Supplementary Material (ESI) for Analyst

An optimized buffer system for NMR-based urinary metabonomics with effective pH control, chemical shift consistency and dilution minimization

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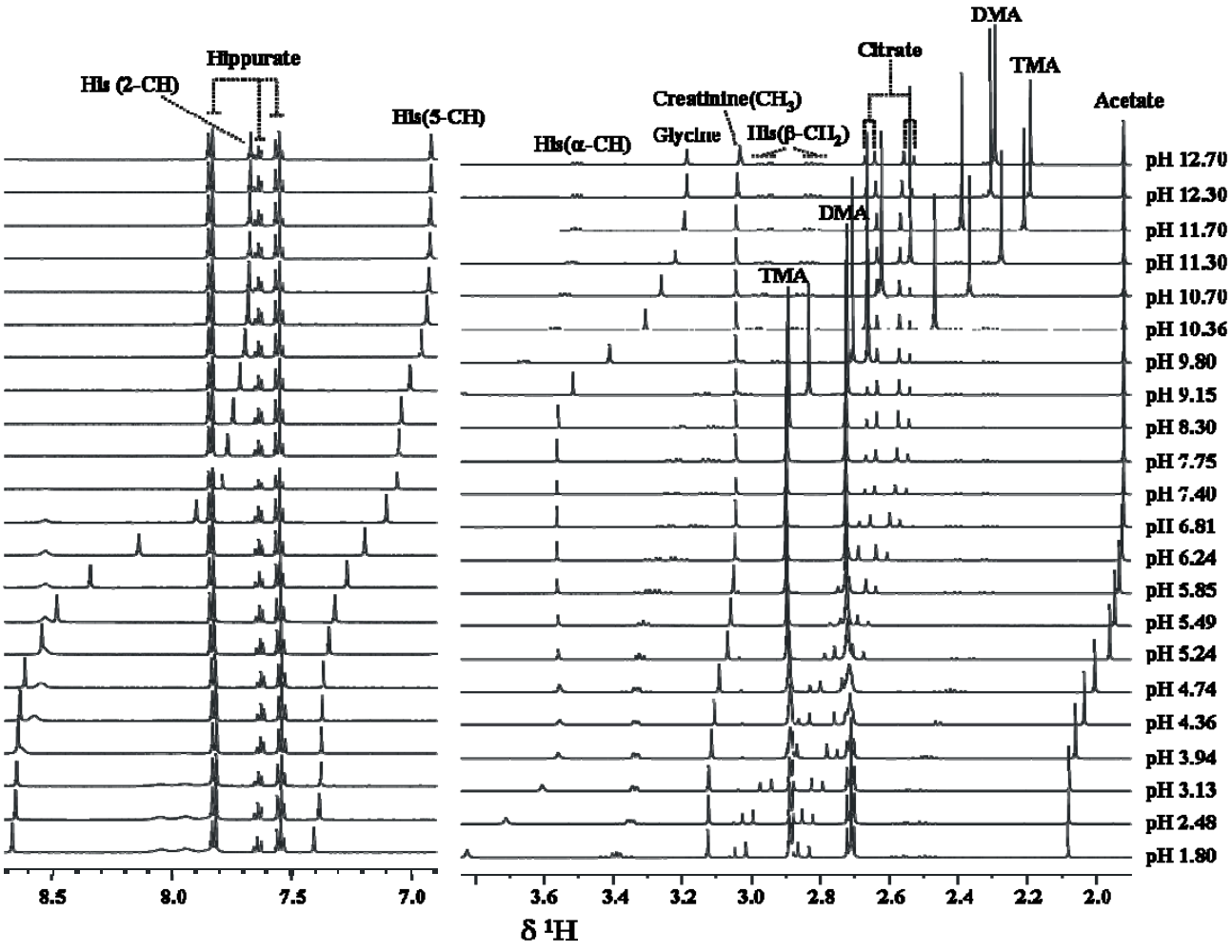

Figure S-1. The ^{1}H NMR spectra for the mixture solutions with different pH values at zero salt.

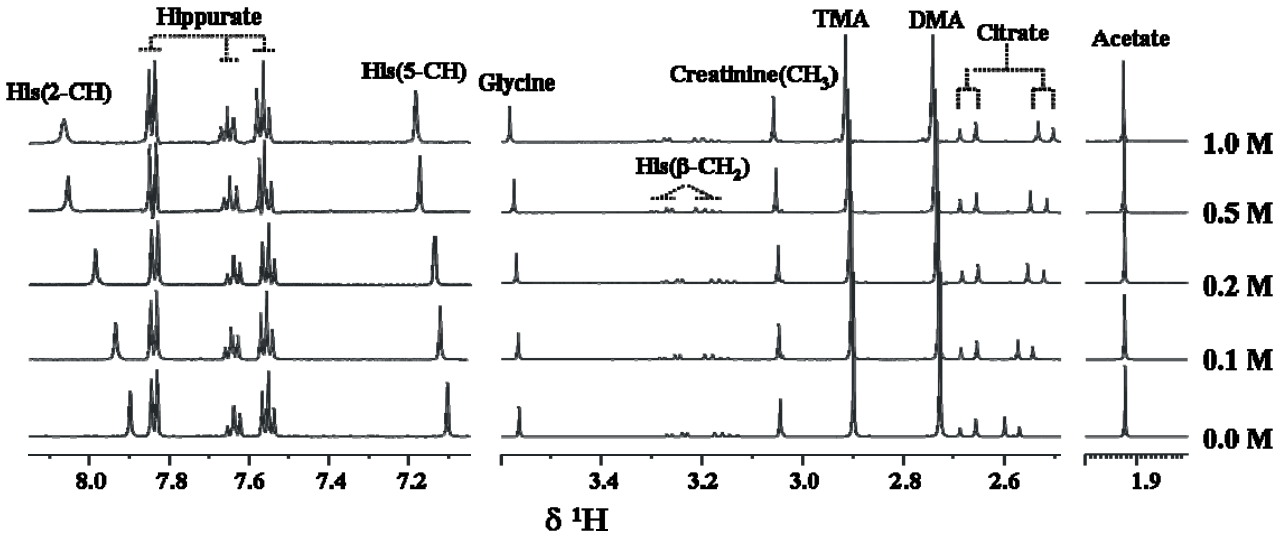

Figure S-2. The ^{1}H NMR spectra for mixture solutions with different salt concentrations at pH ~7.40.

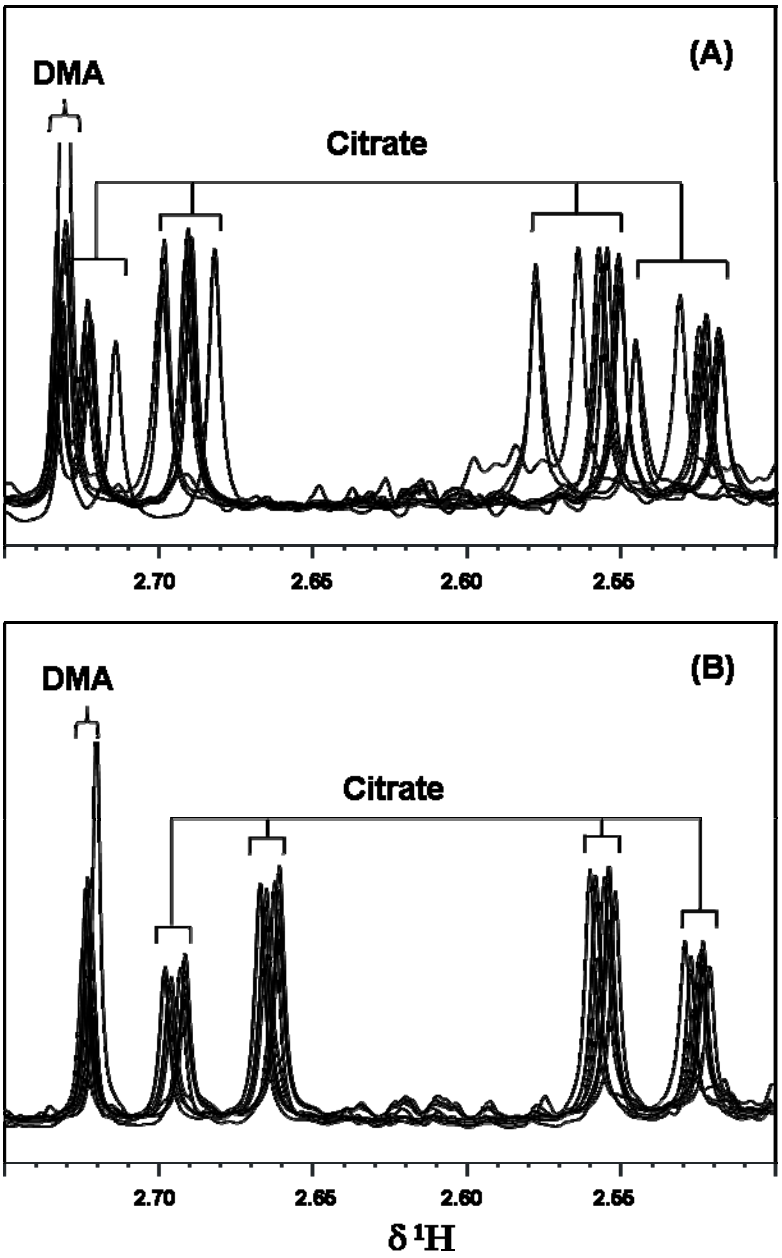

Figure S-3. The chemical shift variations in ^{1}H NMR spectra (δ 2.75–2.50) for 10 human urine samples, (A) with no added buffer and (B) with the final buffer concentration (C_{FB}) of 0.136 M.