ABSTRACT

The aim of this work is to calculate the parameters of substituted bases and chosen phenylguanidinium cations, earlier synthesized at the Department of inorganic and organic chemistry on the Faculty of Pharmacy CU in Hradec Králové, using quantum chemical methods.

I solved chosen problem by using computer programs Gaussian 03W and Hyperchem 8.0.10. I used program Gaussian to optimize the molecules and calculate the energy of the HOMO and LUMO, total energy and the atomic partial charge using the Mulliken population analysis. I used programe HyperChem to calculate the Van der Waals molecular volume; Van der Waals molecular surface; logP; the molar refraction; solvent-accessible surface of the probe size 1.0 Å; 1.2 Å; 1.4 Å; 1.6 Å and the atomic partial charge using methods PEOE.

All parameters of selected substituted phenylguanidines above have been successfully calculated, and listed in the tables in the chapter called results. The calculated results were discussed in chapter called discussion.

The calculated parameters will be used for further correlations and QSAR studies that will help to understand the biological activity of substituted phenylguanidines and hence their effect on the human organism.