Contribution ID: **25** Type: **Poster**

Spectroscopic study of ibuprofen interaction with polyethylene glycol matrix

Friday, November 8, 2024 4:15 PM (3 minutes)

Quantum chemical calculations of the structure and IR spectra of ibuprofen molecule were performed using various methods (HF, DFT, MP2). Several different conformers of ibuprofen were considered. The calculation results were compared with the experimentally registered spectra of ibuprofen. It is shown that MP2 method is the most appropriate for the description of the experimentally registered spectrum of ibuprofen.
FTIR spectra of pure ibuprofen and polyethylene glycol (PEG 400) as well as their solutions with different concentrations were registered and analysed. The obtained results of IR spectroscopy of a mixture of polyethylene glycol and ibuprofen (at a concentration of 30%) indicate the potential for controlled release of ibuprofen in pharmaceutical formulations with a polyethylene glycol matrix. This can contribute to the creation of new dosage forms that provide a constant and controlled release of the active substance, which can improve the effectiveness of therapy and the convenience of use for patients.
The work was supported by the National Research Foundation of Ukraine in the frame of the project "Nanostructural modification of application drugs for military medical technologies"(No. 2023.04/0140).

Type of presence

Presence online

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Session Classification: Poster Session