

Supplementary data:

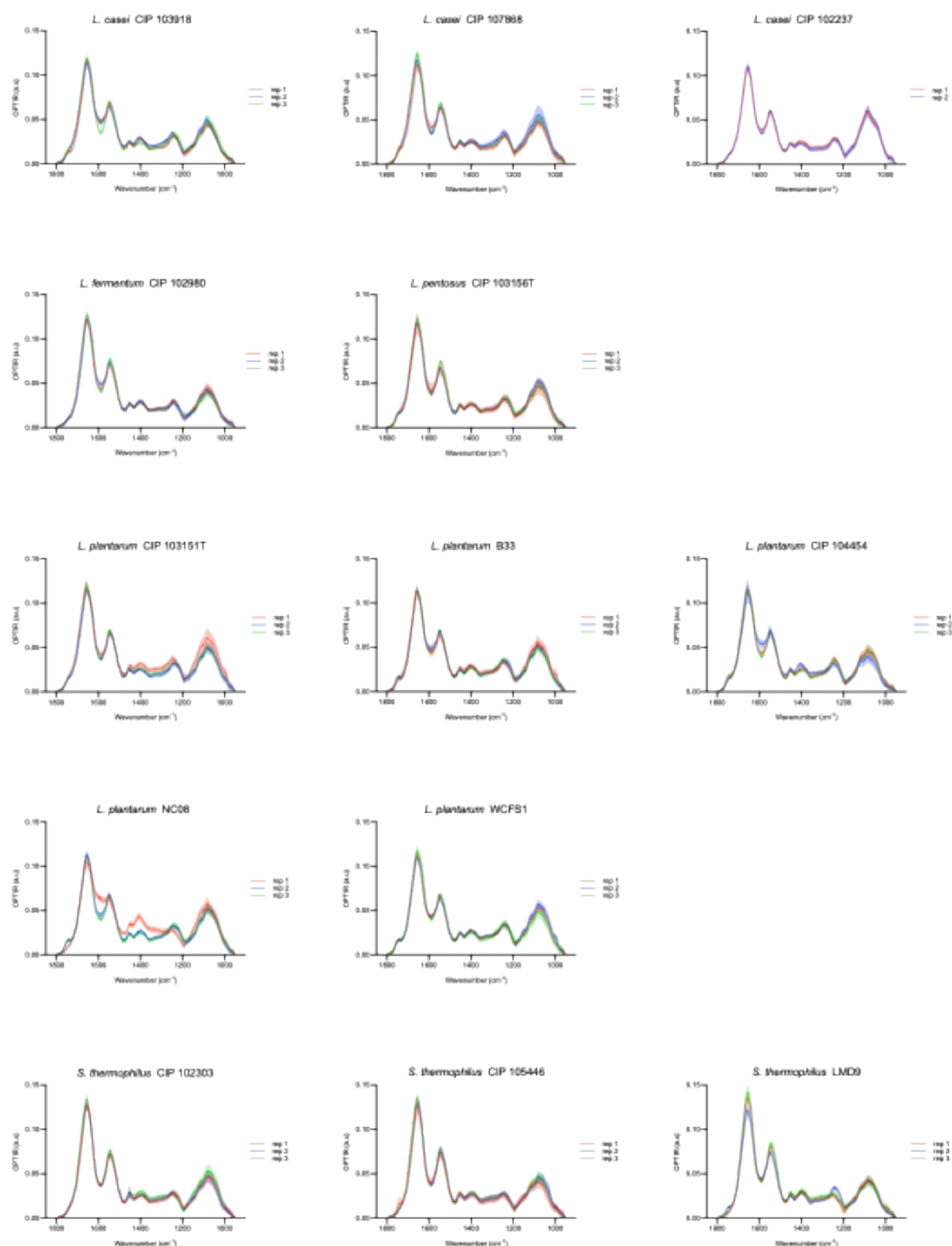


Figure S1: Layout of overlay of average OPTIR spectra (region: 1800 - 950 cm^{-1}) of all 13 strains replicates (red: replicate 1; blue: replicate 2; green: replicate 3). Spectra were vector-normalised, smoothed using the Savitzky-Golay algorithm (window size = 9, polynomial order = 2). The line represents the average (mean) spectrum for each replicate, the shaded area represents standard deviation.

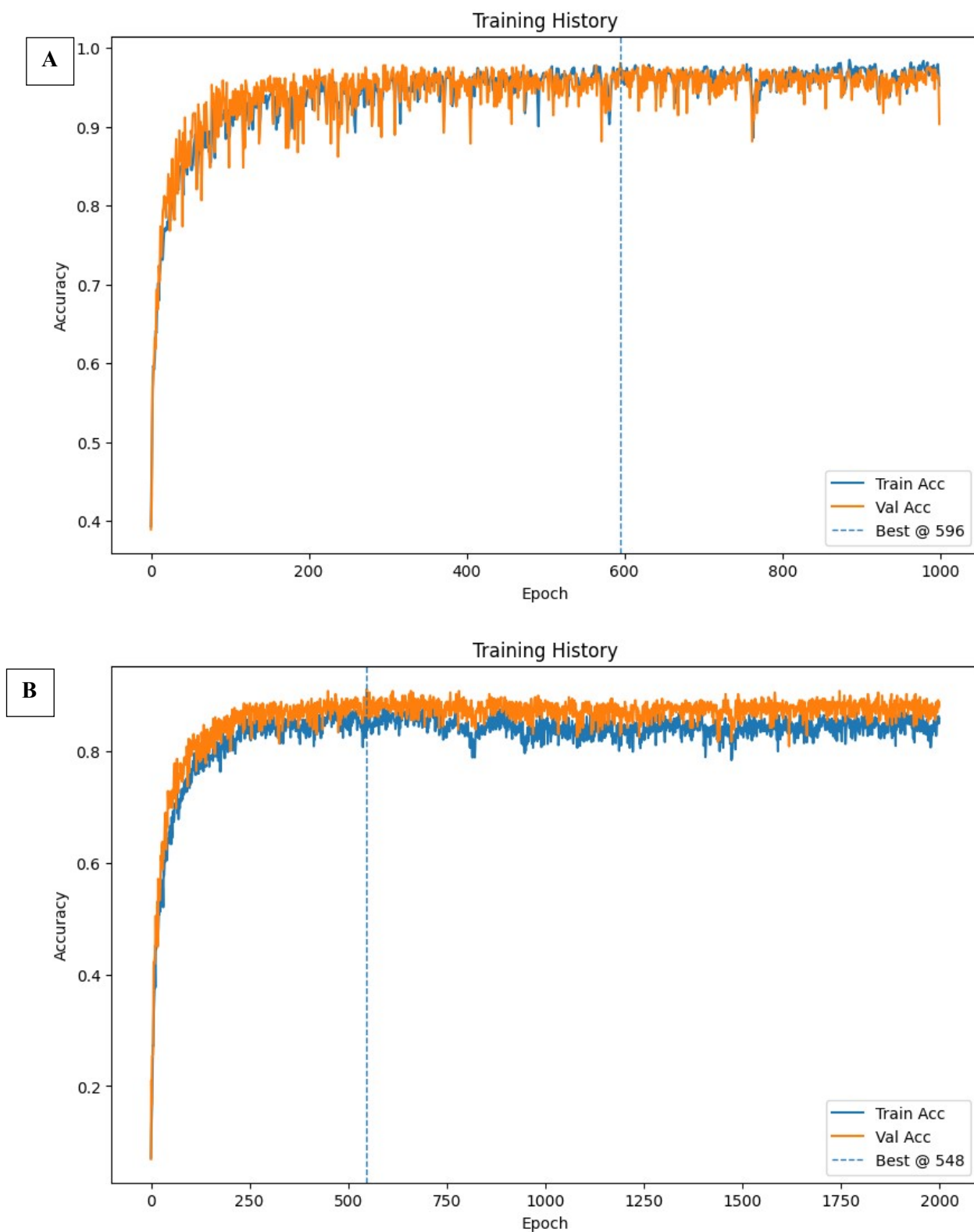


Figure S2: Training/validation accuracy histories to determine best hyperparameters: (A) on species level set (B) on strain level set.