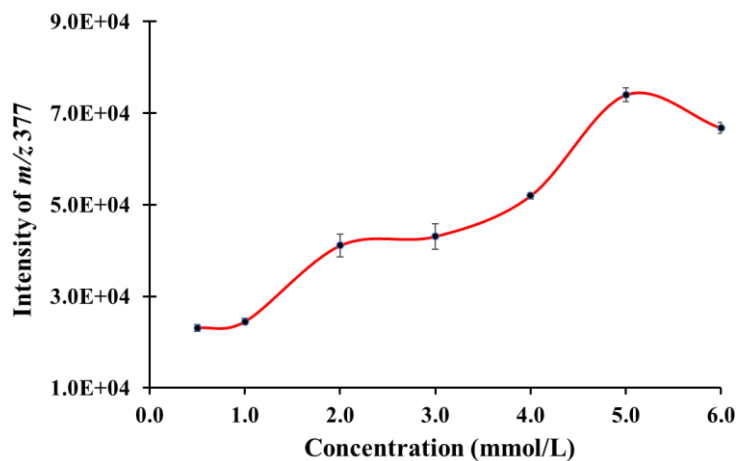


Figure S3. Plot showing effect of chloride concentration on sucrose adduction. Error bars represent standard deviation of five replicates.

4. Effect of Column Flow Rate on Retention Time

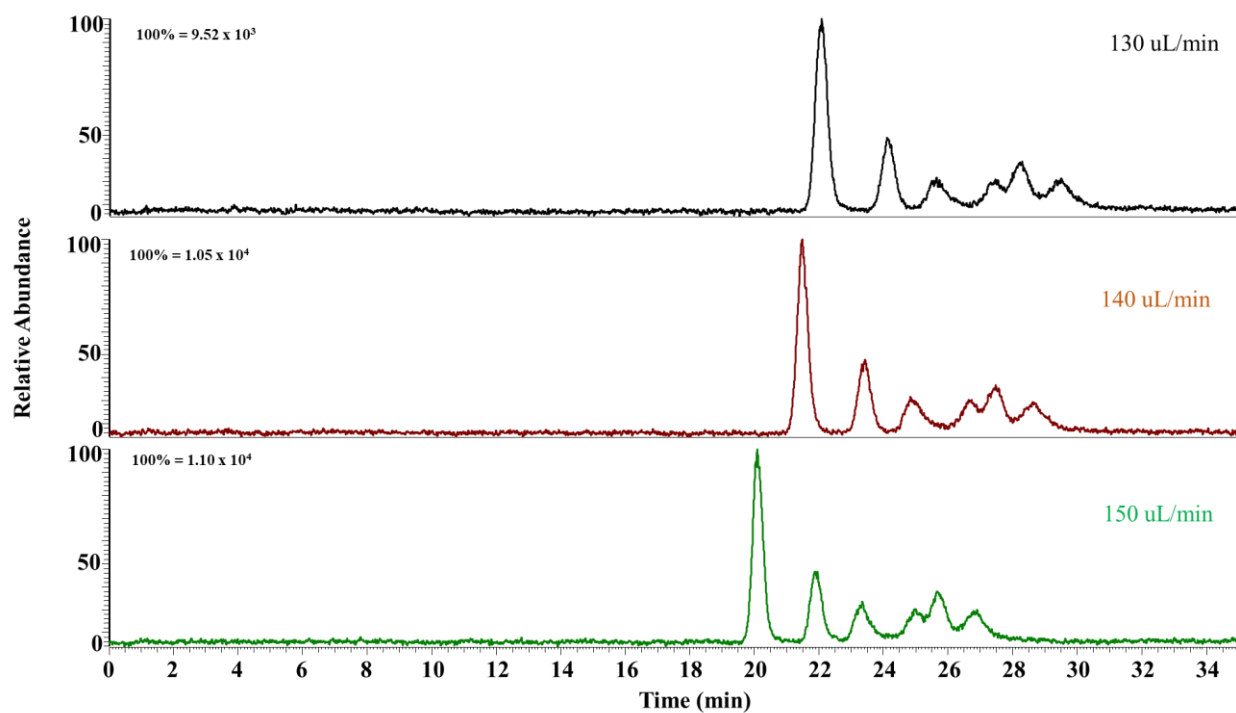


Figure S4. Chromatograms showing separation of mixture of sucrose isomers (2 μ M) at various flow rates (μ L/min).

5. Effect of Column Temperature on Retention Time

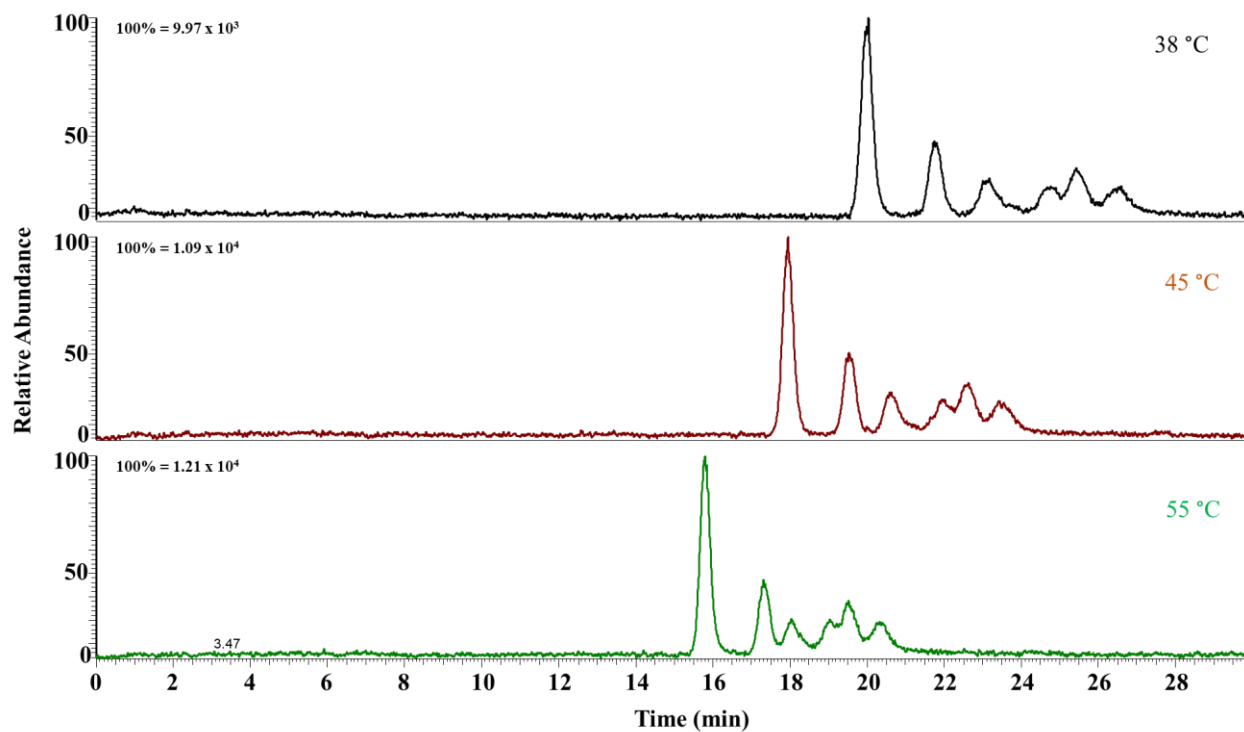


Figure S5. Chromatograms showing separation of mixture of sucrose isomers (2 μ M) at various column temperatures (°C).

6. LC-MS/MS Analysis of Standard Individual Isomers

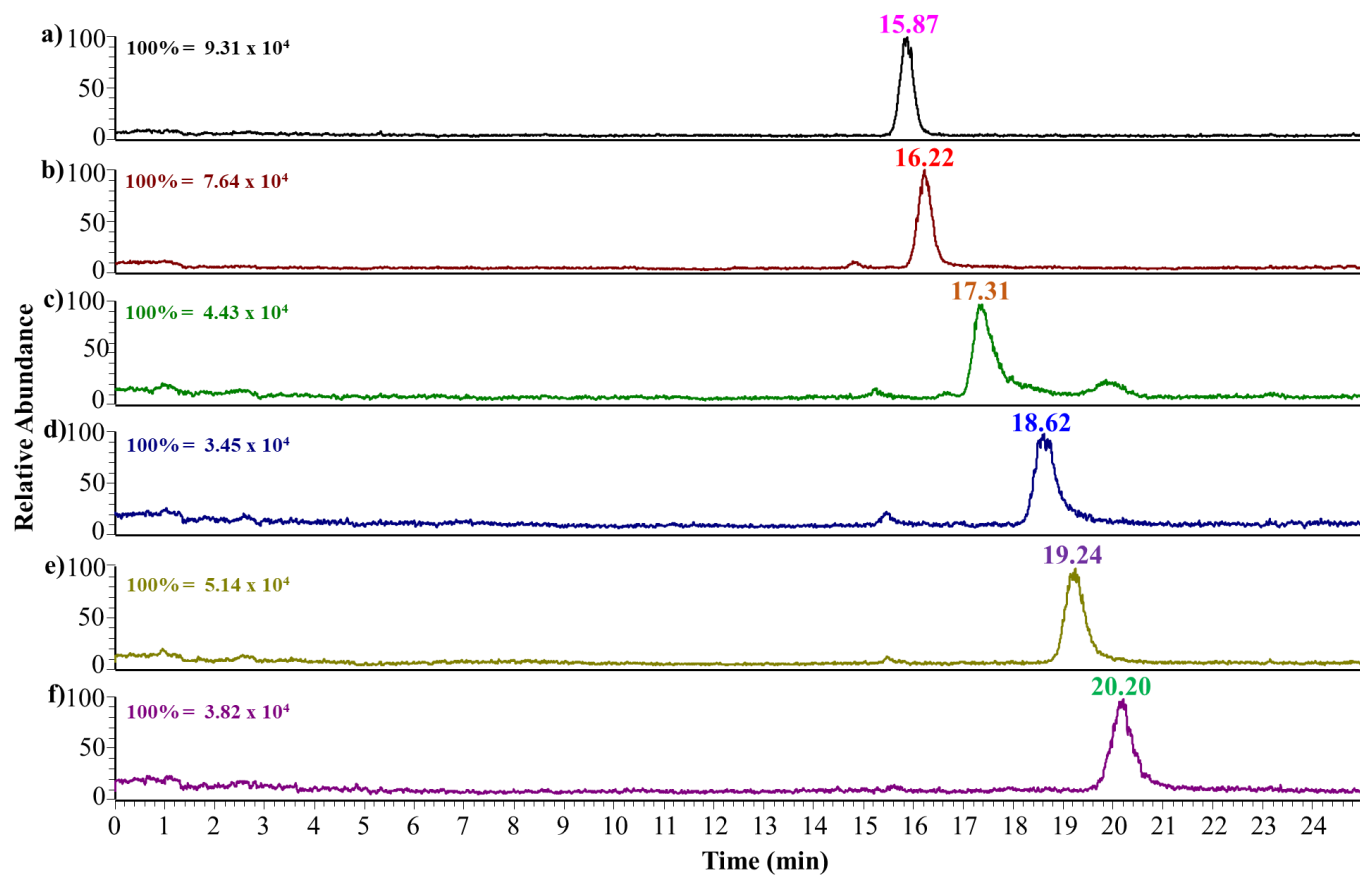


Figure S6. Individual chromatogram for **a)** Sucrose **b)** Turanose **c)** Palatinose **d)** Maltulose **e)** Leucrose **f)** Trehalulose each at concentration of 2 μ M.

7. Tandem MS Analysis of Standard Individual Isomers

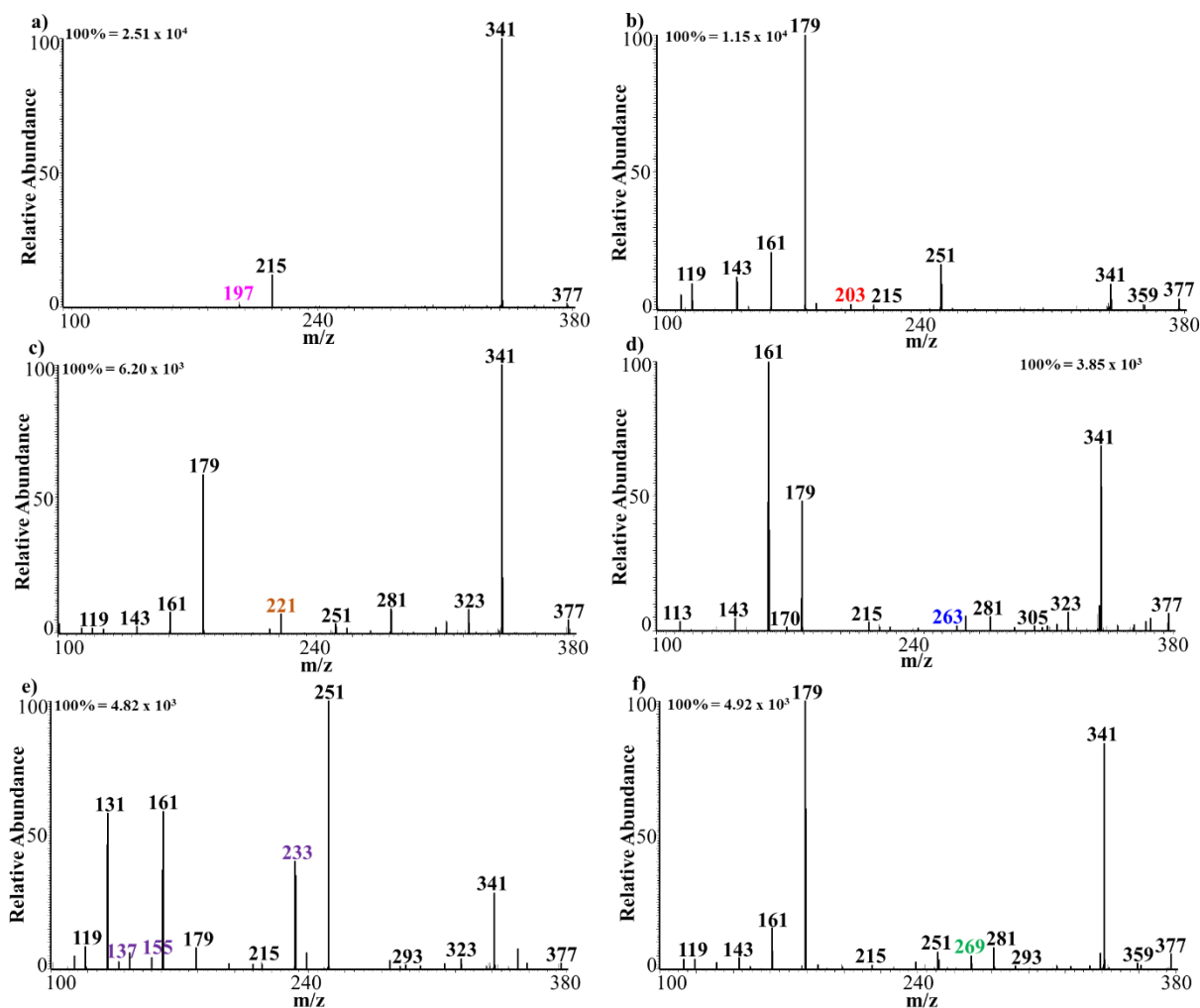


Figure S7. Negative-ion mode product ion spectra for each of the isomers of sucrose (2 μ M) in the standard chromatogram, **a)** Sucrose **b)** Turanose **c)** Palatinose **d)** Maltulose **e)** Leucrose **f)** Trehalulose, all at m/z 377. Different color indicates the diagnostic ions for specific sucrose isomer upon MS/MS.

8. LC-MS/MS Analysis of Isomers in Mixture in Positive ion mode

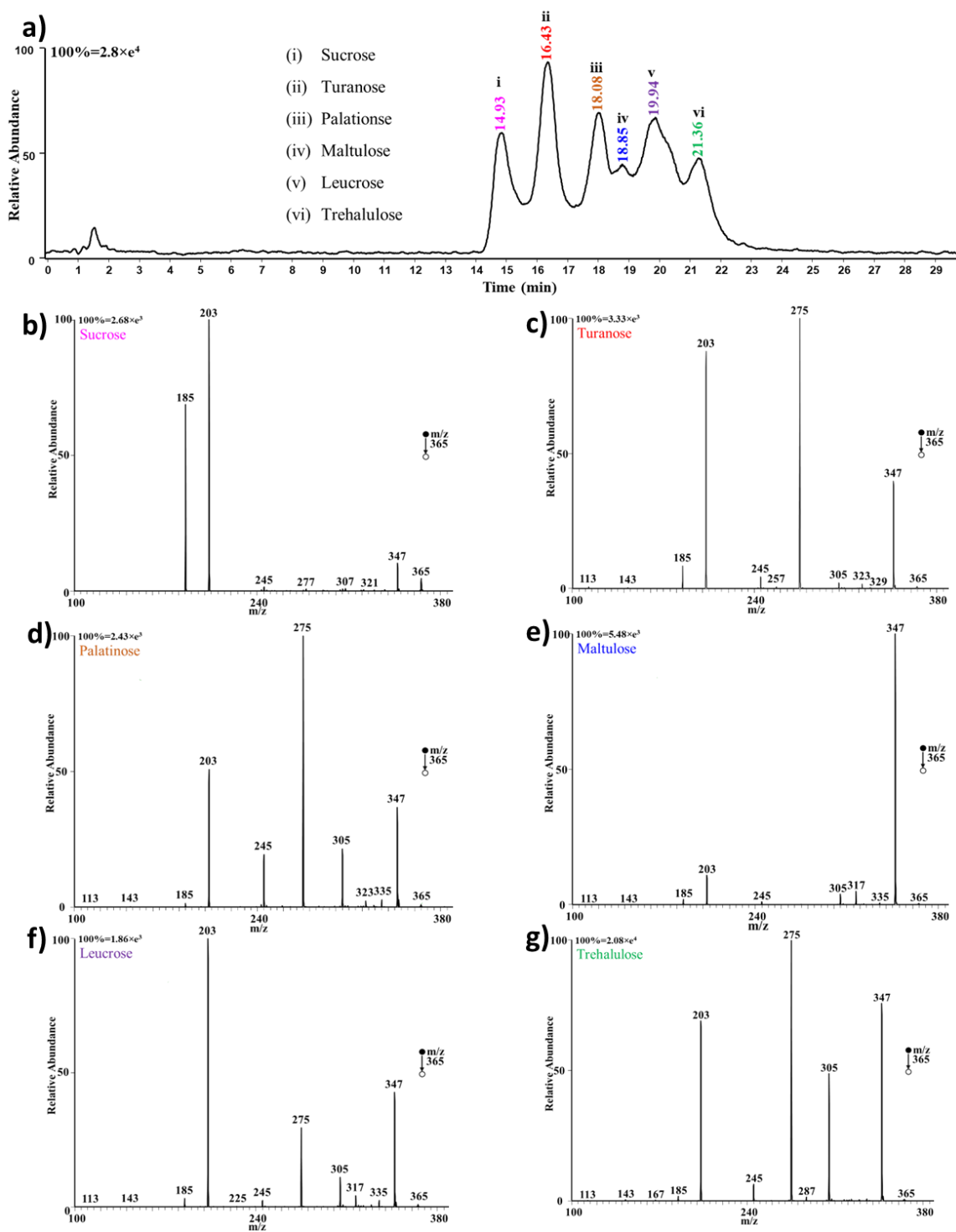


Figure S8. a) Chromatogram generated using LC-MS/MS product ion scanning with sodium adduction
b-g) Positive-ion mode product ion spectra for isomers of sucrose (2 μ M) in the standard chromatogram, all at m/z 365.

9. Calibration Plots of Chloride Adducted Disaccharides

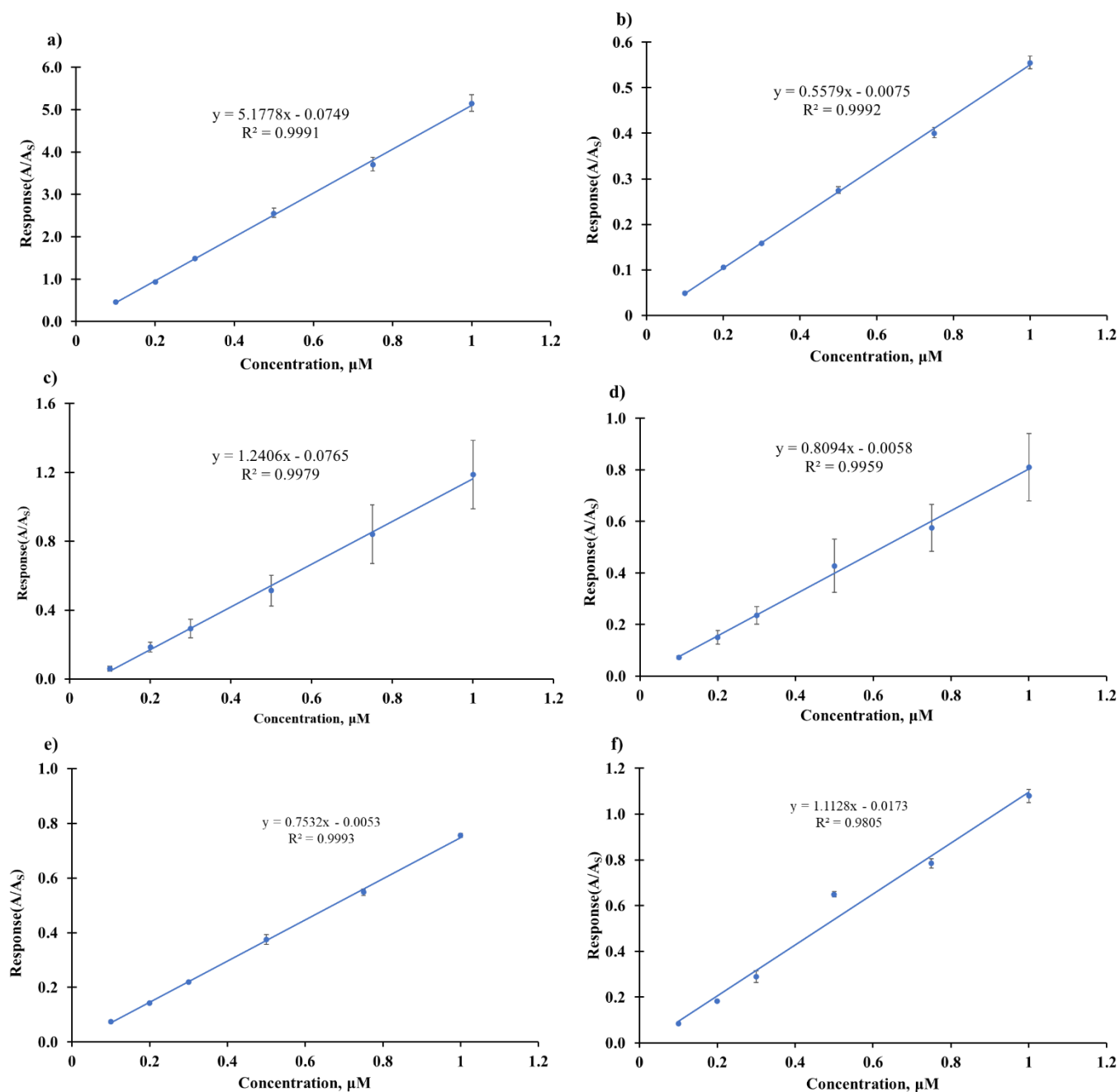


Figure S9. Negative-ion mode chloride adducted calibration plot for **a)** Sucrose **b)** Leucrose **c)** Palatinose **d)** Maltulose **e)** Trehalulose and **f)** Turanose.

10. Calibration Plots of Sodium Adducted Disaccharides

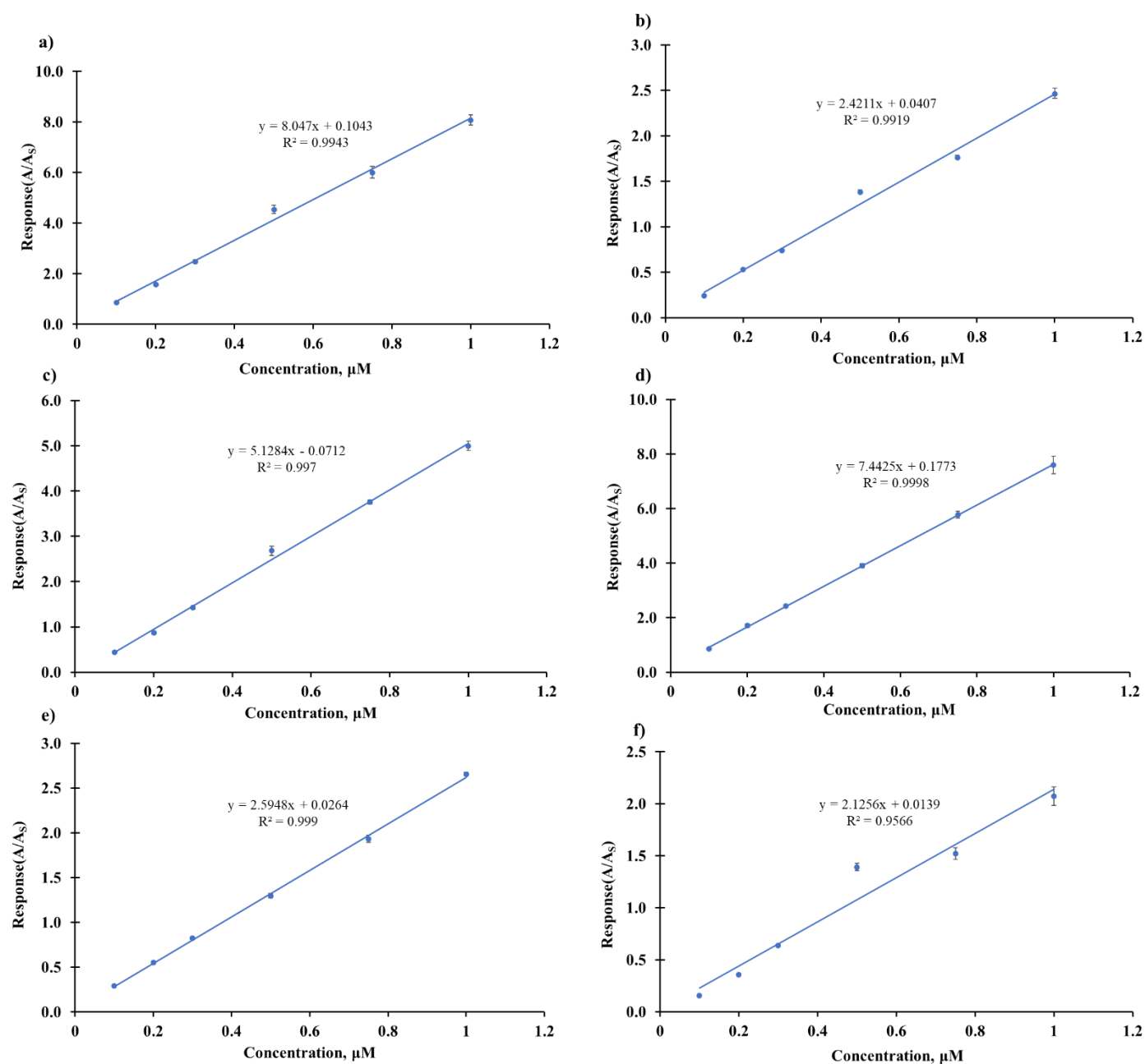


Figure S10. Positive-ion mode sodium adducted calibration plot for **a)** Sucrose **b)** Leucrose **c)** Palatinose **d)** Maltulose **e)** Trehalulose and **f)** Turanose.

11. Intra-day repeatability of sucrose isomers

Table S1. Relative standard deviation of sucrose isomers (n=4) at two different concentrations.

Concentration (μ M)	RSD (%)					
	Sucrose	Turanose	Palatinose	Maltulose	Leucrose	Trehalulose
0.1	2.5	2.0	21.9	14.6	3.4	6.8
0.5	8.7	3.7	20.7	9.1	5.1	9.5

12. Heat Maps for negative and positive- ion mode of analysis

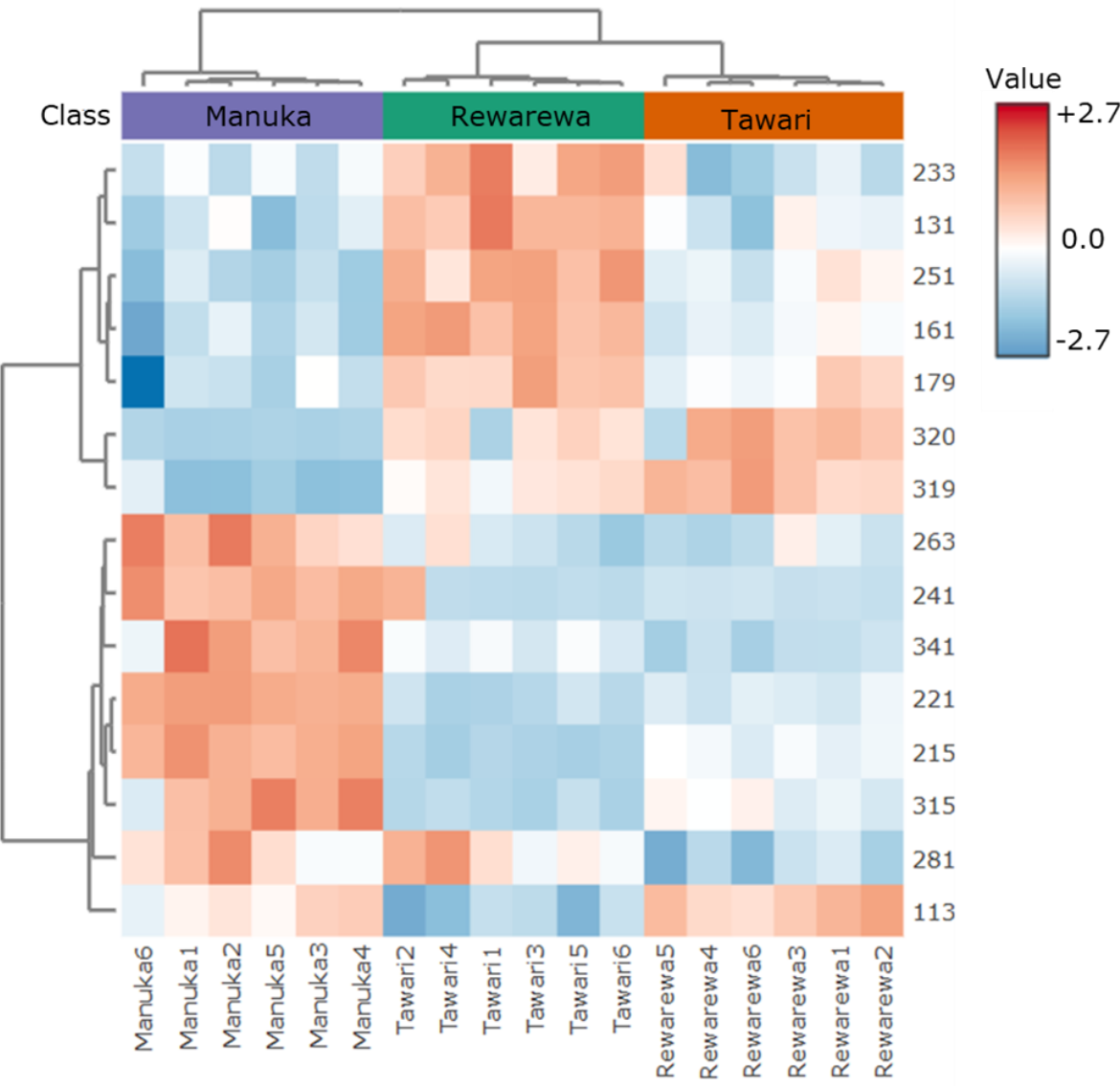


Figure S11. Heatmap results obtained for negative-ion mode tandem MS for sucrose isomers identified in all the honey samples (i.e; Turanose, Palatinose, Maltulose and Trehalulose).

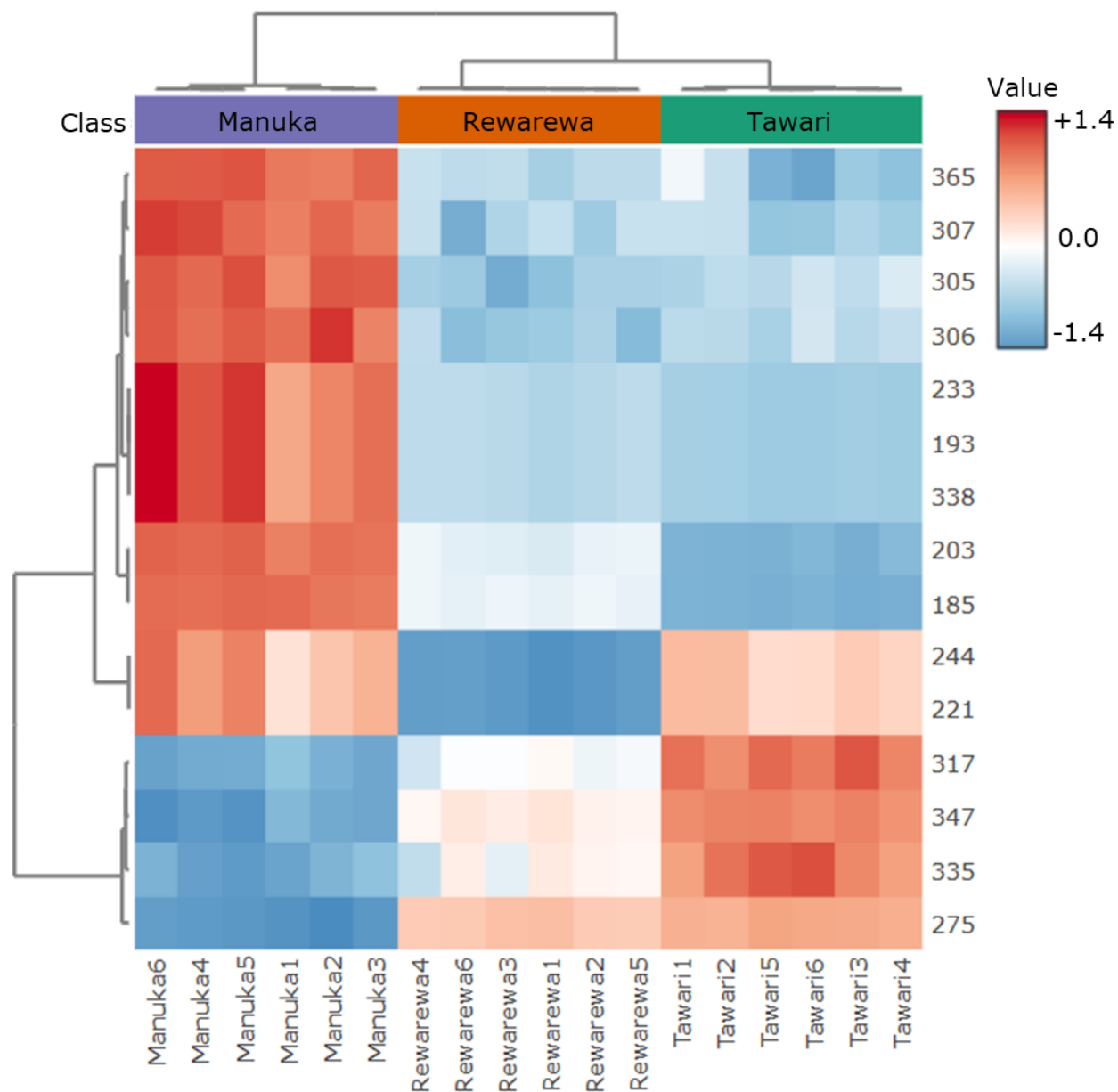


Figure S12. Heatmap results obtained for positive-ion mode tandem MS for sucrose isomers identified in all the honey samples (i.e; Turanose, Palatinose, Maltulose and Trehalulose).