Theoretical and spectral characterization of 5,6-dichloro-2-(2',3'/2',4'/2',5'/3',4'/3',5'-dimethoxyphenyl)-1*H*-benzimidazoles

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Benzimidazole and its derivatives are known to play crucial roles in the structures and functions of a number of biologically important molecules [1]. The benzimidazole ring system is present in clinically approved anthelmintics, antiulcers, antivirals and antihistamines [2].

In this study, theoretical and spectral characterizations of 5,6-dichloro-2-(2',3'/2',4'/2',5'/3',4'/3',5'-dimethoxyphenyl)-1*H*-benzimidazoles (**I** - **V**, Fig. 1) were studied. FT-IR, FT-Raman, NMR, mass and fluorescence spectra of the compounds were investigated. Theoretical calculations were performed by using Density Functional Method (DFT, B3LYP) with 6-32G(d,p) basis set.

According to the calculations the benzimidazole and the phenyl rings are nearly perpendicular to each other (Fig. 1). The highest dipole moment value is belonging to the compound **V** (8.24 D), and the lowest dipole moment with 6.92 D is belonging to **I**.

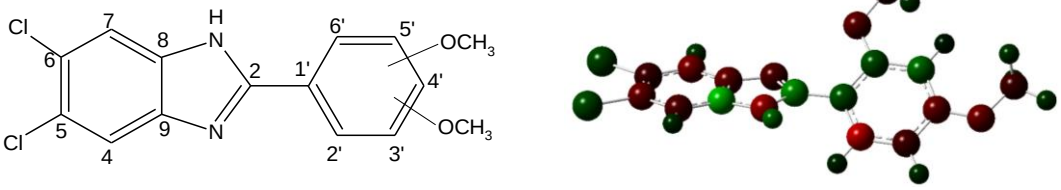

Fig. 1. General formula of the compounds in the study (left) and charge distribution of **II** (right).

[1] Infante-Castillo, R., Rivera-Montalvo, L. A., Hernandez-Rivera, S. P., *J. Mol. Struct.*, 877:10-19, 2008.

[2] Harrel, C. C., Kohli, P., Siwy, Z., Martin, C. R., *J. Am. Chem. Soc.*, 126:15646-15647, 2004.