Supplementary Information

S1: (i) Average spectra and standard deviation of single point spectra used in the PLS-DA analyses. Spectra have been baseline corrected using a 4th order weighted least squares algorithm before averaging. B-cell lines are depicted in shades of red and pink, T-cells are in shade of green. The average spectra and standard deviations obtained appear similar by visual inspection, although Raji and Ramos cell lines appear to have slightly larger standard deviations than the other cell lines, particularly in the high wavenumber region. (ii) Average spectra and standard deviation obtained for B- and T-cells (top panel) and difference spectrum obtained by subtracting the average T-cell spectrum from the average B-cell spectrum (bottom panel). The difference spectrum was obtained by further baselining the average spectra of all B- and all T-cells by making the following points zero and interpolating between them, 528, 666, 916, 1027, 1150, 1402, 1533, 1808, 2384, 2615, 2802 and 2984 cm⁻¹. The two spectra were then normalised to the intensity of the Raman band at 1454 cm⁻¹ before subtraction. (iii) Comparison of the difference spectrum obtained from the average B- and Tcell single point spectra and the b-vector obtained from the PLS-DA analysis of all B- and all T-cell single point spectra. Although bands in the b-vector tend to be much sharper than those in the difference spectrum, a number of bands in the fingerprint region show similarities between the two spectra. The high wavenumber region, however, is markedly different with large bands present in the difference spectrum that are not present in the b-vector.







S2 Comparison of spectra obtained from single point and image measurements. Single point spectra shown were chosen at random from those used in the PLS-DA analysis. One Raji and one Jurkat spectrum are shown. Image spectra were obtained from one cell acquired following the same procedures as performed for the image analysis described in the last section of the paper. Spectra shown are an average of all the pixels present in a single cell (36x34 pixels for both Raji and Jurkat). As can be anticipated by the markedly different exposure conditions for each measurement regime the spectra obtained show substantially different Raman spectral intensities. Additionaly, the single point spectra provide better defined bands than the imaging spectra, particularly in the fingerprint region, and are not as greatly affected by the presence of bands originating from the quartz substrate as the imaging spectra are.

