MS22-P05 | CHARGE DENSITY ANALYSIS OF A SERIES OF 4-METHYLTHIOSTILBENE DERIVATIVES

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The microtubular system with its dynamic nature characterized by the polymerization and depolymerization of α,β-tubulin heterodimers, is essential in a variety of cellular processes, including cell division. Because of this function microtubules are one of the significant and more successful molecular target for designing of new active molecules possessing anticancer activity. Among this group of compounds chalcones (1,3-diphenylprop-2-en-1-on derivatives) represent a promising class of compounds with a simple structure, taking the possibility of structural modifications that improve their anticancer properties. Our successful investigation on novel inhibitors of tubulin polymerization from group of combretastatin A-4 thioderivatives [1] prompted us to extend our research on chalcone scaffold.

In the course of these studies, a series of stilbene derivatives, bearing methylthio group at position 4 of one phenyl rings and different number and positions of mehoxy groups connected with the second phenyl ring, has been synthesized and structurally characterized. The influence of the substituents on the geometry and electron density distribution was studied by means of the charge density analysis, based on the high-resolution X-ray diffraction studies for well-diffracted crystals as well as on the transfer of the multipolar parameters, obtained from this analysis, to the samples of lesser quality. Multipolar Hansen-Coppens model was applied for building of electron density distribution, and the Atoms-In-Molecules approach for analysis of intra- and intermolecular interactions.

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[1] Stefański, T. et al. Eur. J. Med. Chem. 2018, 144, 797-816