Electronic Supplementary Material (ESI) for Food & Function

Supporting information

Phenolic Promiscuity in the cell nucleus - Epigallocatechingallate (EGCG) and theaflavin 3, 3ʻdigallate from green and black tea bind to model cell nuclear structures including histone proteins, double stranded DNA and telomeric quadruplex DNA

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1. Molecular ion weight calculation from MS spectra

Since TOF mass spectrometer is used, the peaks are well-resolved and isotope pattern can be used to determine to molecular weight of nucleic acids. The calculation of MW is done using the difference in m/z between peaks in Fig. S1.

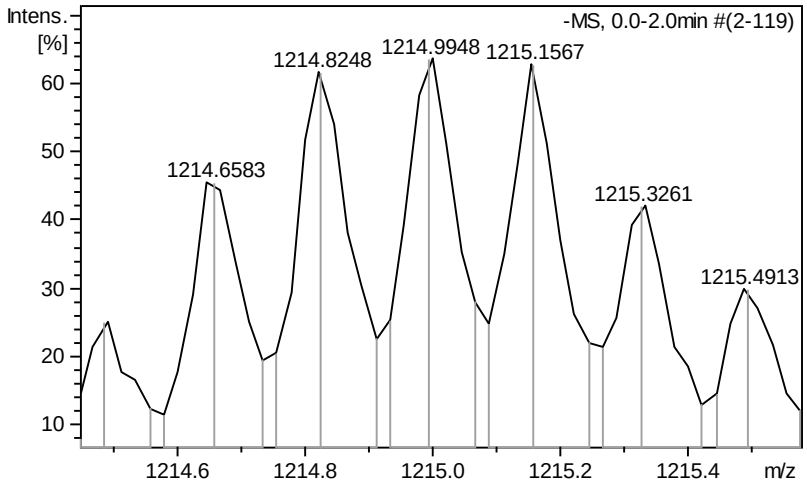

Figure S1. The spectrum of clearly resolved peak of 22AG (zoomed in Fig. 5A).

In singly charged ion spectrum the difference between isotopes is m/z = 1. If multiply charged ion is observed, its isotope pattern is n times denser, where n – charge of molecular ion. Thus, the charge of molecular ion is calculated using the following equation:

$$n = \frac{1}{[m/z]_x - [m/z]_{x-1}}$$

Where x and x-1 denote two neighboring peaks. Precision can be improved if the difference between more peaks (y – number of peaks) is taken because error even out in that case:

$$n = \frac{1}{([m/z]_x - [m/z]_{x-y})y}$$

An example using spectrum in Figure S1:

$$n = \frac{1}{([m/z]_x - [m/z]_{x-y})y} = \frac{1}{(1215.4913 - 1214.6583)5} = 6.0024 \approx 6$$

Charges for all other peaks were calculated analogously.

2. Mass spectra of pure compounds

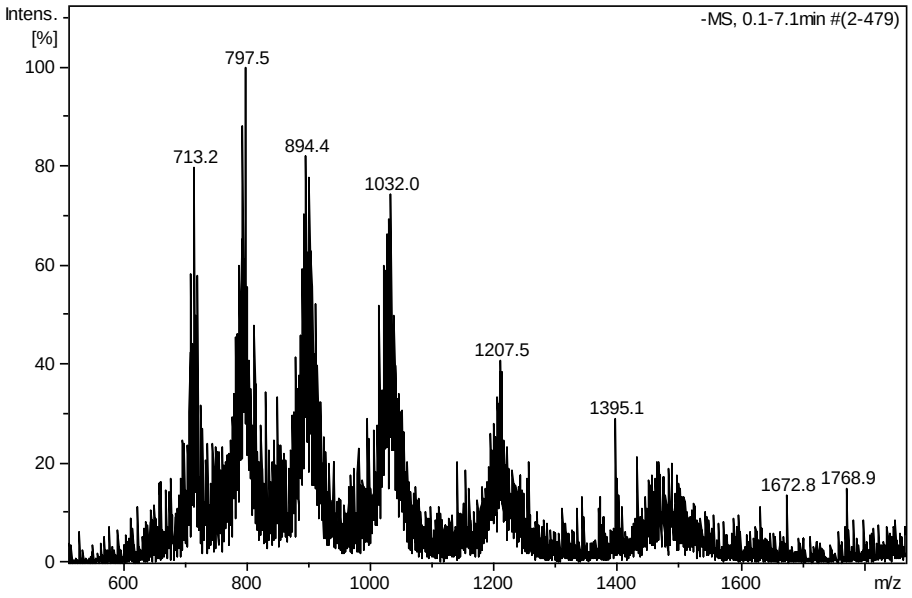

Figure S2. Negatively ionized mass spectrum of 22AG using ESI-Ion Trap mass spectrometer

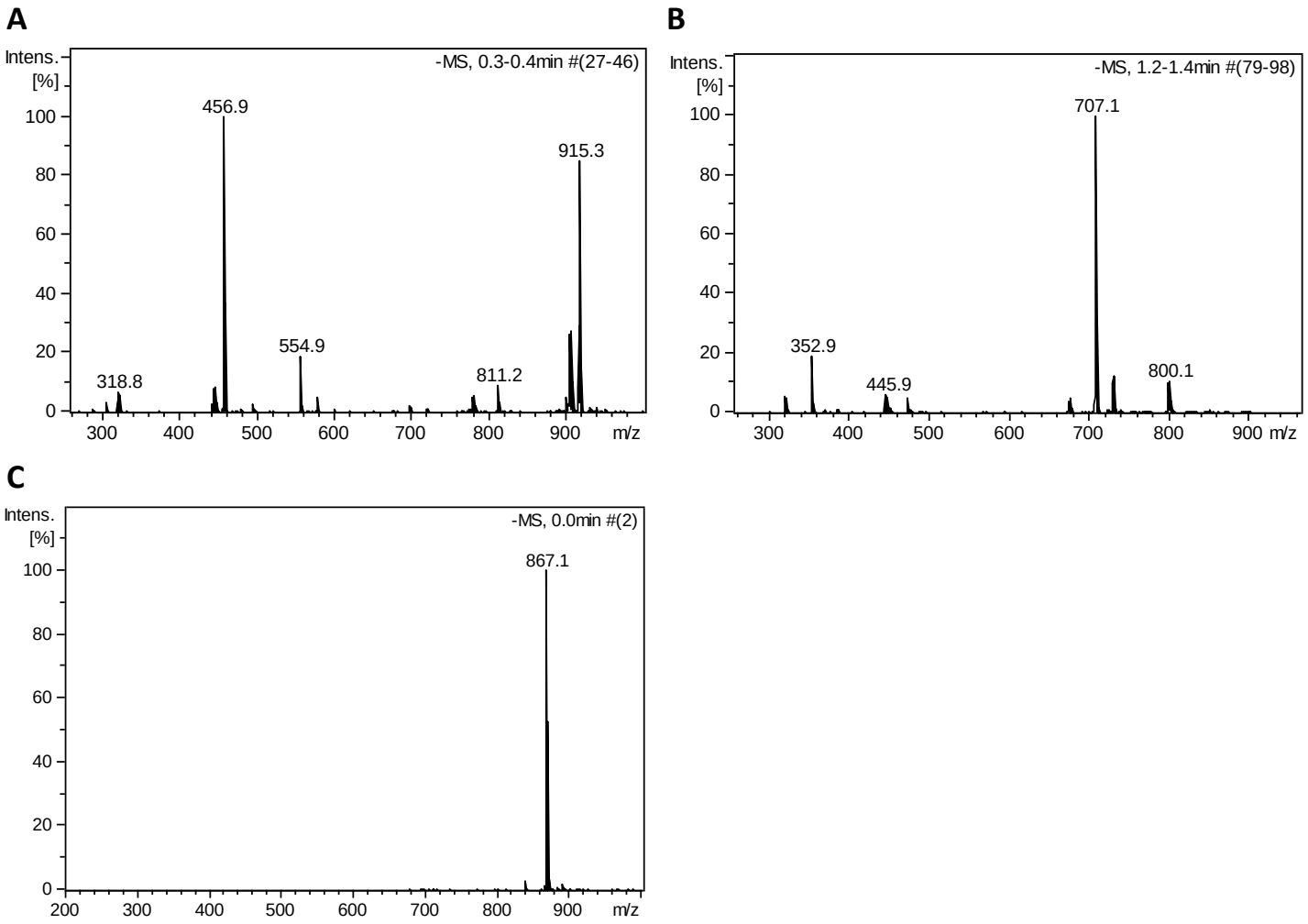

Figure S3. Negatively ionized mass spectra of polyphenols. (A) Chlorogenic acid (CGA); (B) Epigallocatechin-3-gallate (EGCG); (C) Theaflavin-3,3'-digallate.

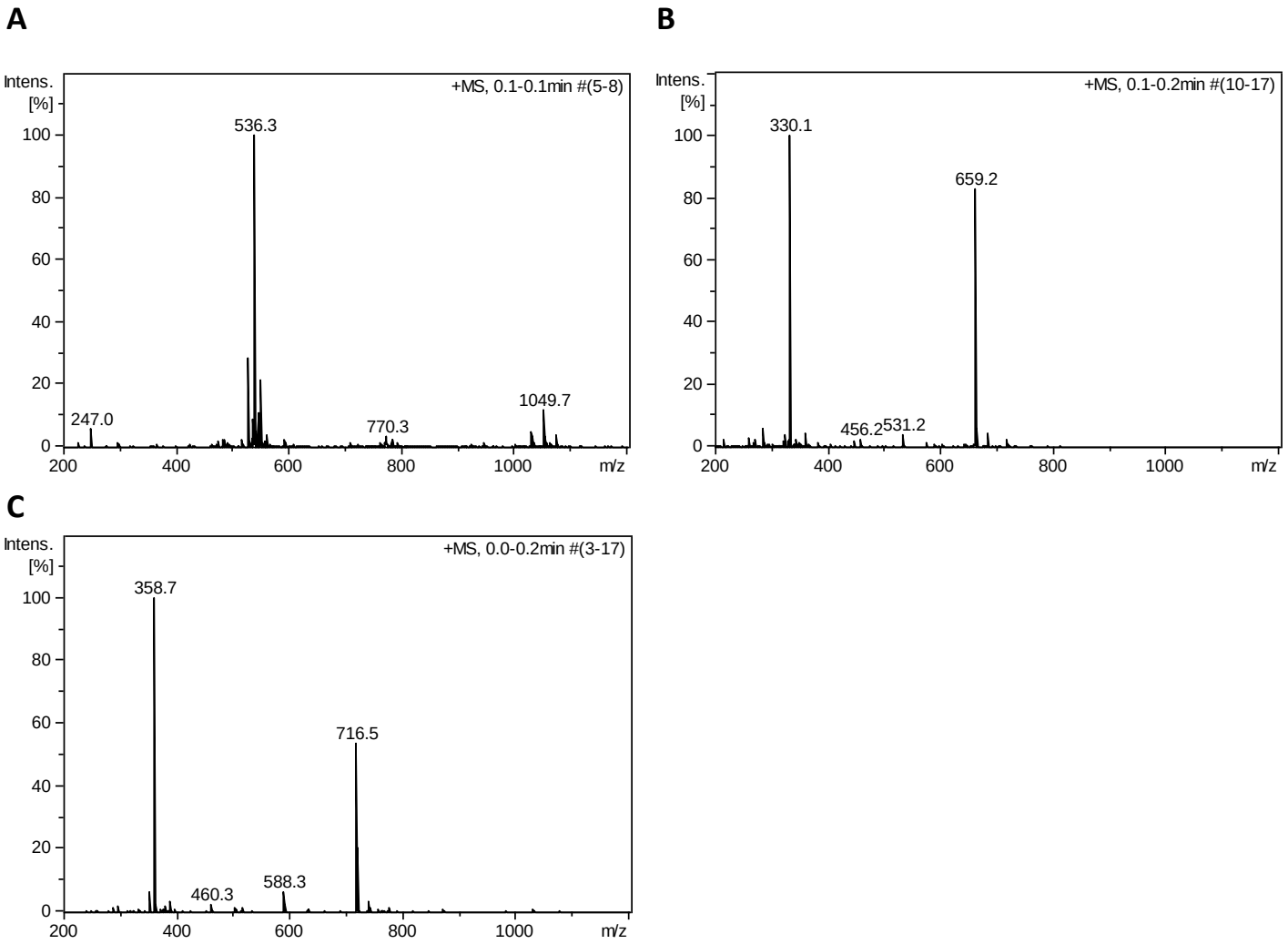

Figure S4. Positively ionized mass spectra of peptides. (A) Pep1 (QSVIKPGELG); (B) K_3AGAG; (C) K_4GAG

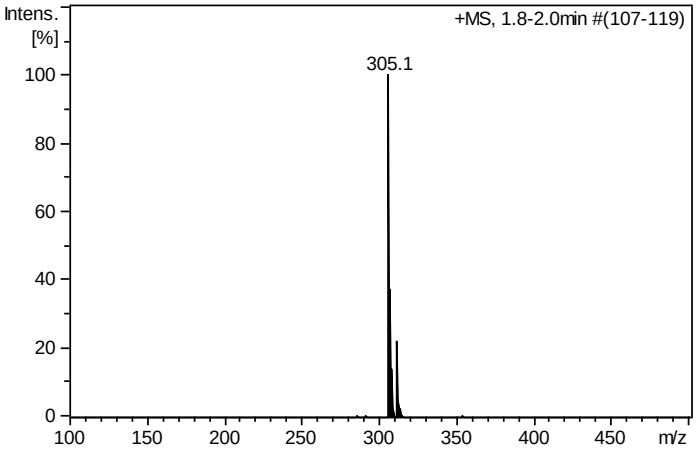

Figure S5. Positively ionized mass spectra of thiazole orange (TO)

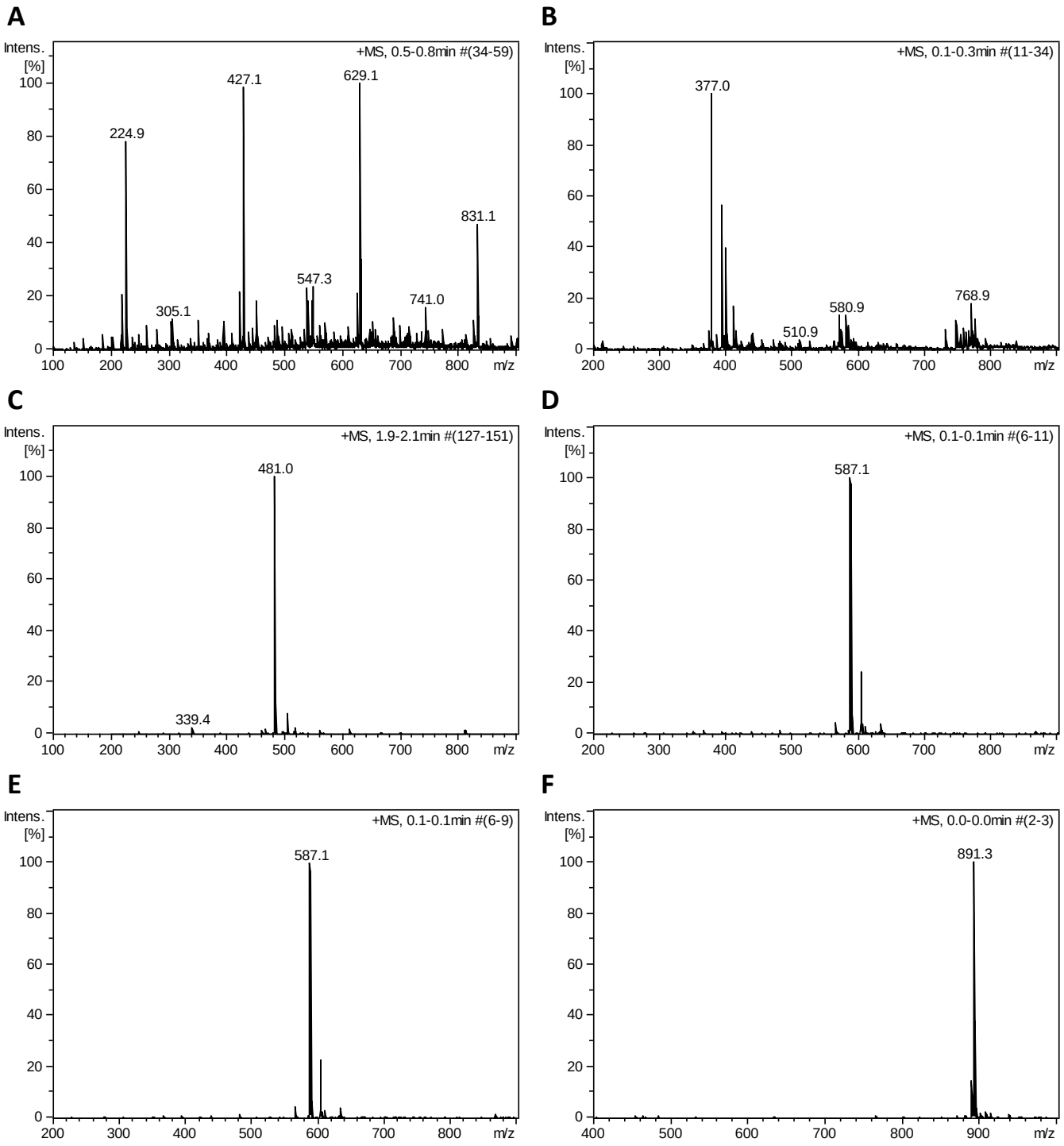

Figure S6. Positively ionized mass spectra of polyphenols. (A) Caffeic Acid; (B) CGA; (C) EGCG; (D) Rutin; (E) Theaflavin; (F) TFDG.

3. Peptide-polyphenol interaction spectra

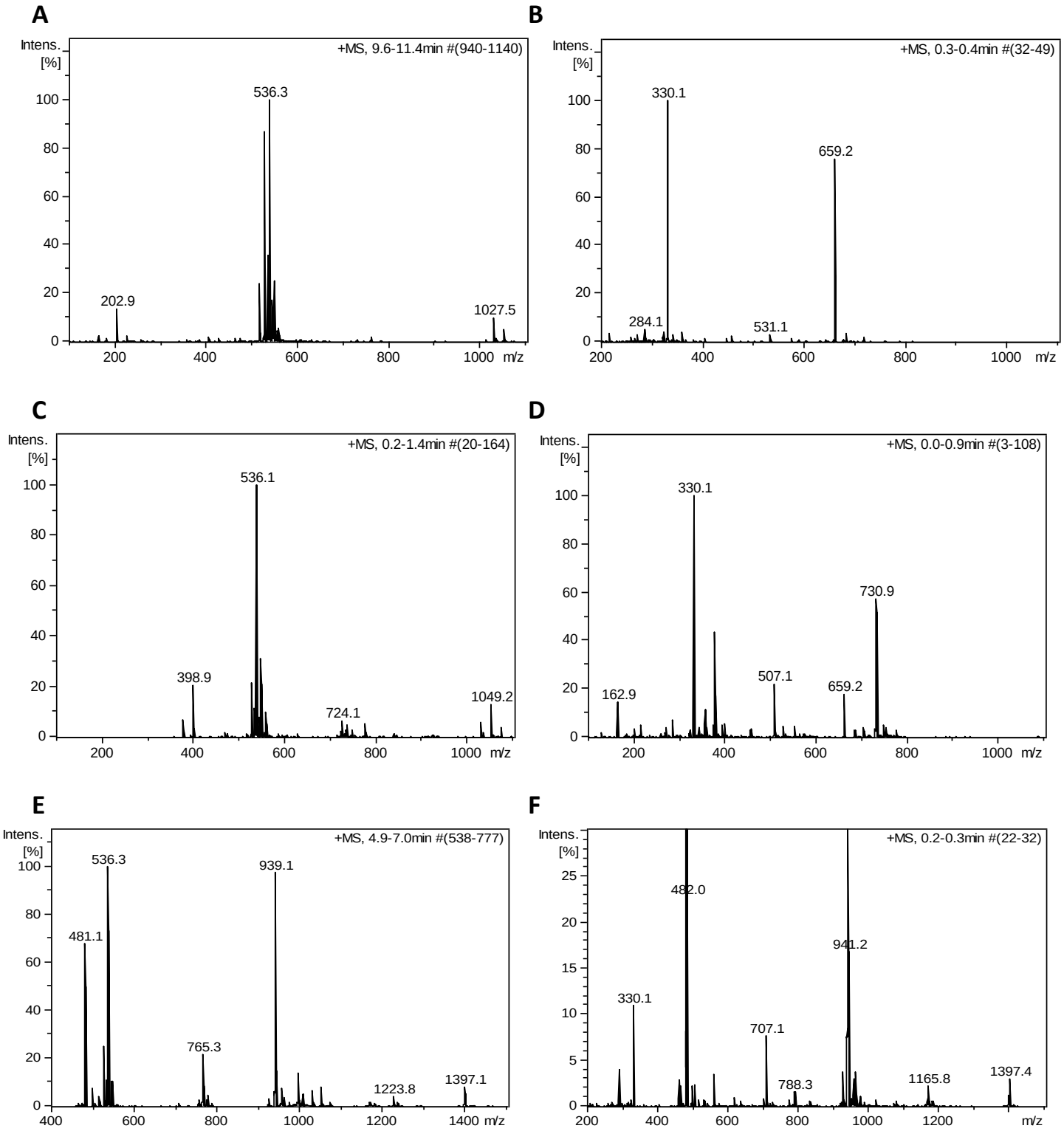

Figure S7. The ESI-Ion trap mass spectra of interactions between polyphenols *2–7* and peptides Pep1 (QSVIKPGELG) and K_3AGAG. (A) Pep1–caffeic acid; (B) K_3AGAG– caffeic acid; (C) Pep1–CGA; (D) K_3AGAG– CGA; (E) Pep1– EGCG; (F) K_3AGAG– EGCG; Continued on the next page.

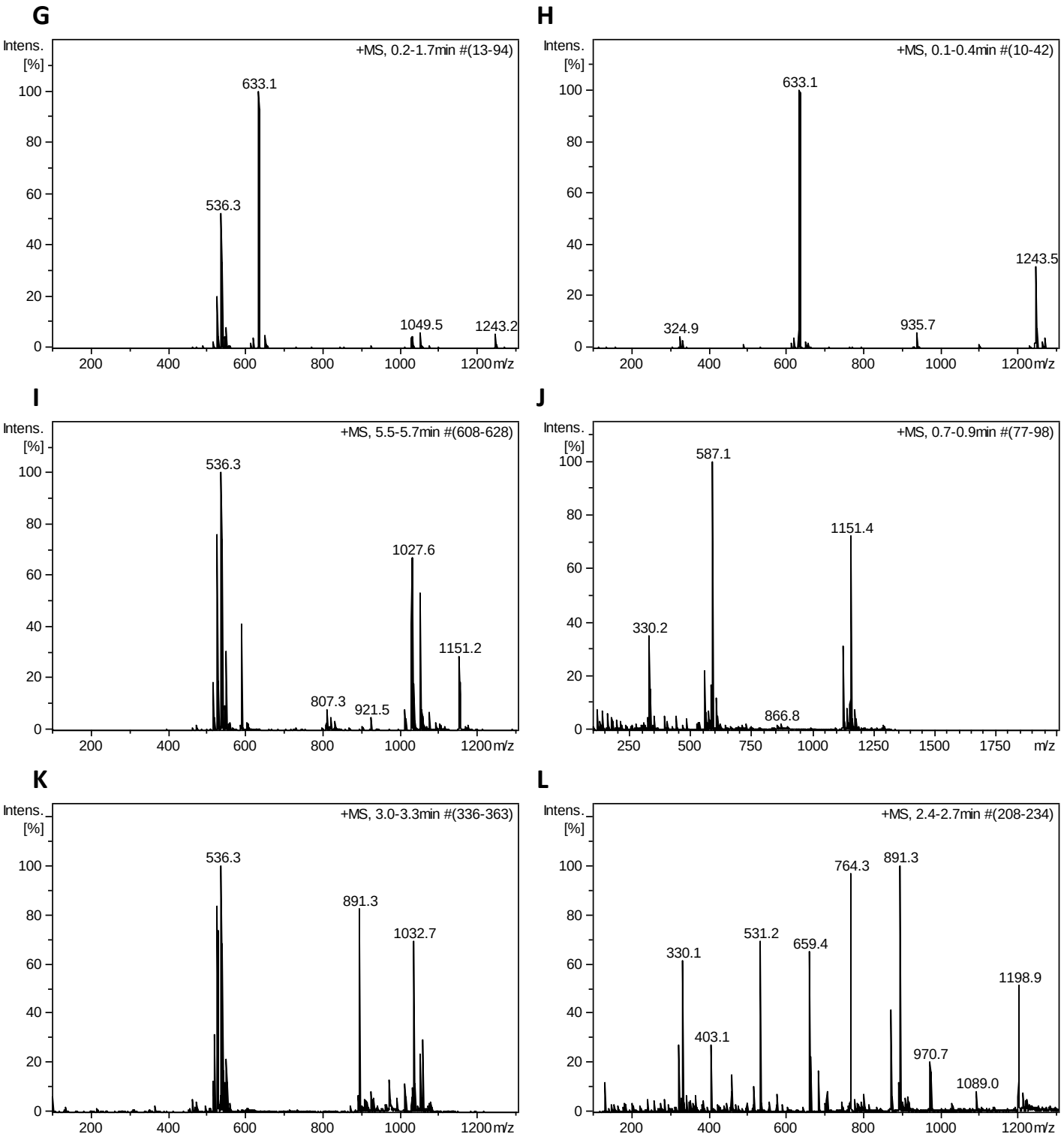

Figure S7. Continued: The ESI-Ion trap mass spectra of interactions between polyphenols *2–7* and peptides Pep1 (QSVIKPGELG) and K_3AGAG.; (G) Pep1–rutin; (H) K_3AGAG – rutin; (I) Pep1–theaflavin; (J) K_3AGAG – theaflavin; (K) Pep1–TFDG; (L) K_3AGAG – TFDG;

4. CD spectra

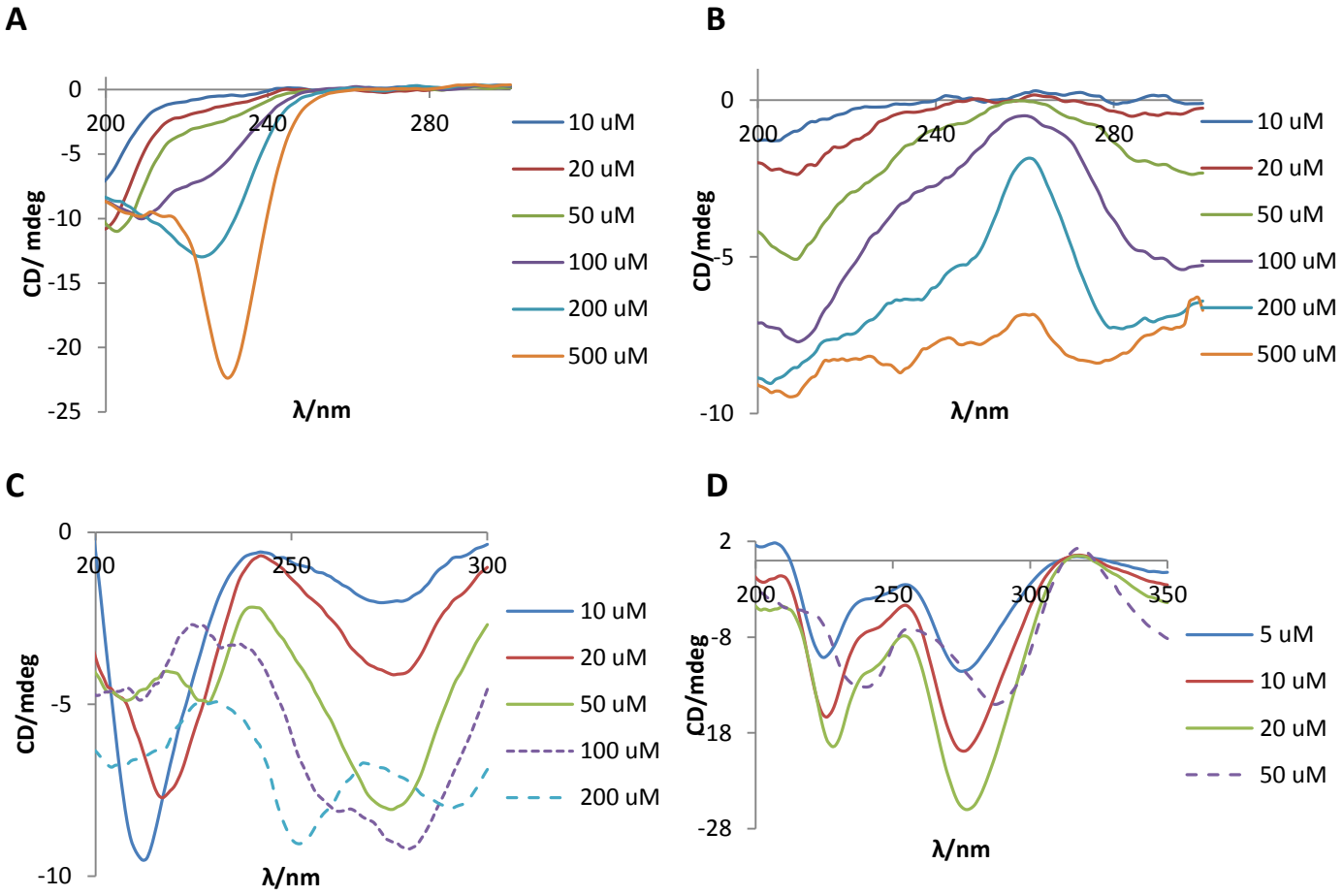

Figure S8. Circular dichroism spectra of varying concentrations of peptide Pep1 and polyphenols used in CD experiments. (A) Pep1; (B) CGA; (C) EGCG; (D) TFDG.

5. FID spectrum

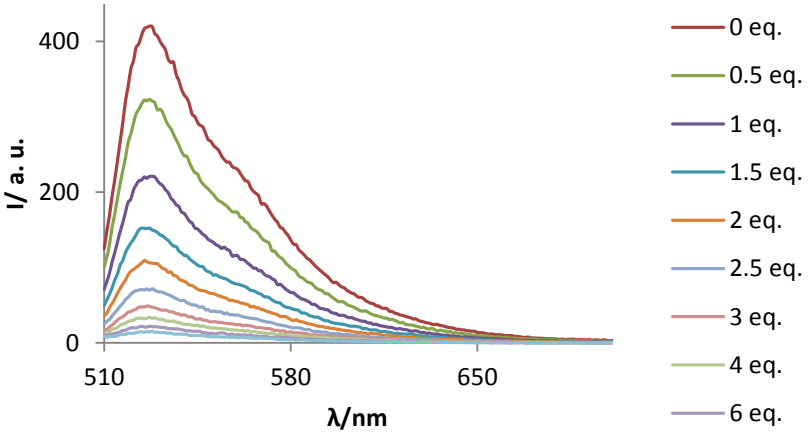

Figure S9. Fluorescence spectra obtained from titrations of 22AG and TO with a solution of TFDG

6. CGA-peptide CD titration

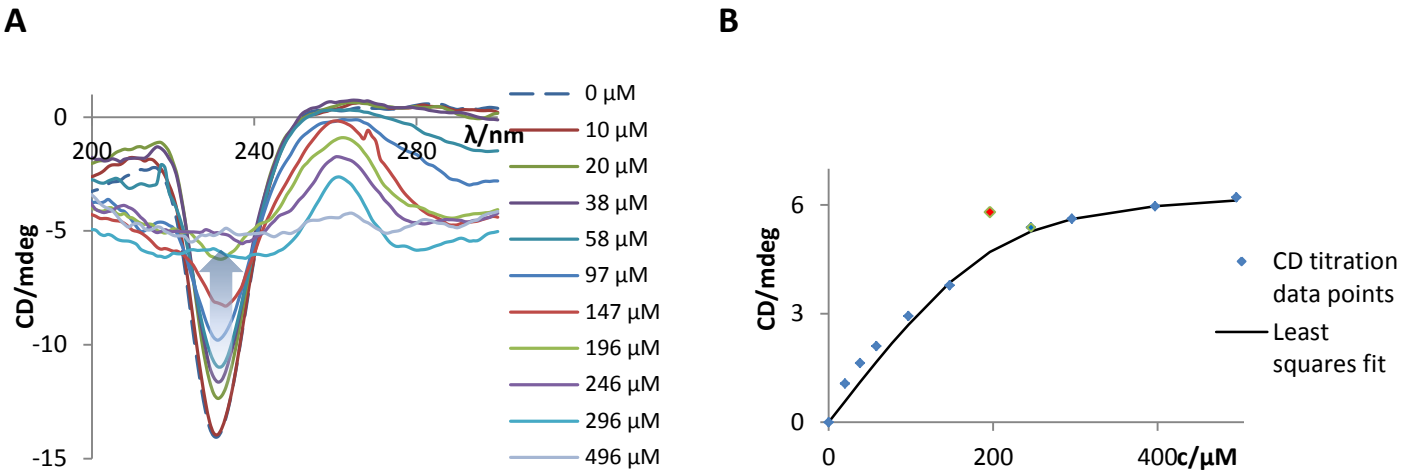

Figure S10. (A) Circular dichroism (CD) titration spectra of mixtures between a random peptide Pep1 (sequence QSVIKPGELG, c = 200 µM) and varying concentrations of chlorogenic acid (CGA); (B) The change in the peptide Pep1 CD of the negative maximum (averaged over 225-240 nm for higher precision) with the varying conc. of CGA.