Supplementary

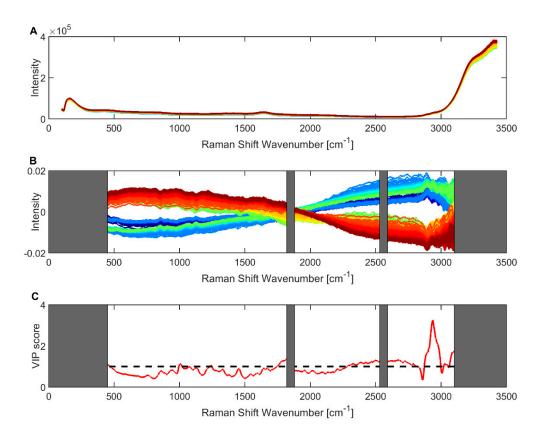


Figure S1. Acquired Raman spectra of the calibration set of ROT1: **A** contains the raw spectra **B** shows the pretreated spectra eliminating Raman shift wavenumber regions (100–450 cm⁻¹, 1820–1880 cm⁻¹, 2530–2590 cm⁻¹ and 3100–3425 cm⁻¹). **C** contains the Variable Importance in Projection of the calibrated PLS model for ROT1.