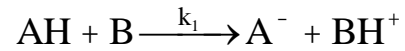
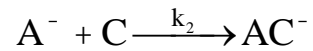


Example – wavelength selection

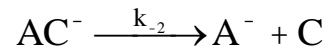
◆ Consider:



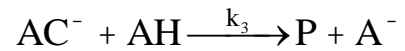
$$r_1 = k_1 c_{\text{AH}} c_{\text{B}}$$



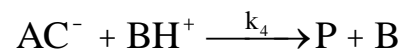
$$r_2 = k_2 c_{\text{A}^-} c_{\text{C}}$$



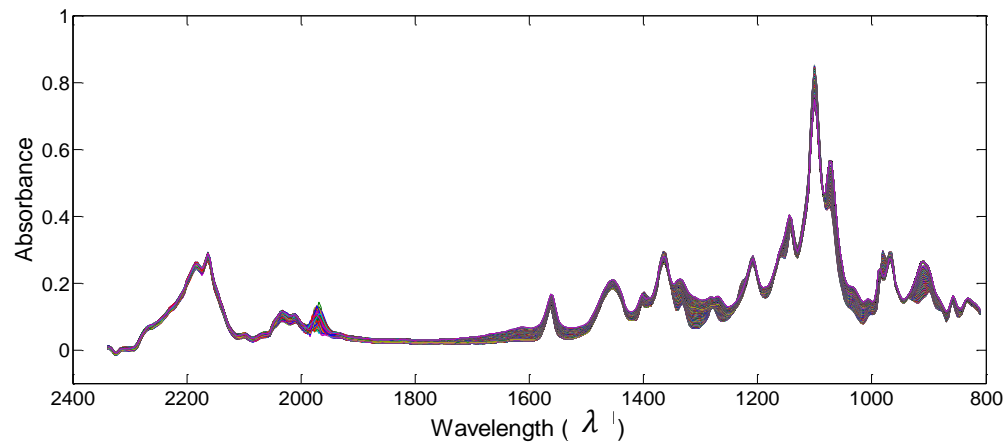
$$r_{-2} = k_{-2} c_{\text{AC}^-}$$



$$r_3 = k_3 c_{\text{AC}^-} c_{\text{AH}}$$



$$r_4 = k_4 c_{\text{AC}^-} c_{\text{BH}^+}$$



$$\frac{dV}{dt} = \begin{cases} \text{const flowrate}, t < 3.5h \\ 0, t > 3.5h \end{cases}$$

$$\frac{dc_{\text{AH}}}{dt} = -r_1 - r_3 - \frac{\dot{V}}{V} c_{\text{AH}}$$

$$\frac{dc_{\text{B}}}{dt} = -r_1 + r_4 - \frac{\dot{V}}{V} c_{\text{B}}$$

$$\frac{dc_{\text{A}^-}}{dt} = r_1 - r_2 + r_{-2} + r_3 - \frac{\dot{V}}{V} c_{\text{A}^-}$$

$$\frac{dc_{\text{BH}^+}}{dt} = r_1 - r_4 - \frac{\dot{V}}{V} c_{\text{BH}^+}$$

$$\frac{dc_{\text{C}}}{dt} = -r_2 + r_{-2} - \frac{\dot{V}}{V} c_{\text{C}} + \begin{cases} m_{\text{C_add}} / V, t < 3.5h \\ 0, t > 3.5h \end{cases}$$

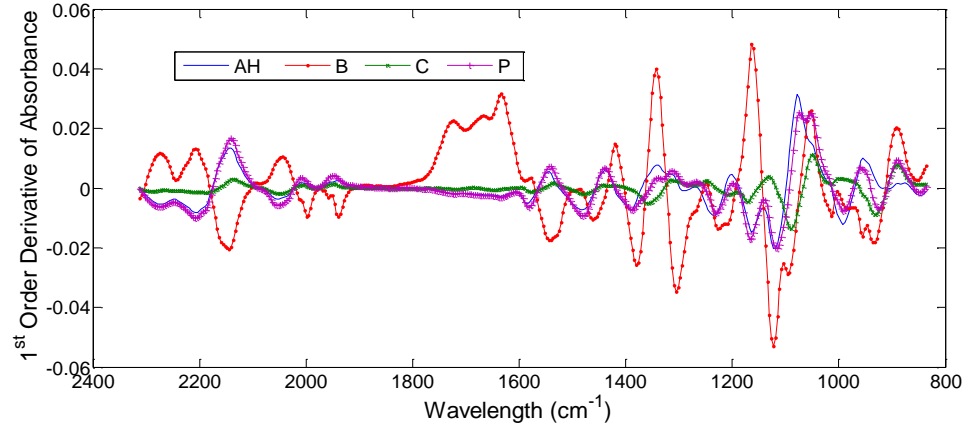
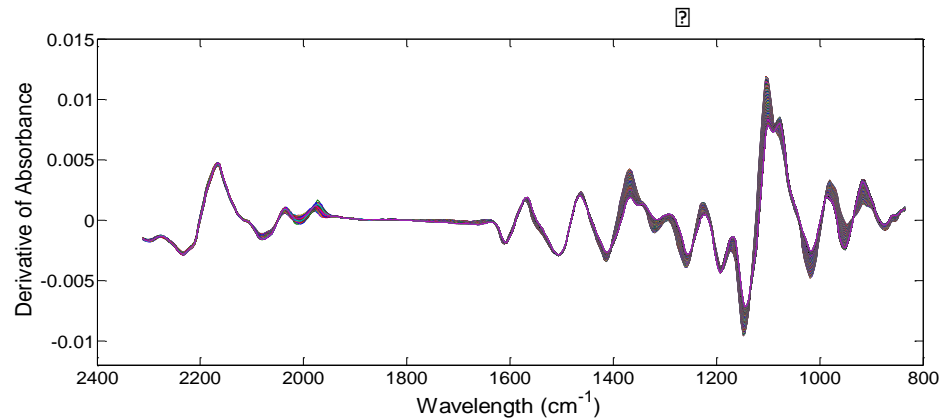
$$\frac{dc_{\text{AC}^-}}{dt} = r_2 - r_{-2} - r_3 - r_4 - \frac{\dot{V}}{V} c_{\text{AC}^-}$$

$$\frac{dc_{\text{P}}}{dt} = r_3 + r_4 - \frac{\dot{V}}{V} c_{\text{P}}$$

Example – wavelength selection

◆ Using MSC + SG

Parameters	k_1	k_2	k_2	k_3	k_4
Upper bound	10	100	10	50	150
Value	3.46252×10^{-2}	61.5544	2.36893	4.04948	150
Variance	2.14×10^{-8}	12.78	3.15×10^{-2}	6.74×10^{-4}	3.85×10^{-10}
Standard Deviation	1.46×10^{-4}	3.57	1.77×10^{-1}	2.60×10^{-2}	1.96×10^{-5}

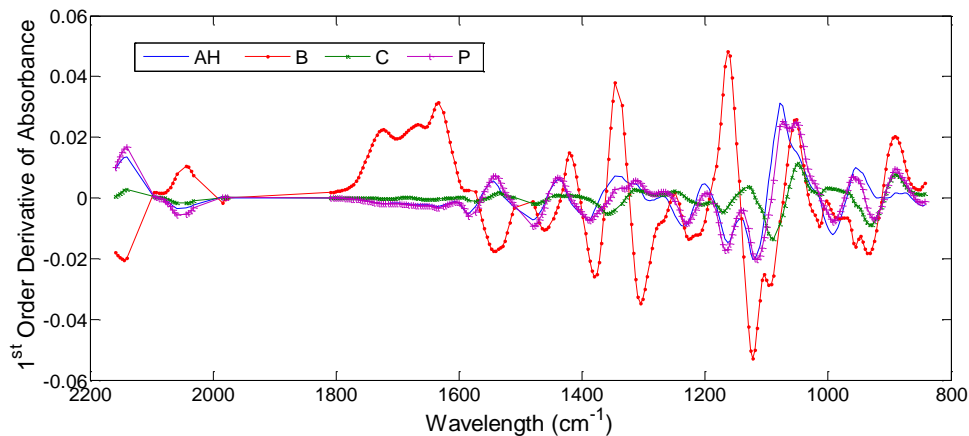
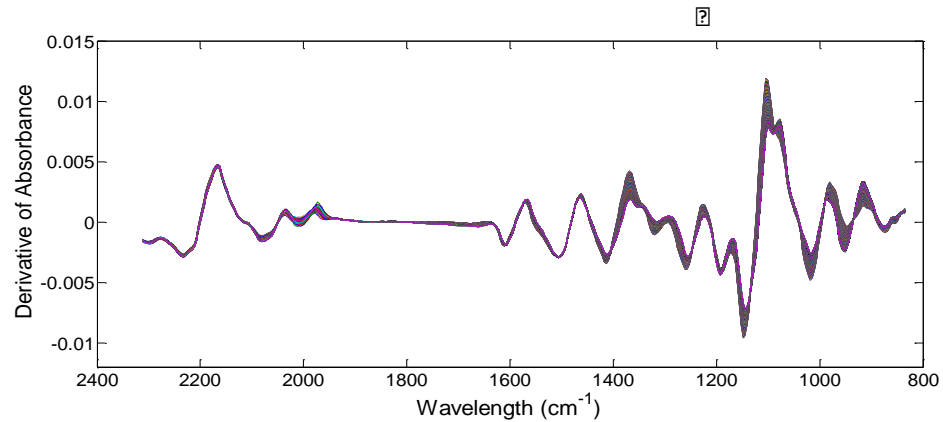


Using entire spectra

Example – wavelength selection

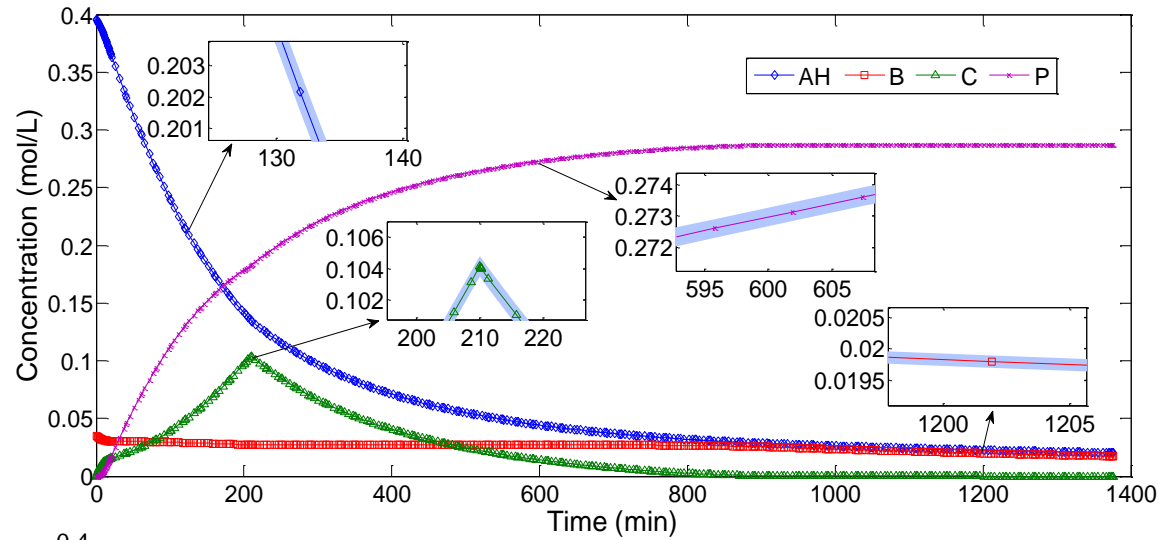
◆ Using MSC + SG

Parameters	k_1	k_2	k_{-2}	k_3	k_4
Upper bound	10	150	10	50	150
Value	3.46445×10^{-2}	96.0931	4.17568	4.12065	150
Variance	2.17×10^{-10}	1.67×10^{-9}	6.17×10^{-7}	2.27×10^{-6}	6.00×10^{-10}
Standard Deviation	1.47×10^{-5}	4.08×10^{-5}	7.85×10^{-4}	1.51×10^{-3}	2.45×10^{-5}

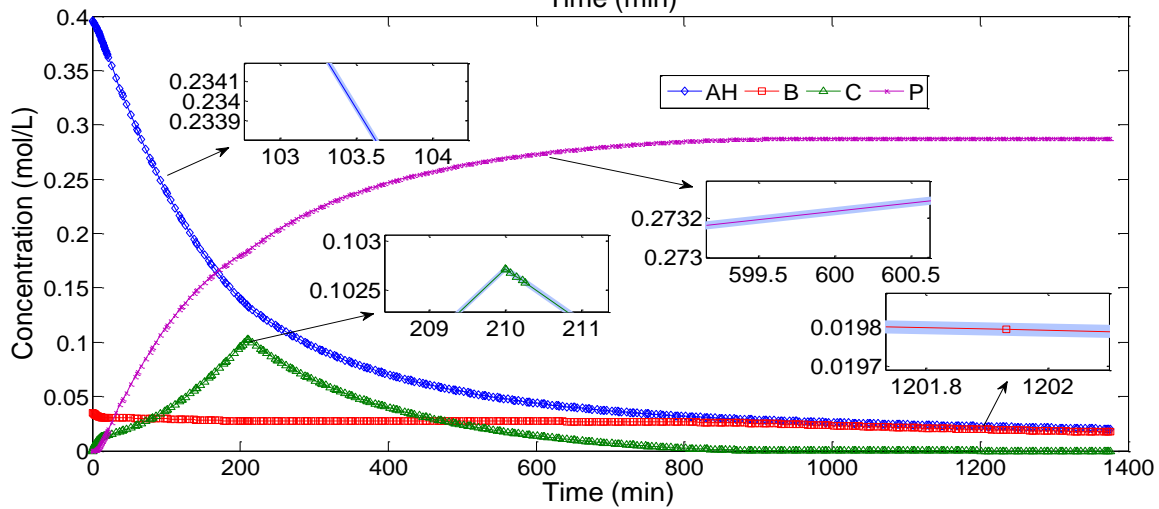


Using NLP to select channels
Reduction in LOF of 66%.

Example – wavelength selection



All spectra



With NLP
wavelength
selection