Spectra simulations in near-infrared spectroscopy of biomolecules and food adulterants

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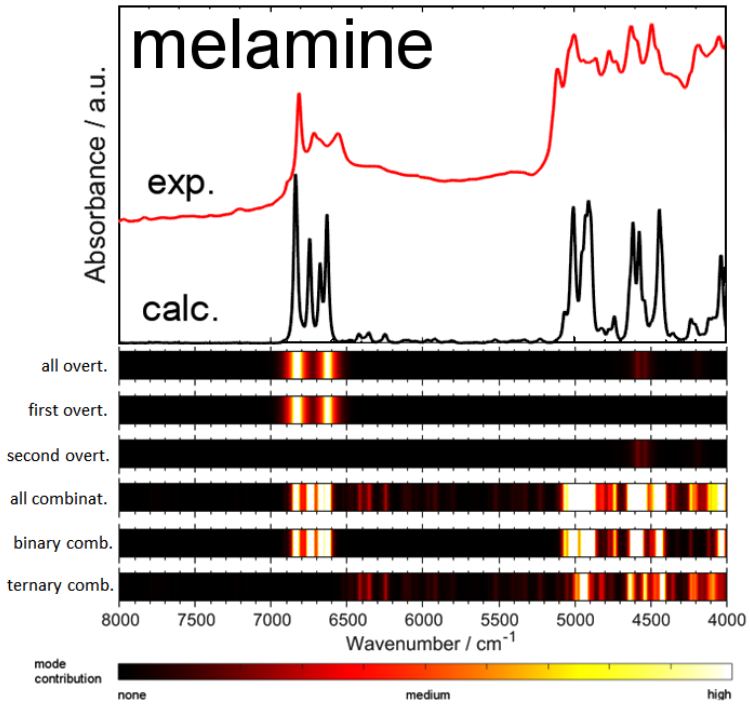
Near-infrared (NIR) spectroscopy is a powerful qualitative and quantitative analytical tool with increasing importance throughout science and industry. Difficult interpretability of the spectra hampers the evolution of NIR spectroscopy in certain areas, e.g. structural discrimination and identification. Recently, new opportunities for enhancing the qualities of NIR spectroscopy appeared through theoretical simulations of NIR bands. We present our achievements in developing this promising lane of research on the relevant examples – molecules of high importance in applied spectroscopy. Fatty acids (short-, medium-, and long-chain) are key biomolecules existing in most kinds of biomaterials. Their spectral signature is highly specific, yet interpretation of their complex NIR spectra remained mostly speculative. Melamine attracts high attention of analytical NIR spectroscopy due to its misuse as a food adulterant [1]. Our current goal is to develop new strategies for analytical spectroscopy, which will take advantages from hyphenated application of theoretical spectra simulations.



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[1] Grabska J., Beć K.B., Kirchler C.G., Ozaki Y., Huck C.W. *Molecules* **2019**, 24, 1402