

8. APPENDIX: SUPPLEMENTARY DATA†

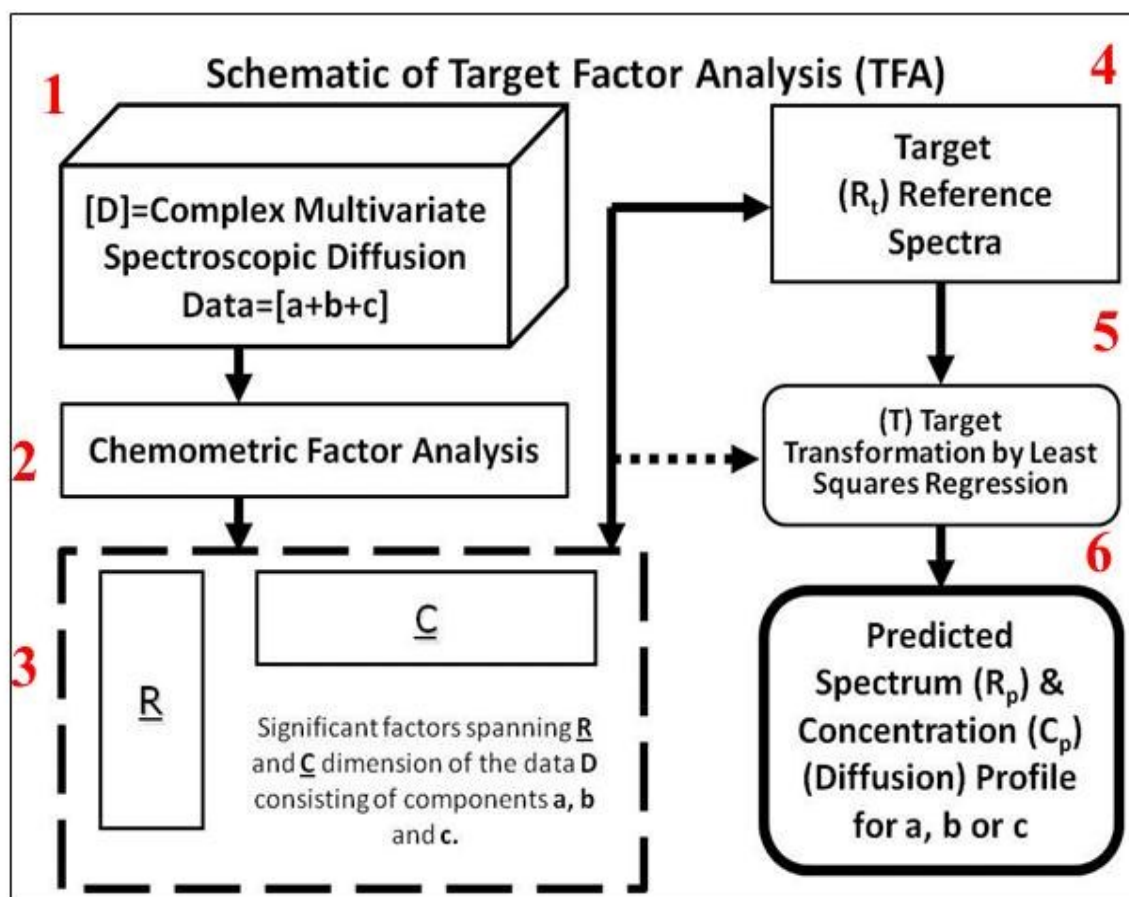


Figure S1: Schematic layout of the target factor analysis process: (1) complex data matrix ($\underline{D}$); (2) chemometric factor analysis; (3) significant factors affecting data matrix; (4) target reference spectra (R_t) used in combination with the $\underline{R}$ and $\underline{C}$; (5) target transformation through least square regression; (6) predicted spectrum (R_p) and concentration profile (C_p).

A typical data analysis using 2% mucin on POL-CAR-BLK in the wavenumber window 1400-1700cm⁻¹, with a spectral correlation minimum limit of 0.8, is shown below. Figures S2a and S2b show a typical data set obtained from the ATR-FTIR setup equivalent to data matrix D in the schematic figure S1 (box 1). The data was subjected to chemometric factor analysis to obtain the significant factors in row domain R and corresponding column domain C as shown in S1 (box 2). These significant factors for the diffusion of 2% mucin through POL-CAR-BLK film are shown in figure S2 c, d and e. The significant factors were estimated using various methods such as factor indicator function (Figure S2c), the percentage significant level (Figure S2d) and the cumulative percentage variance (Figure S2e) to determine true factor space. Detailed background on the determination of the significant factors is described elsewhere (Malinowski, 1991). Figure S3 shows the deconvoluted diffusion output of the 2% mucin through the POL-CAR-BLK film and other factors within the same spectra window used for the analysis. It is clear that besides mucin (e.g. in figure S1 box 6), two other factors (e.g. b and c in figure S1 (box 6) also contributed to the diffusion process. These hidden profiles would be very difficult to know without the use of multivariate target factor analysis. The diffusion profile obtained in figure S3 (b) enabled the relative diffusion coefficient to be calculated by determining the slope of the curve before the film or wafer was saturated (i.e. before the plateau of the curve). The process described above was used to analyse all other formulations to deduce the diffusion profiles for the mucin and thus enable direct comparison of the relative rate of diffusion between the different formulations by normalisation of data.

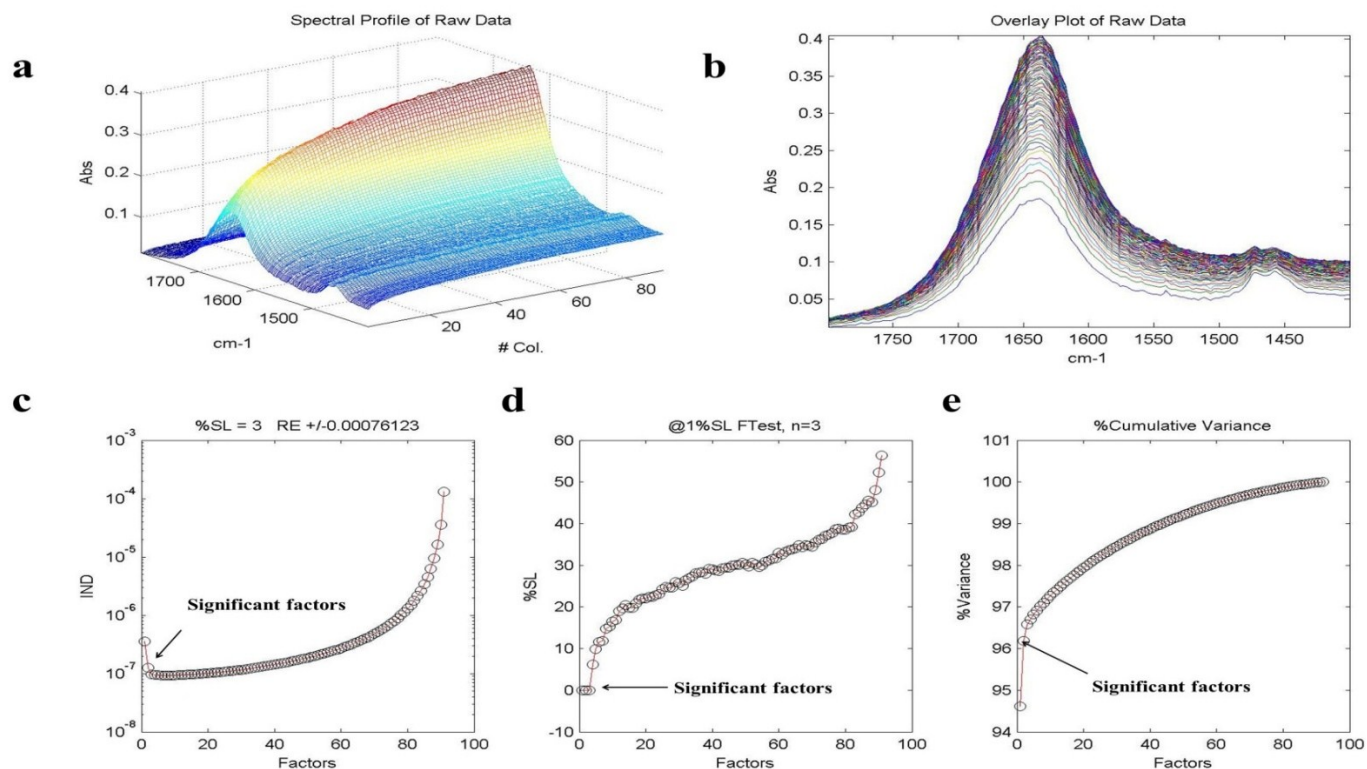


Figure S2: (a) shows a typical ATR-FTIR 3D spectral profile for the selected window 1400-1700 cm⁻¹ (b) overlay plot of raw ATR-FTIR spectral profile (c) significant factor calculated using factor indicator function (IND) (d) percentage significant level (%SL) plotted against the number of factors (e) cumulative percentage variance (CPV) accounted for the abstract factor reproduction. The arrow indicates the cut off point for the selection of number of significant factors.

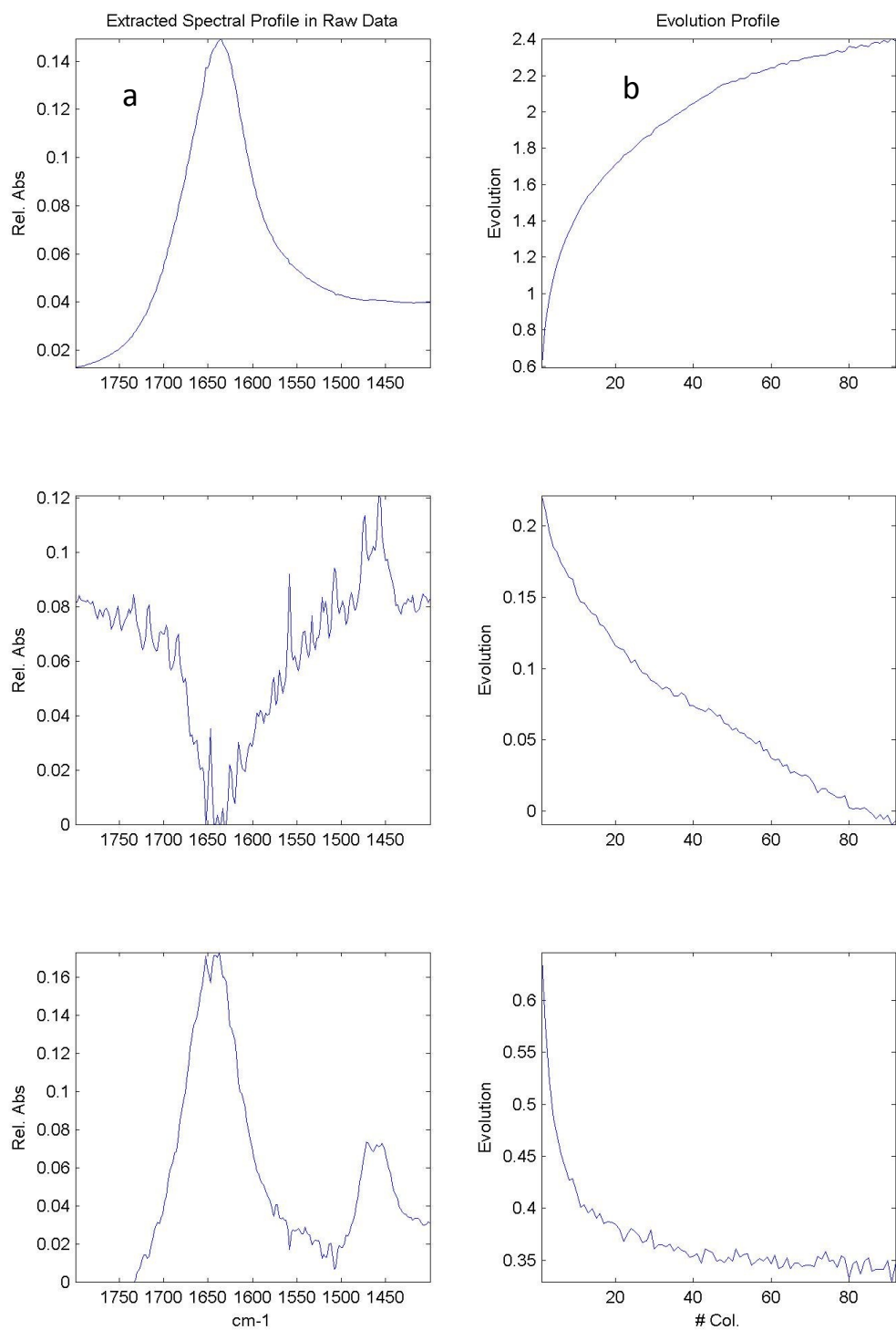


Figure S3: The deconvoluted diffusion output of the 2% mucin and other factors within the spectrum window 1400-1700cm⁻¹ used for the analysis.