Supplementary material

Ion mobility mass spectrometry workflows for characterizing bioactive isomer conformation, isomerization and drug-protein-liposome interaction

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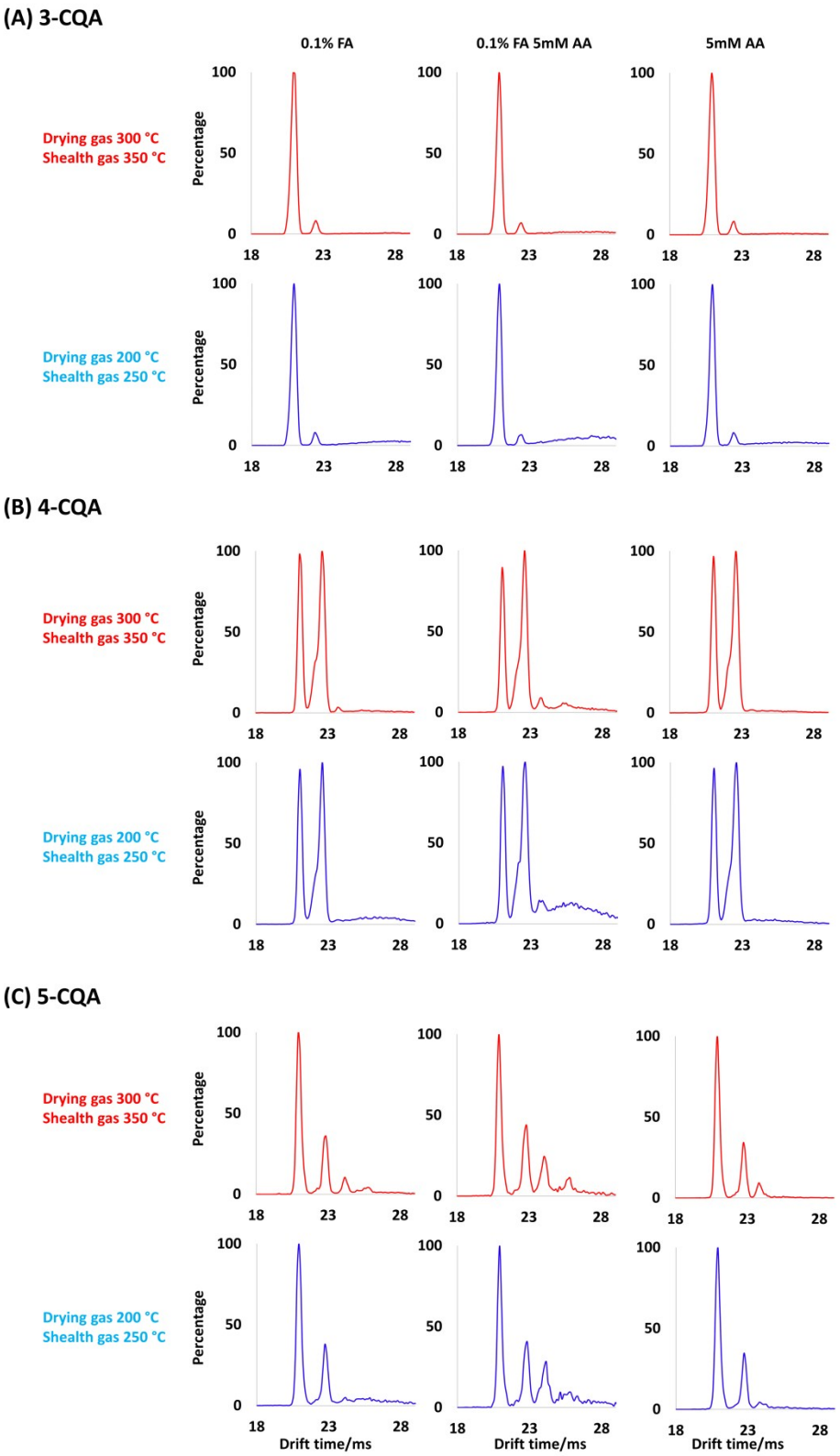

Fig. S1. The DT profile of 3-CQA (A), 4-CQA (B) and 5-CQA (C) at different ion source temperatures (drying gas and sheath gas temperature) and buffer systems.

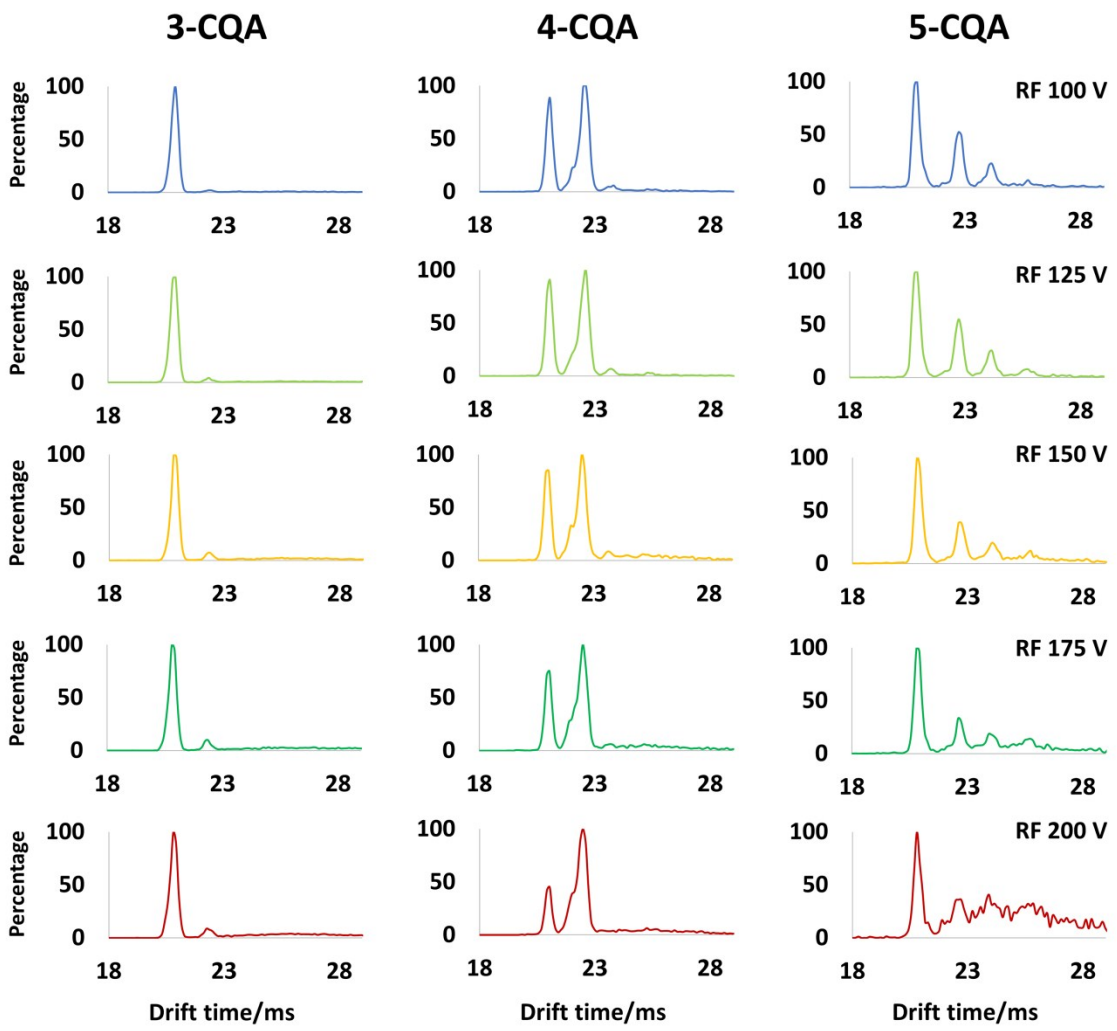

Fig. S2. IM DT profile of 3-CQA, 4-CQA and 5-CQA at different RF voltages.

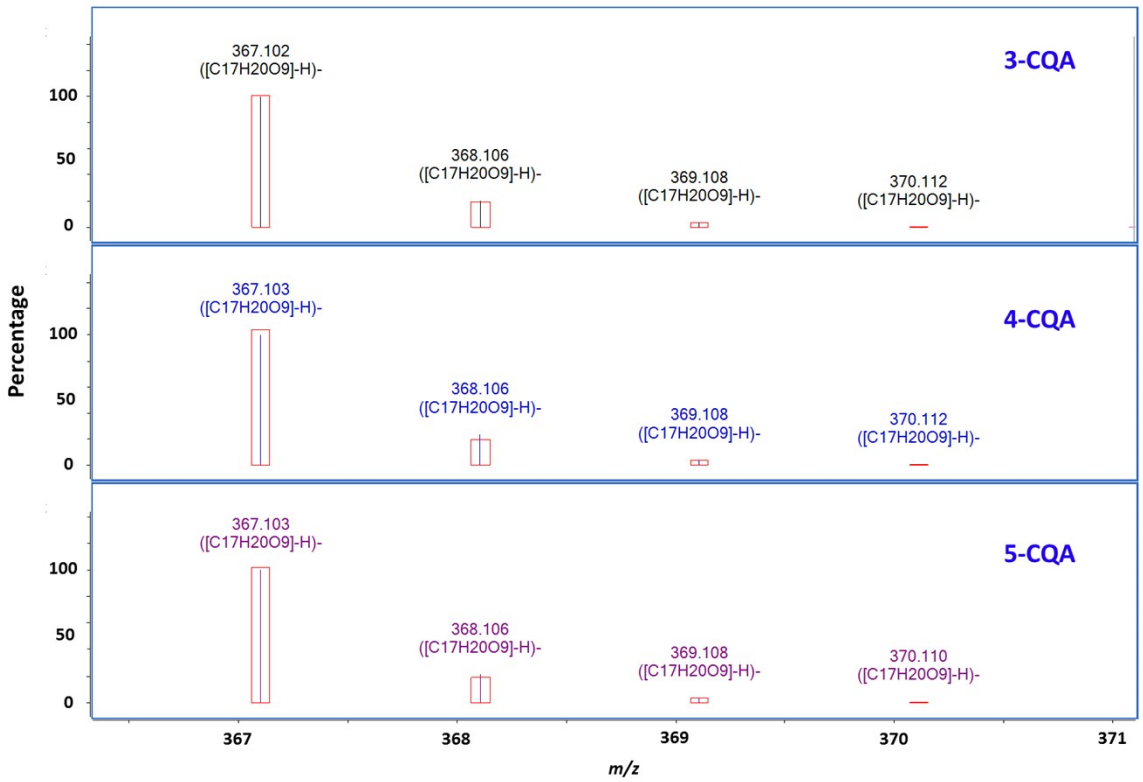

Fig. S3. The mass spectra of methylated CQA (C17H20O9) observed in the CQA standards. The mass spectra fitted well with the red squares, which indicated the theoretical accurate mass and isotopic distribution of C17H20O9.

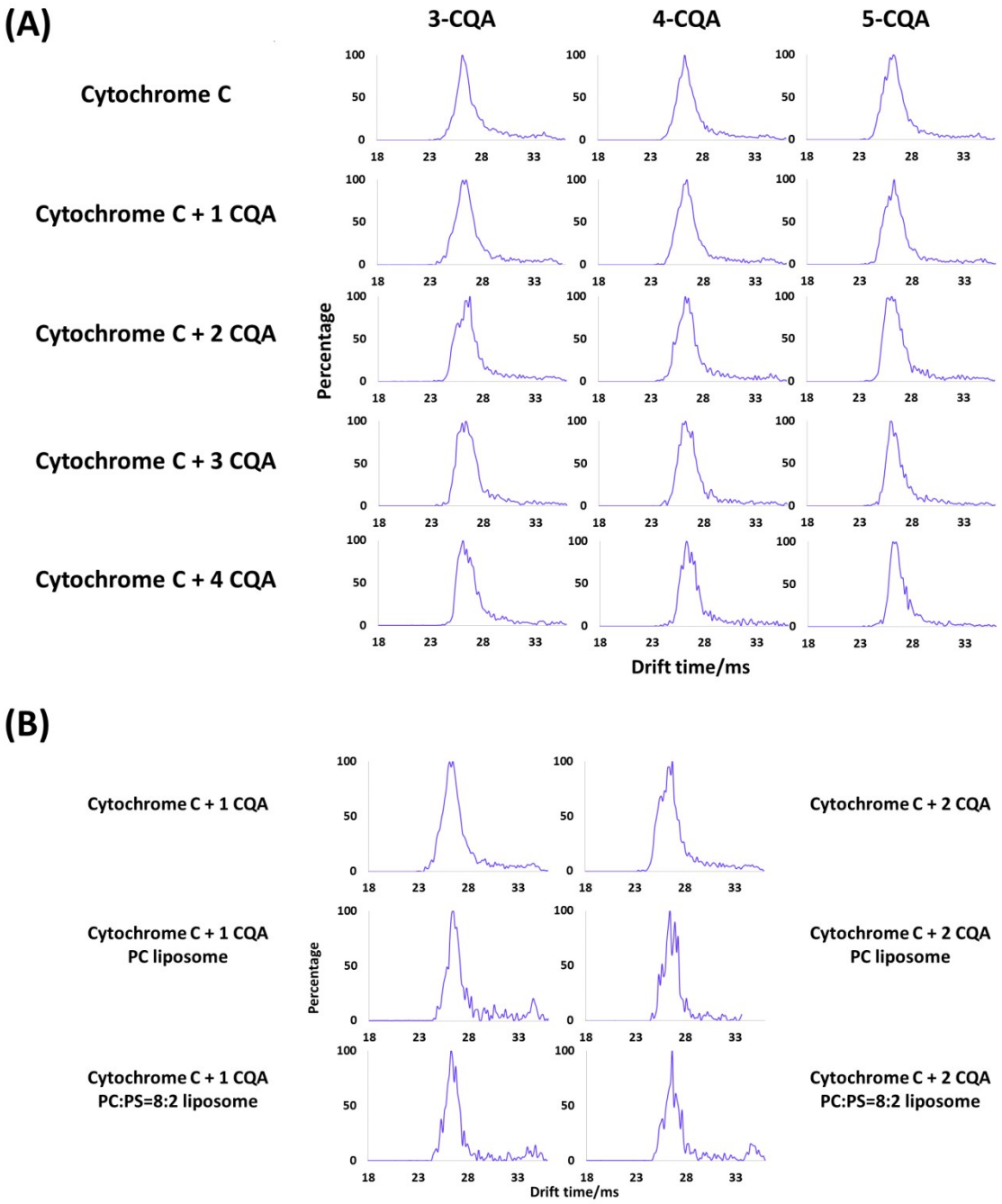

Fig. S4. (A) The DT distribution of +8-charge state of Cytochrome C and various CQA binding Cytochrome C. No significant DT difference is observed for the species. (B) The DT distribution of +8-charge state of one and two CQA binding Cytochrome C without liposome and with two different liposomes. No significant DT difference is observed for the species.