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Characterization of ibuprofen by IR-spectroscopy and other complementary methods

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The main purpose of this study is to investigate the physicochemical properties of a pharmaceutical substance called ibuprofen. The research of medicines is crucial for the promotion and improvement of the healthcare system. The first aim of the study is to check the purity of the ibuprofen sample obtained in the pharmacy and its analysis in comparison with the information provided in the relevant literature. Various research methods are used to test ibuprofen. The following experimental methods were used: differential scanning calorimetry (DSC), X-ray powder diffractometry (XPRD), IR, NMR and RAMAN spectroscopy. The work presents a preliminary description of these methods, as well as the experimental results obtained for the tested ibuprofen sample. The NMR spectroscopy method revealed that the sample contains pure ibuprofen and can be used for further investigations. The powder X-ray diffraction method showed that the studied ibuprofen sample was in a crystalline form. The oscillation frequencies obtained from experimental measurements closely corresponded to the values calculated using the density functional theory (DFT) approximation, demonstrating a high degree of agreement. Linear correlations were found between the experimental oscillation frequencies and the frequencies calculated by DFT method.

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