Assessment of Beeswax Adulteration by Paraffin and Stearic Acid Using ATR-IR Spectroscopy and Multivariate Statistics—An Analytical Method to Detect Fraud

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Table S1. Paraffin and stearic acid calibration samples.

Paraffin	**CP1**	**CP2**	**CP3**	**CP4**	**CP5**	**CP6**	**CP7**	**CP8**
Paraffin concentrations (% w/w)	0.00	5.02	9.69	15.10	20.07	25.15	49.69	100
Stearic acid	**CA1**	**CA2**	**CA3**	**CA4**	**CA5**	**CA6**	**CA7**	**CA8**
Stearic acid concentrations (% w/w)	0	0.68	1.14	4.9	14.89	25.65	50.64	100

Figure 5 indicates that samples 16 and 22 may contain amounts of tri-stearin and/or beef fat, in addition to paraffin and/or stearic acid. An independent way of investigating this assumption is illustrated in Figure S1, where the experimental IR spectrum of sample 22 and a calculated spectrum to simulate the former are presented. The calculated spectrum is computed by linear combinations of the reference spectra of beeswax, stearin, paraffin and stearic acid. Each reference spectrum was multiplied with a weighting factor and then all four weighted spectra were added together. The weighting factor is considered as a rough approximation of the presence of each substance. The linear combination used in Figure S1 is the following:

Simulated spectrum = (0.4*Beeswax) + (0.29*Paraffin) + (0.25*Stearin) + (0.06*Stearic Acid)

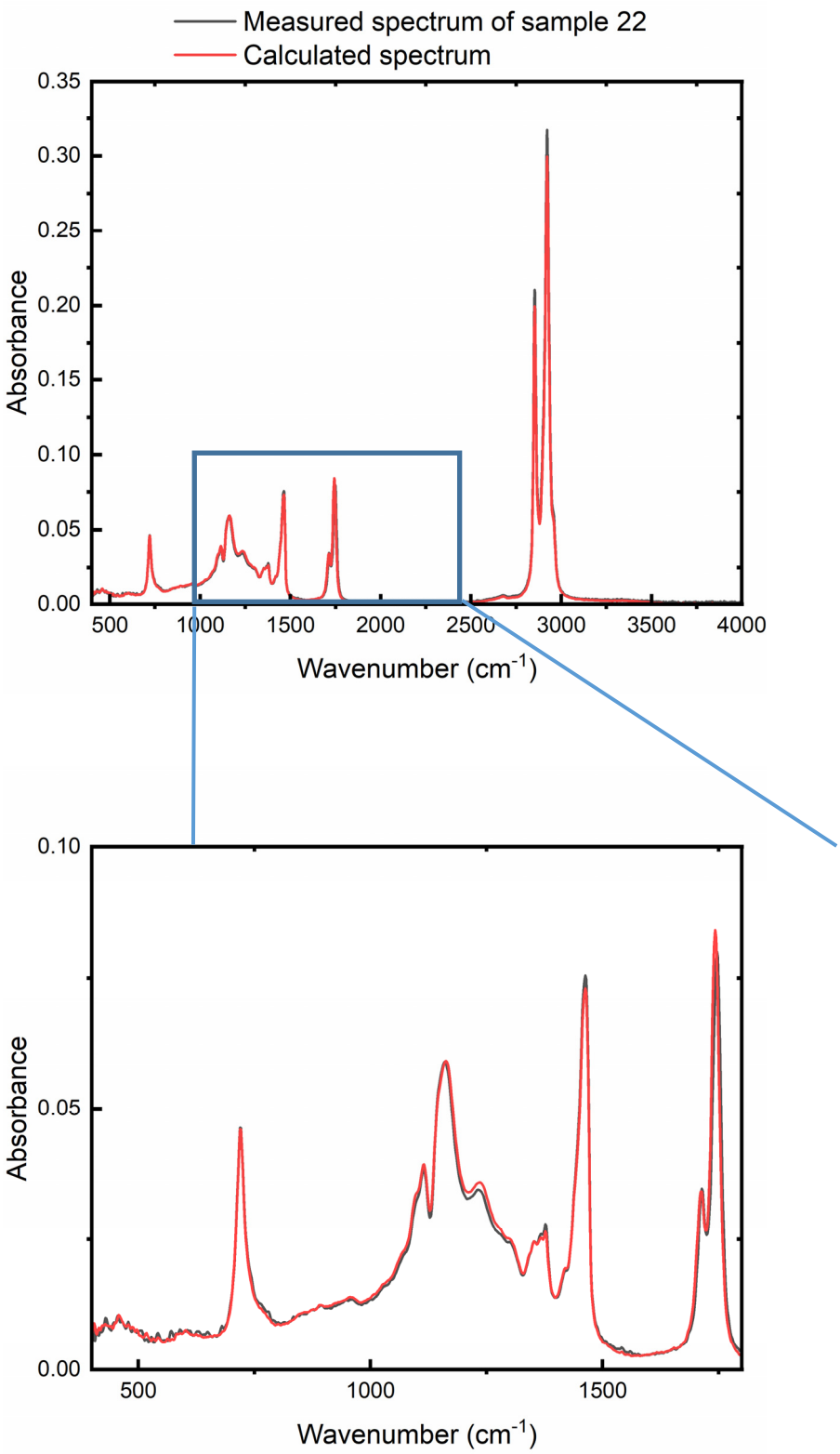

Figure S1. **Top:** Comparison of the experimental and simulated IR spectra in the 400 – 4000 cm^{-1} range**. Bottom:** Enlarged view of the same spectra in the 400 – 1800 cm^{-1} range for better visualization.