Supporting Information

^{13}C-Formylation for ^{1}H-^{13}C 2D NMR Profiling of Amino Metabolites in Biofluids

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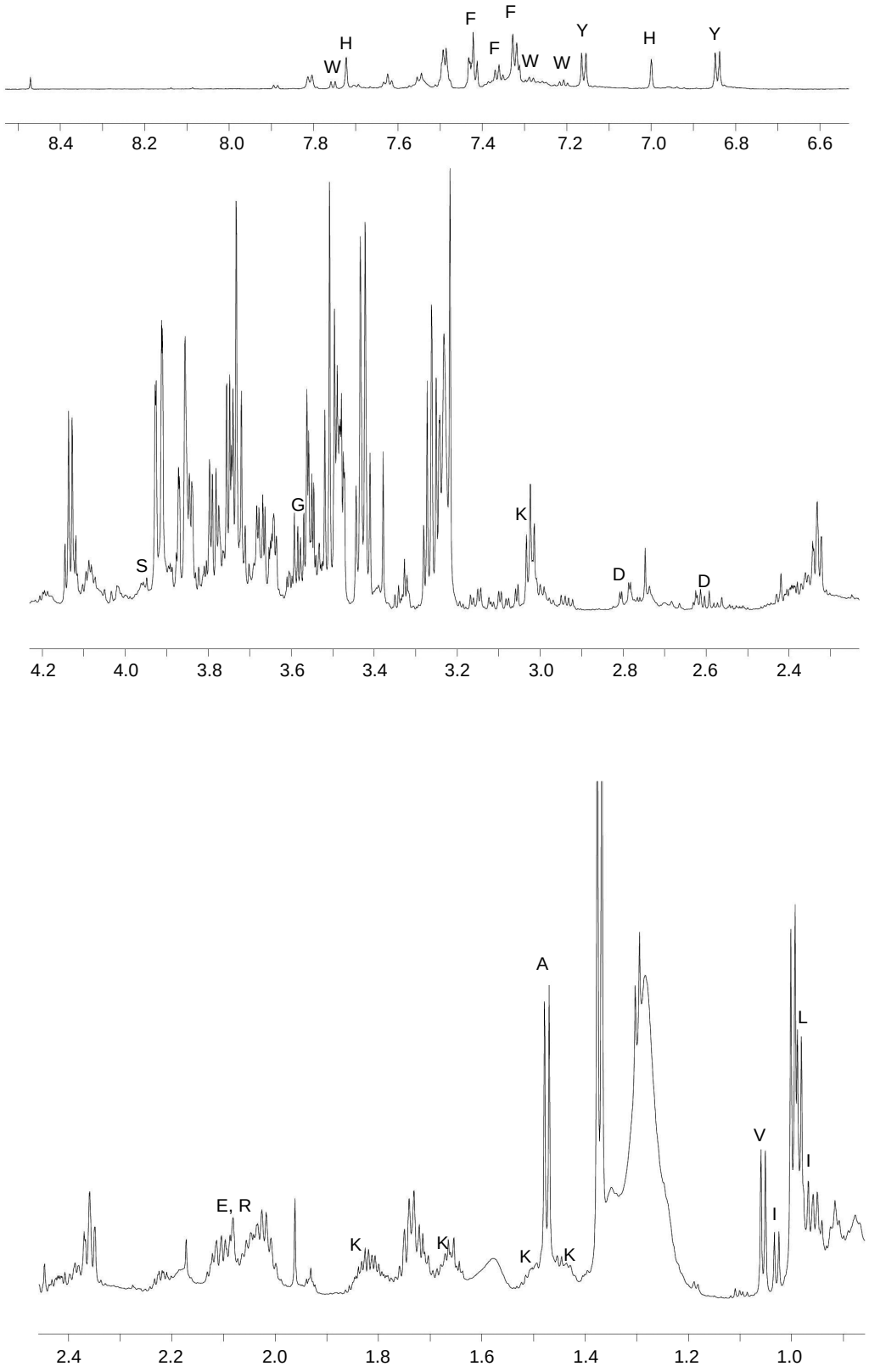

Figure S1. 1D ^{1}H NMR spectrum of the serum sample before ^{13}C-formylation with peak assignment.

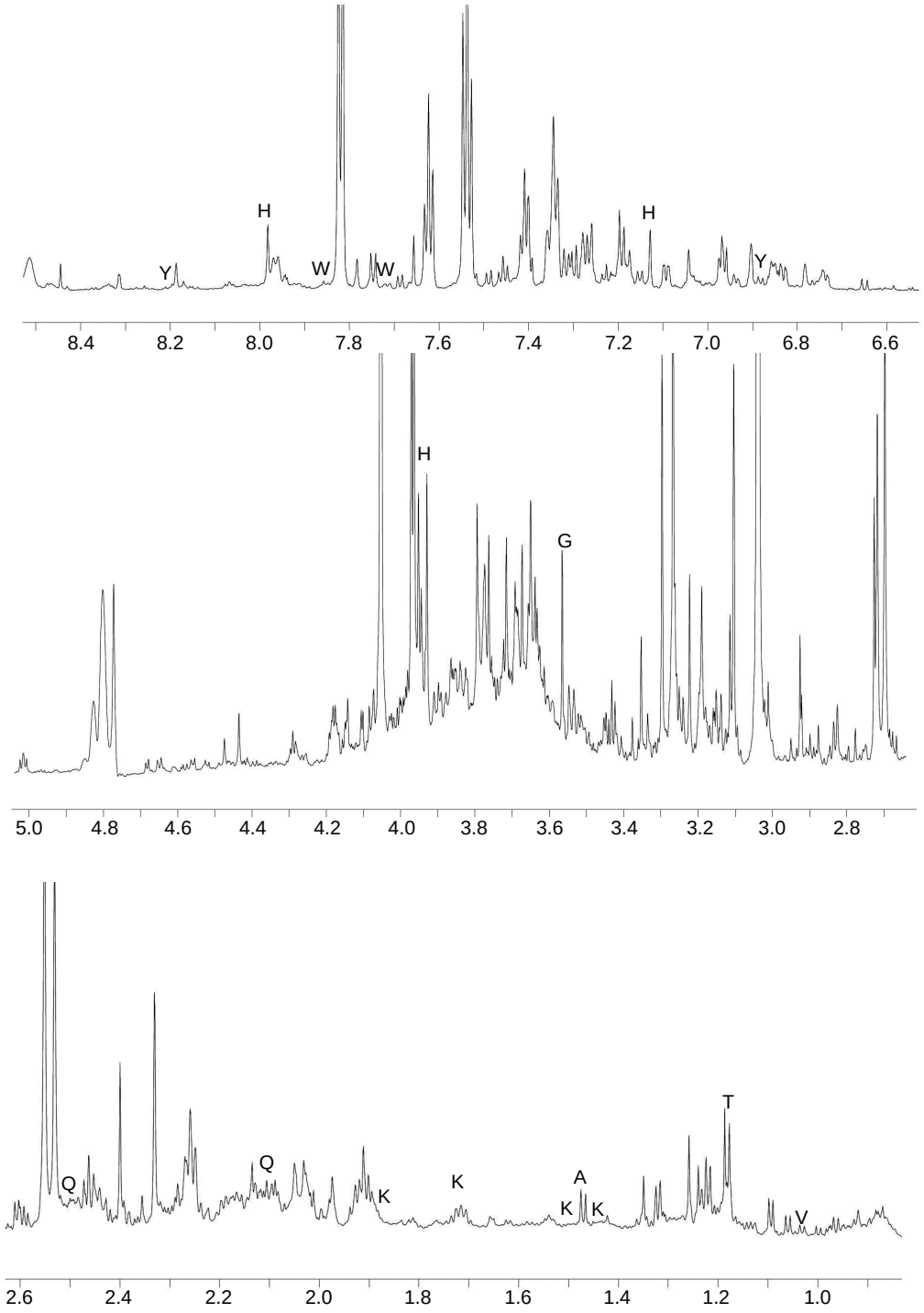

Figure S2. 1D ^{1}H NMR spectrum of the urine sample before ^{13}C-formylation with peak assignment.

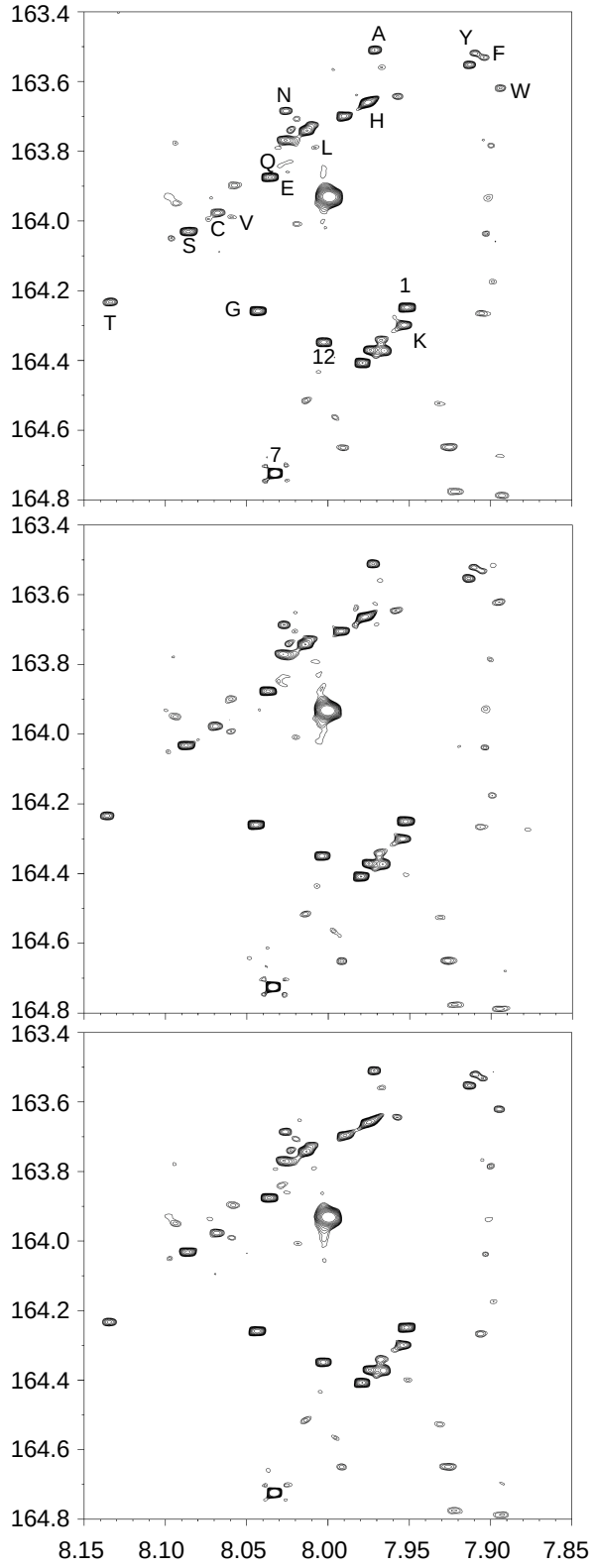

Figure S3. ^{1}H-^{13}C 2D NMR spectra of a split of healthy human urine sample obtained by individual ^{13}C-formylation and HSQC analysis.

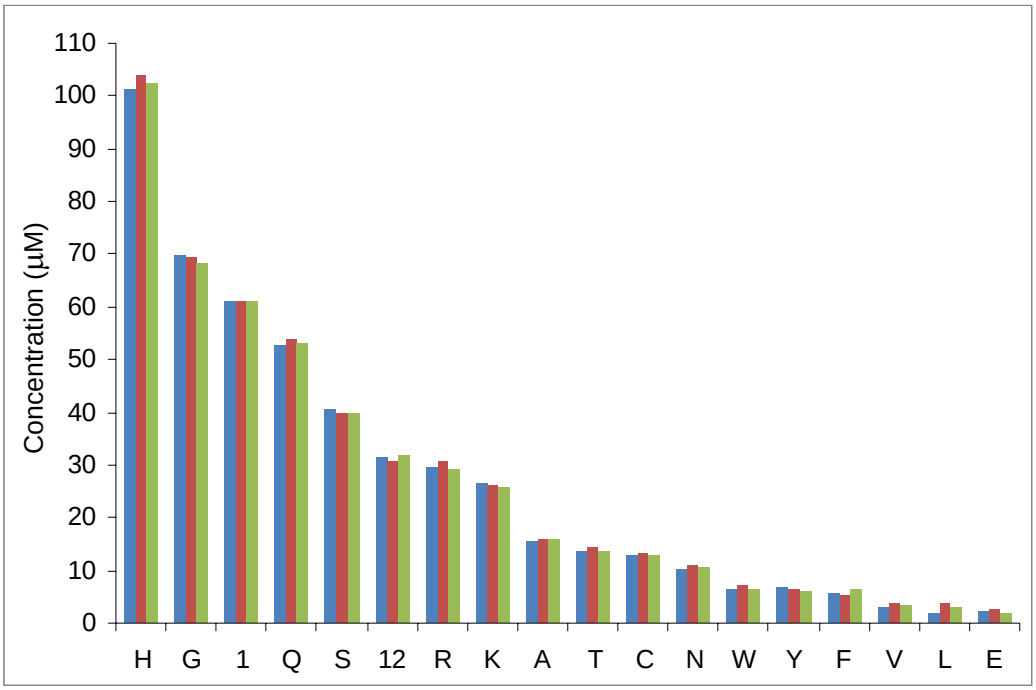

Figure S4. Concentrations of amino metabolites obtained from the triplicate reaction and analysis of a split of human urine sample. Metabolites in the same split sample are represented by the same color. Concentrations were measured by integrating 2D signals referencing to ^{13}C-tagged 0.2 mM ethanolamine (internal standard). The average coefficient of variation (CV) is 2% for 12 metabolites above 10 μM and 11% for 6 metabolites below 10 μM (SNR are less than 8 for 3 metabolites below 4 μM, which contributes to the observed error).

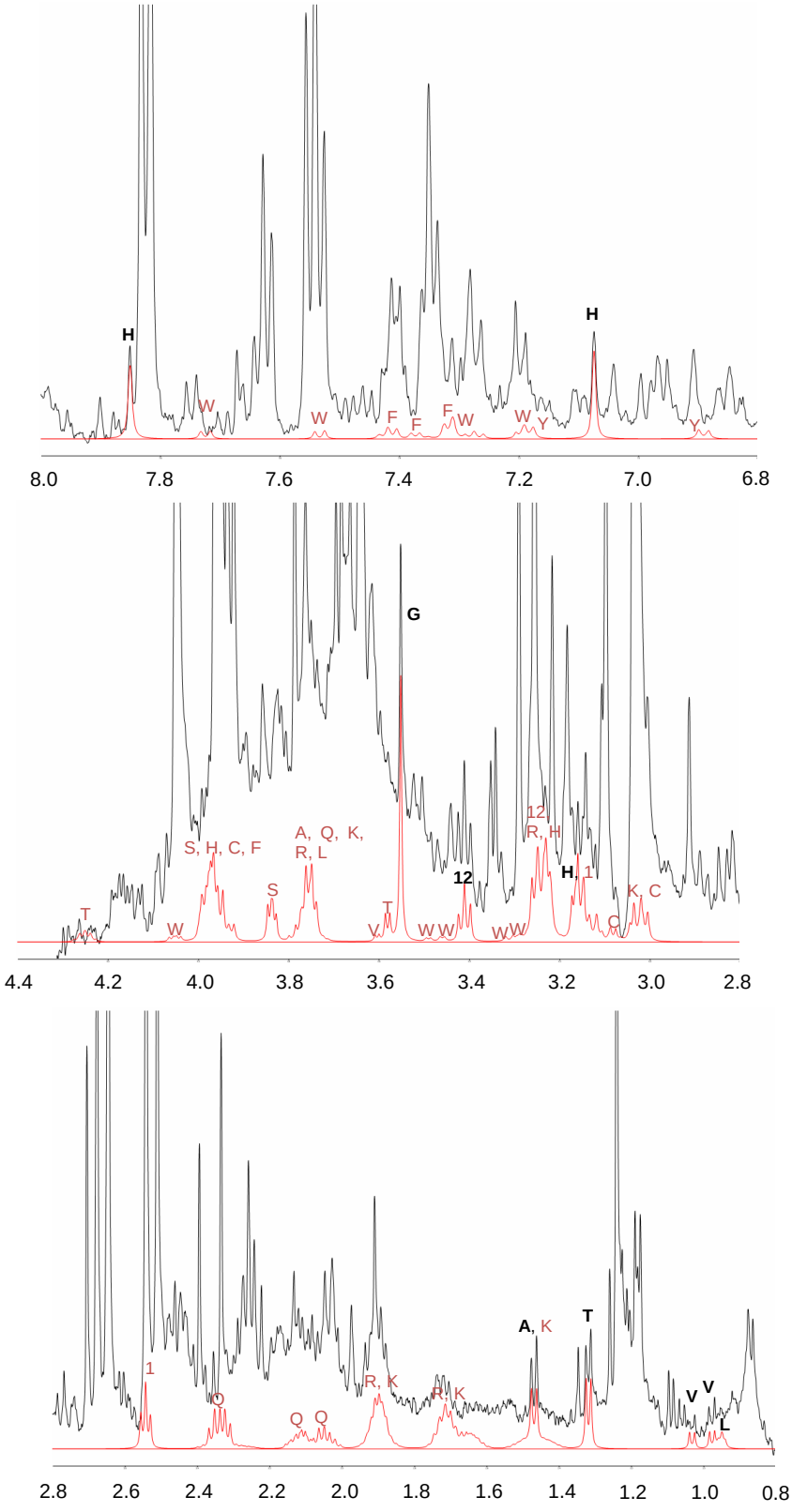

Figure S5. 1D ^{1}H NMR spectrum of the same human urine sample used for triplicate analysis as in Figure S3. Recognizable signals of amino metabolites are assigned in black; the simulated spectrum generated by Chenomx NMR Suite professional 5.1 (Chenomx, Inc.) with assignments of metabolites observed through ^{13}C-formylation is shown in red.