Emerging possibilities of scientific and industrial applications of near-infrared spectroscopy. Towards efficient marriage between computational chemistry and analytical spectroscopy

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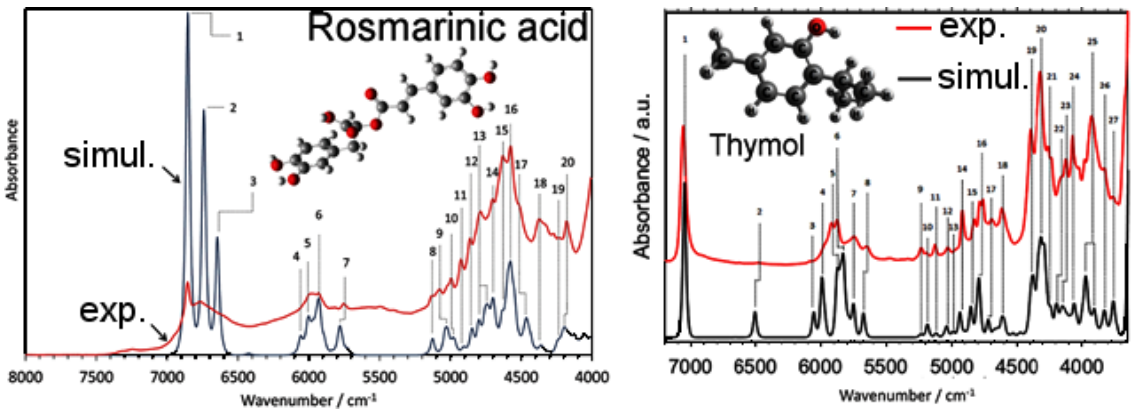
Near-infrared (NIR) spectroscopy has become a major analytical technique with various applications throughout academia and industry. Yet, due to the intrinsic complexity of spectra, NIR data has been mostly used without real physicochemical and molecular interpretation. Accordingly, the qualitative (structural discrimination and identification) and quantitative capabilities of NIR spectroscopy yet remain to be exploited to their real potential. We present our unique accomplishments in the emerging area of theoretical simulations of NIR spectra [1], and provide thorough overview of the unique possibilities, which emerge for academic and industrial research as the black-box nature of NIR spectroscopy is being successfully removed step-by-step. The examples range from basic molecules to biomolecules and practical materials with key importance in analytical spectroscopy, e.g. phytopharmaceuticals (Figure) or food adulterants.



This work was supported by the Austrian Science Fund (FWF), M2729-N28.

[1] Bec KB, Huck CW. Breakthrough potential in near-infrared spectroscopy: spectra simulation. A review of recent developments. *Front. Chem.* **2019**, 7:48.