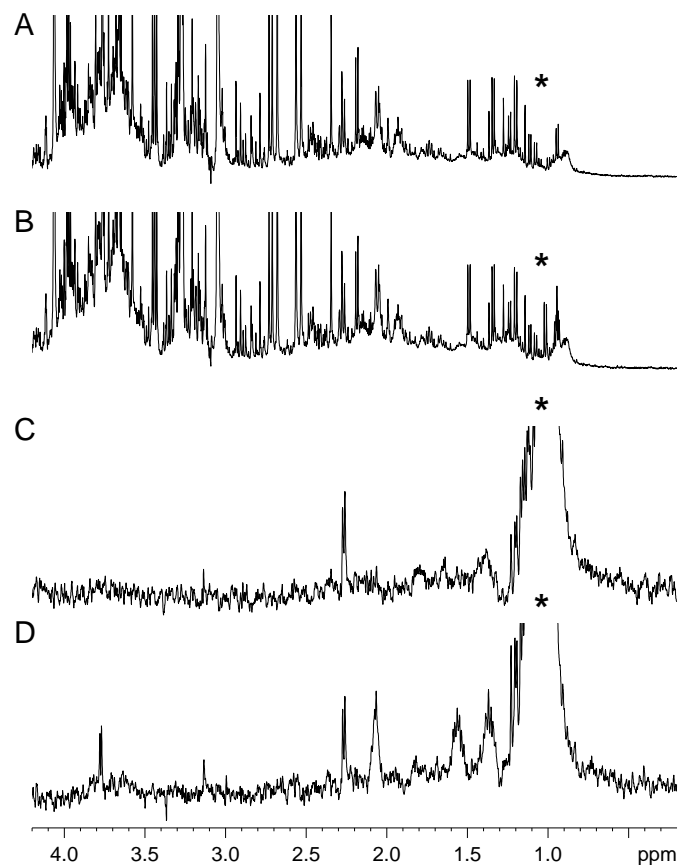
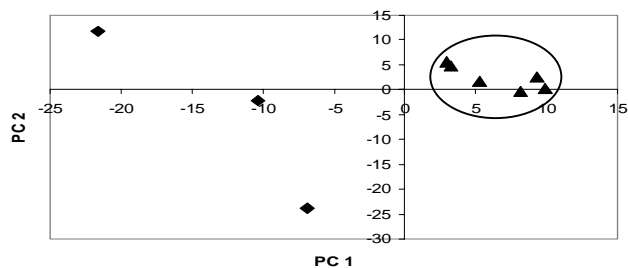


SUPPLEMENTARY RESULTS

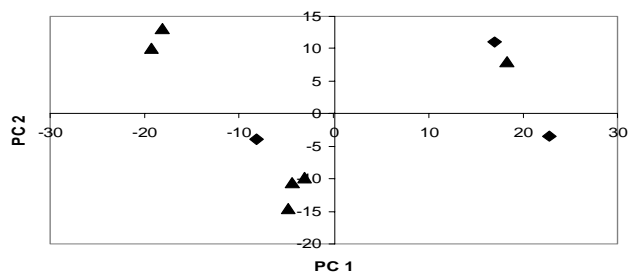


Supplementary Figure 1: (A) High field expansion of proton NMR spectrum of human urine. (B) High field expansion of the proton NMR spectrum of human urine sample from A spiked with 250 μM isoleucine. (C) High field expansion of semiselective TOCSY spectrum of human urine sample from A. (D) High field expansion of semiselective TOCSY spectrum of human urine sample from A spiked with 250 μM isoleucine. Both TOCSY spectra were taken with SP = 10 msec centered at a frequency of 1.00 ppm (*).

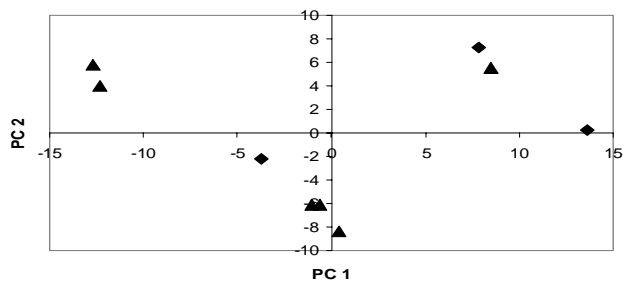
A Semiselective TOCSY Based PCA Score Plot (0.2 to 4.2 ppm)



B 1D Proton NMR Based PCA Score Plot (0.2 to 4.2 ppm)



C 1D Proton NMR Based PCA Score Plot Isoleucine Peaks Only – Including Methyl Peaks



Supplementary Figure 2: PC1 vs PC2 score plots from the isoleucine spiking study of human urine. (A) Score plot from PCA calculated using 398 bins of the semiselective TOCSY spectra as data inputs (0.2 to 4.2 ppm data with selective excitation at 1.00 ppm). (B) Score plot from PCA calculated using 398 bins of the 1D proton spectra as data inputs (0.2 to 4.2 ppm data). (C) Score plot from PCA calculated using the 129 bins of the 1D proton spectra containing isoleucine peaks (including methyl peaks at 0.90 to 1.1 ppm) ▲ = isoleucine spiked, ◆ = control.