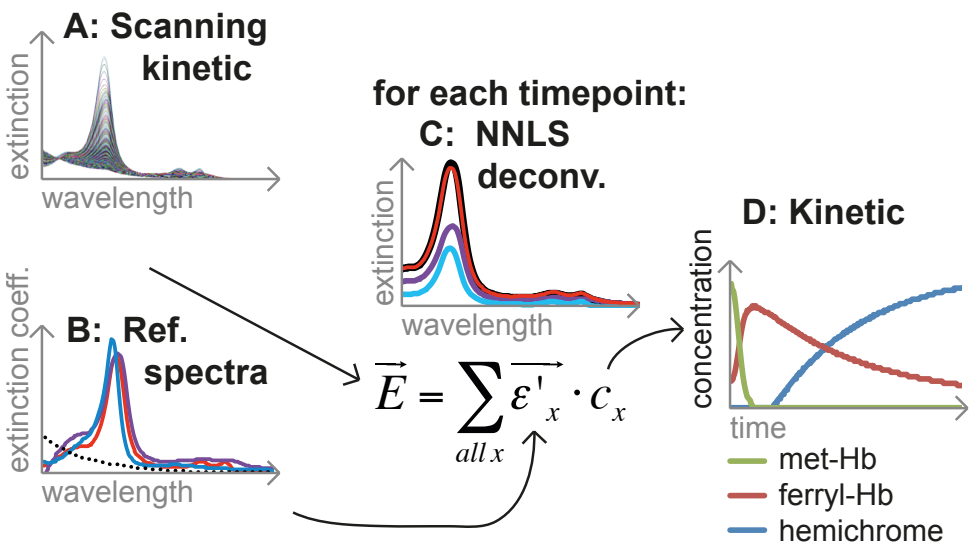
SUPPLEMENTARY FIGURE 6



Principle of spectral deconvolution for the determination of Hb oxidation species.
(A) A continuous spectrum of the reaction mixture is recorded every minute in the range of 300-700nm in 2nm steps. **(B)** Reference spectra of known concentrations of each expected compound in the reaction are recorded in the same spectral range. **(C)** For every individual time-point the concentration of each compound is calculated using the Non-Negative Least Squares (NNLS) algorithm to solve the linear equation* (using R[REF] in a python [REF] script). **(D)** Final result of the spectral deconvolution procedure plotted as compound concentration versus time.

* the equation applies the Beer-Lambert-Law: E is the measured Extinction (as a vector including all measured wavelengths), ε'_x the extinction coefficient vector and c_x the compound x concentration.