Comment on “Optimization of Alkylresorcinols Extraction from Triticale Bran Using Response Surface Methodology [Agil et al. (2012), Food and Bioprocess Technology, 5(7), 2655–2664]”

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In their article, Agil et al. (2012) make the following statement regarding the assignment of FTIR spectra for the standard and extracted alkylresorcinols: “The 2,900–3,000 cm^{-1} absorption bands were attributed to C–H and CH_2 vibration of aromatic hydrocarbons.” In contrast, an aromatic group cannot have a “ CH_2 vibration.” The authors have incorrectly assigned the 2,900–3,000 cm^{-1} absorption bands as belonging to the aromatic C–H stretches on the alkylresorcinols. These absorption bands are due to the aliphatic C–H stretches on the long alkyl chains. Aromatic C–H stretches show up generally between 3,000 and 3,100 cm^{-1} , not between 2,900 and 3,000 cm^{-1} as Agil et al. (2012) erroneously claim.

The IR spectra in Fig. 6 from Agil et al. (2012) have apparently been manipulated. When the regions around 3,100 cm^{-1} in Fig. 6a and b are examined closely, it becomes clear that the spectral lines are discontinuous, and it appears that different portions of the spectra (or from different spectra) have been moved around in the x – y space in order to construct some type of desired final spectra. Further suggestions of image manipulation come from the spectrum in Fig. 6b, whereby a peak between about 1,100–1,200 cm^{-1} is also discontinuous, suggesting regions of the spectrum had been “cut-and-pasted” together. These regions are shown in Fig. 1 herein.

a Region around 3100 cm^{-1} in Fig. 6(a) from Agil et al. (2012)

b Region around 3100 cm^{-1} in Fig. 6(b) from Agil et al. (2012)

c Region around 1100–1200 cm^{-1} in Fig. 6(b) from Agil et al. (2012)

Fig. 1 Regions from Fig. 6 in Agil et al. (2012) showing evidence of potential FTIR image manipulation

References

- Agil, R., Oomah, D. B., Mazza, G., & Hosseini, F. S. (2012). Optimization of alkylresorcinols extraction from triticale bran using response surface methodology. *Food and Bioprocess Technology*, 5(7), 2655–2664.

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