

Supporting Information
for

Quantitative insights into tightly and loosely bound water in hydration shells of amino acids

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Fig. S1. DSC melting heat flow curve of pure water

Fig. S2. DSC melting curves of 20 amino acids and water mixtures in the W_C range of 0 to 8

Fig. S3. The change curves of the T_{onset} and ΔH_w values against W_C for different amino acids

Fig. S4. Linear dependencies of the normalized melting enthalpy changes on the W_C for 20 amino acids

Fig. S5. Raman SC spectra of six amino acid aqueous solutions

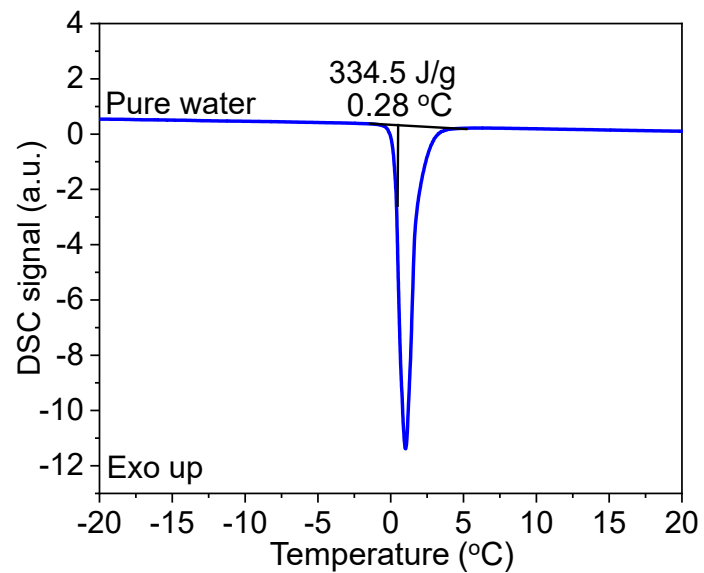


Fig. S1 DSC melting heat flow curve of pure water. The onset transition temperature (T_{onset}) and the obvious melting enthalpy change (ΔH_{obs}) of pure water are shown in the figure ($T_{\text{onset}} = 0.28 \text{ }^{\circ}\text{C}$, $\Delta H_{\text{obs}} = 334.5 \text{ J/g}$).

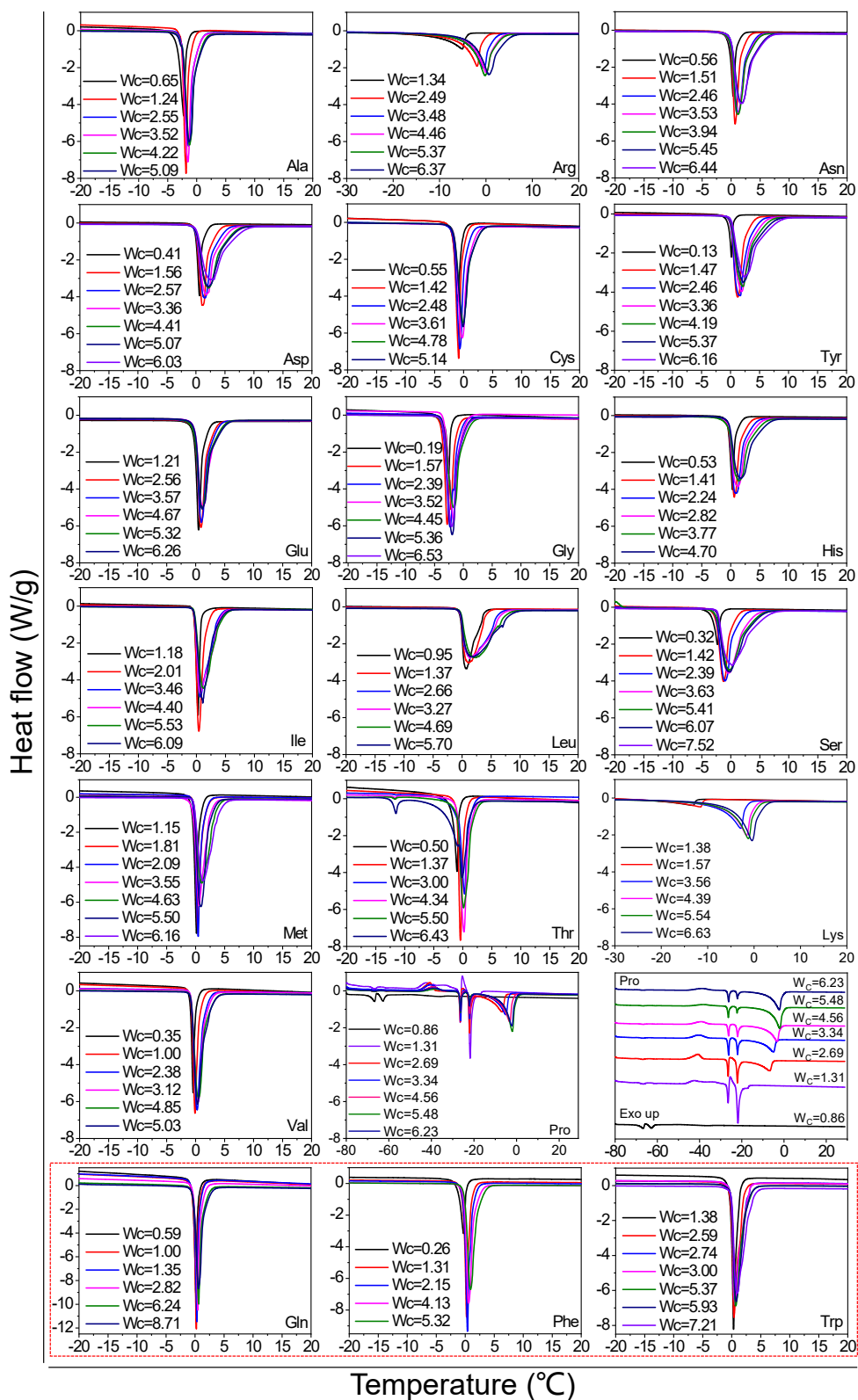


Fig. S2 DSC melting heat flow curves of 20 amino acids and water mixtures in the W_C range of 0 to 8. The curves of Gln, Phe and Trp are shown in the lowest panel, and their heat flow curves are almost unchanged in the W_C ranges of 0 to 8.

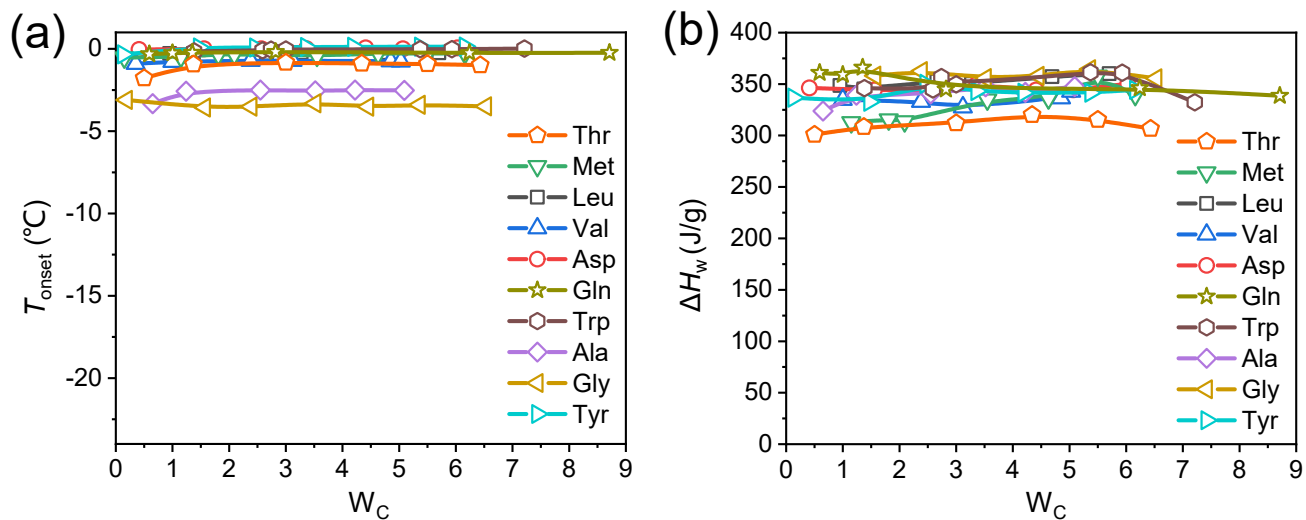


Fig. S3 The change curves of the T_{onset} and ΔH_w values against W_C for different amino acids. (a) Onset transition temperature (T_{onset}) values of amino acids and water mixtures against W_C for different amino acids. (b) Melting enthalpy ΔH_w values (normalized to the water weight) of water molecules against W_C for different amino acids.

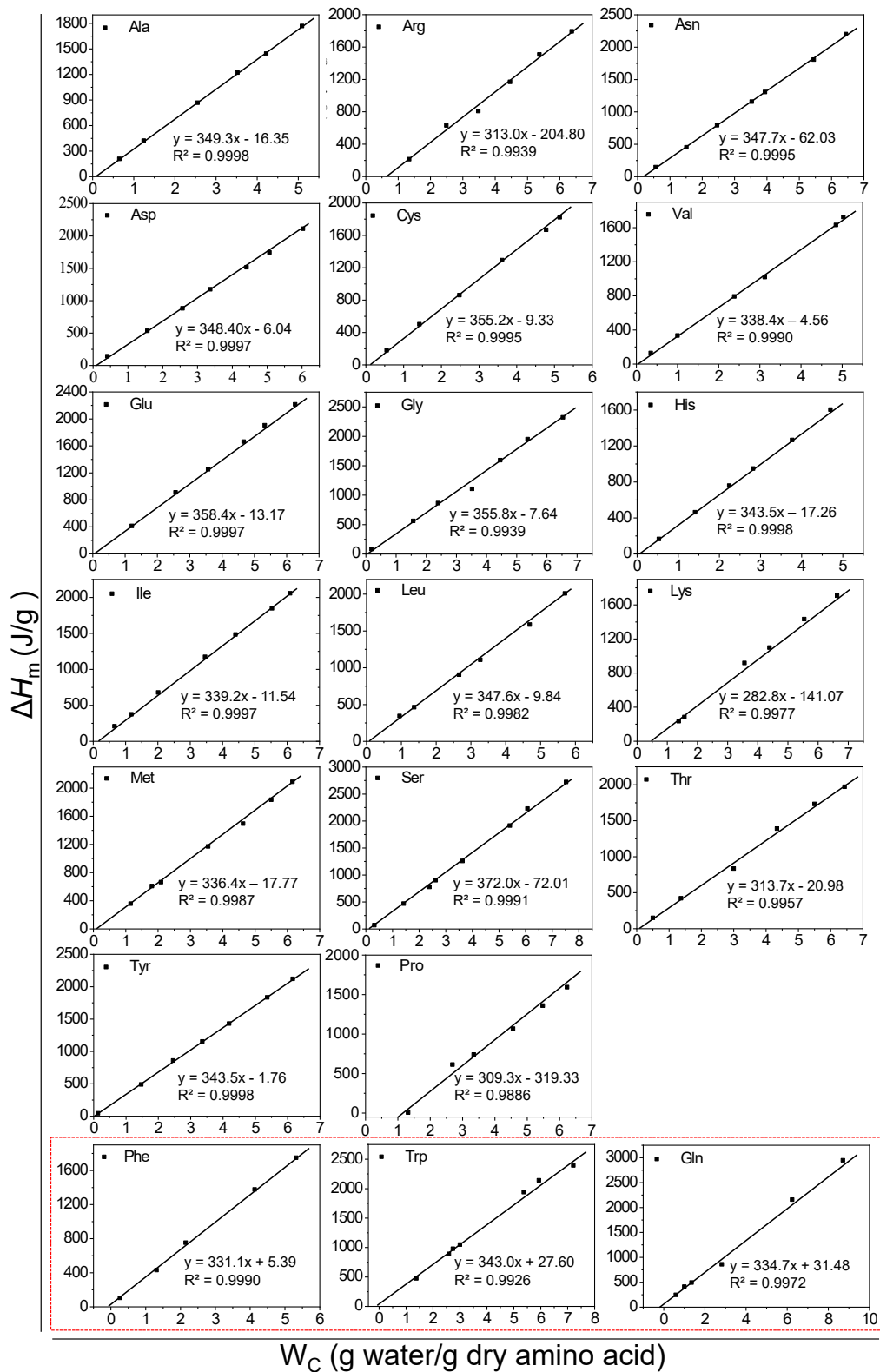


Fig. S4 Linear dependencies of the normalized melting enthalpy changes on the W_C for 20 amino acids. The melting enthalpy changes (ΔH_m) are normalized to the amino acid weight, and plotted as a function of water content (W_C) of amino acids. The x-intercept represents the amount of tightly bound water. The negative x-intercept values of Phe, Trp and Gln are shown in the lowest panel.

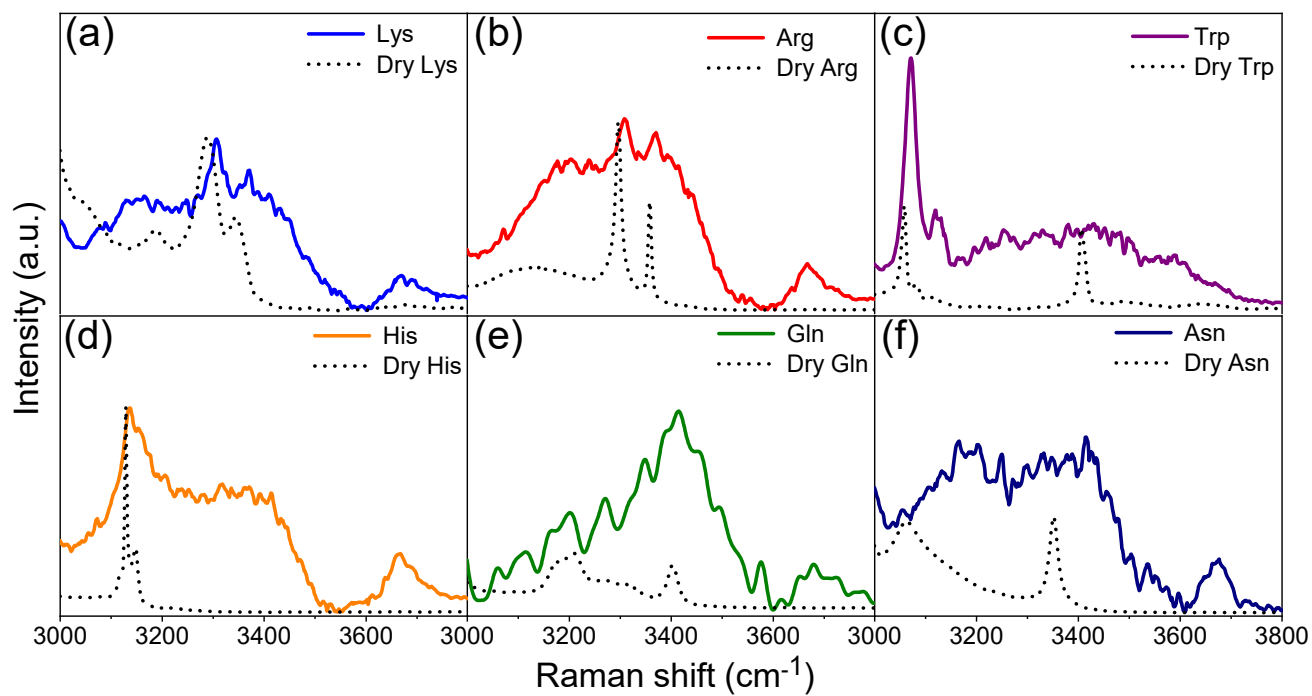


Fig. S5 Raman SC spectra of six amino acid aqueous solutions. Raman SC spectra of 0.10 M Lys (a), 0.10 M Arg (b), 0.05 M Trp (c), 0.10 M His (d), 0.05 M Gln (e) and 0.10 M Asn (f), and the Raman spectra of their corresponding dry amino acid samples (black, dash) are also presented for comparisons.