The interaction between myosin and aldehydes during heating process by molecular docking simulation and multi-spectroscopy techniques

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Objectives: The flavor is a critical factor influencing consumers' preference, especially for volatile compounds. Aldehydes, especial- ly short linear aldehydes, are the predominant volatile compounds in meat and meat products (Liu et al., 2021; Qi et al., 2021). The protein is an ideal food matrix binding volatile compounds (Pe´rez-Juan, Flores, & Toldra´, 2007). However, the synergistic effects between the protein rheological behavior and protein-ligand interactions on the small molecule ligand retention are not fully re- ported. This study clarified how aldehydes bind to myosin during the constant thermal treatment by combination of multi-spectros- copy techniques and molecular docking simulation.

Materials and Methods: The myosin solution was prepared by myosin standard diluted to 2 mg/mL (pH 5.42) in a phosphate buffer (0.02 M, pH 5.42) containing 0.6 M NaCl. The solution was heated for 0 s, 30 s, 60 s, 120 s, and 180 s at 91°C water bath until the core temperatures of samples reached 25°C, 47°C, 64°C, 75°C, and 79°C, respectively. After that, the vial was immediately cooled to room temperature in the ice water. The unheated sample (25°C) was considered the control group. The heated myosin solution under different temperature was used to detected its secondary structure, tertiary structure, particle size distribution, microstructure and rheological characterization. The interaction between myosin and pentanal was simulated using a molecular docking method (Mhatre & Patravale, 2021). The binding ability of myosin with aldehydes was determined by GC-MS.

Results and Discussion: The thermal treatments (25-64°C) significantly enhanced ($P < 0.05$) the values of absolute zeta potential, particle size distribution, and morphologic property of myosin, whereas their values were not different ($P > 0.05$) at 75-79°C. The percentages of aldehydes in the headspace of myosin were significantly decreased ($P < 0.05$) during the constant thermal treatment. No significant changes ($P > 0.05$) in the headspace percentages of free aldehydes in myosin were observed at 120-180 s (75-79°C). Both shear viscosity and stress of the myosin solution were increased ($P < 0.05$) at 30-60 s, whereas their values were decreased ($P < 0.05$) at 120-180 s in comparison with the control group. Interestingly, the secondary structure contents of myosin at 120 s and 180 s were highest ($P > 0.05$), followed by 60 s and 30 s ($P < 0.05$). The lowest surface hydrophobicity was observed in the control group (43.56), followed by the samples at 30 s and 60 s ($P < 0.05$), while the samples at 120 s (91.99) and 180 s (96.60) presented the highest surface hydrophobicity ($P < 0.05$). Notably, the fluorescence quenching behaviors of myosin were increased ($P < 0.05$) with the increase of pentanal concentration and heating temperature. Synergistic effects between the rheological behavior of myosin and the myosin-aldehyde molecular interaction might predominantly contribute to the aldehyde retention. The key residues of pentanal binding to myosin were Thr125, Pro128, Trp131, and Val187, which might be key sites between myosin and pentanal, among which the chemical forces were the conventional hydrogen bond, alkyl, pi-alkyl, and alkyl hydrophobic among them, re-spectively.

Conclusions: The increase of binding ability of myosin with aldehydes might depend on not only the increased rheological behavior but also the increased hydrophobic interaction, reactive sulfhydryl contents, and hydrogen bonds at 25-64°C. The latter might play a major role in the aldehyde retention at 75 - 79°C. The key amino acid residues of pentanal binding to myosin might be Thr125, Pro128, Trp131, and Val187. Among them, the chemical forces were the conventional hydrogen bond, alkyl, pi-alkyl, and alkyl hy- drophobic, respectively.

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Key words: Rheological behavior, Hydrophobic interaction, Trp131, Molecular docking simulation, Multi-spectroscopy techniques