



Demonstrating the importance of visual inspection of reference spectra matching results

MCR-ALS resolved pure component spectra from Raman microspectroscopic images of cross-sections of hybrid aspen wood fibers are used as examples (see “good example” in Figure 6), with spectra of pure cellulose, lignin and D-glucuronic acid used as references (see the Materials section)

a) The percentage matches based on Euclidean distances (dot products)

b-f) Area normalized spectra plots showing each component (thick black line), cellulose (blue), lignin (red) and D-glucuronic acid (green).

As can be seen, all matches to D-glucuronic acid can be discarded despite the high percentage hits, since none its characteristic bands match the component spectra (most notably the band at  $1750\text{ cm}^{-1}$ , resulting from  $\text{-C=O}$  stretching, is absent). Component 1 matching lignin and component 2 matching cellulose can be confirmed as legitimate matches. Component 3 and 4 can have contributions from cellulose too, while component 5 is clearly an unresolved mixture, containing both lignin and cellulose.