Supporting Information

Quantitative Measurement of Solvent Accessibility of Histidine Imidazole Groups in Proteins

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Temperature effect on the pH of D_2O buffers*

In order to determine the effect of temperature on the D_2O buffers, we measured the 100 mM pyridine buffer (pH* 6.04 at 25°C) and 100 mM N-ethylmorpholine buffers (pH* 6.86 and 7.94 at 25°C) at 30, 35, 40, and 45°C. Fitting the data points to a linear equation yielded linear regression lines corresponding to the three buffers (Figure S1). The slope values of the three linear regression lines were comparable as shown. We therefore averaged the three slope values and derived the following equation to estimate the pH* values at a specific temperature, T in Celsius.

$$^{T}pH^{*} = 0.0135 \times (T - 25) + {}^{25}pH^{*}$$

where ^{T}pH* and ^{25}pH* are the pH* at T and 25°C. The equation was used to estimate the pH* of the D_2O buffers at 31 and 37°C.

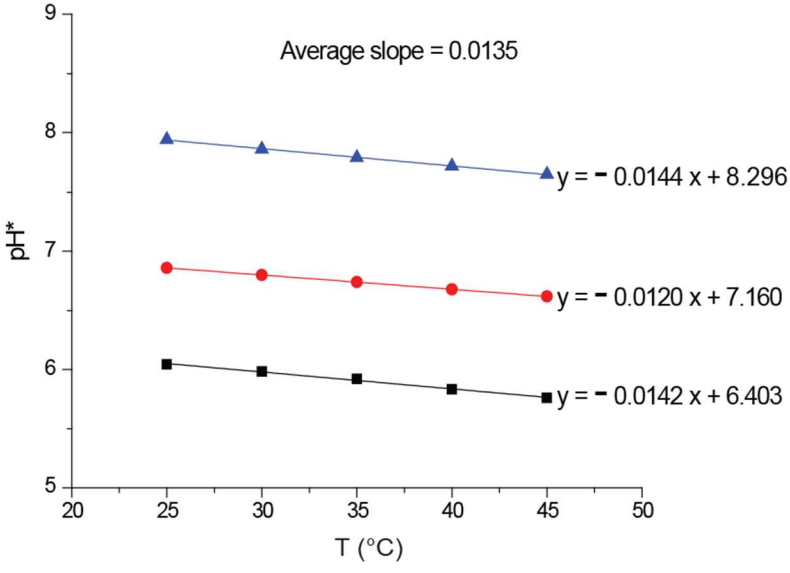
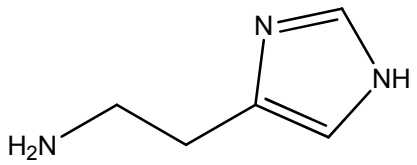
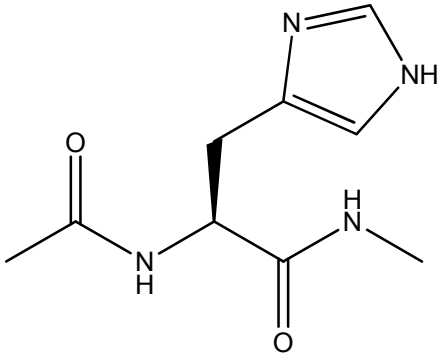


Figure S1: Effect of temperature on the pH* of D_2O buffers.

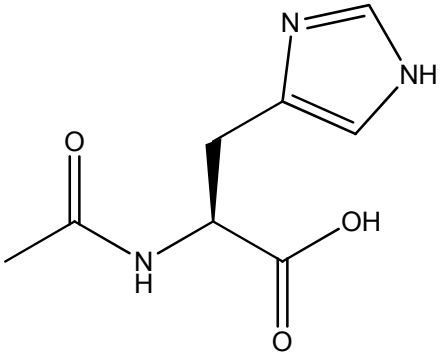
Structures of histamine, Ac-His-NHMe, Ac-His-OH, and IPA



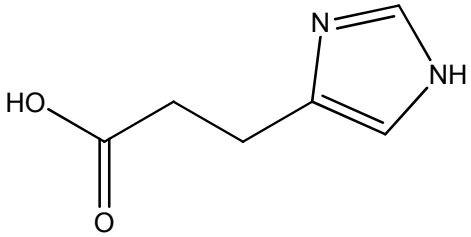
Histamine



Ac-His-NHMe



Ac-His-OH



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