[P37] Development and Applications of Electronic-Structure Informatics

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Electronic structures of molecules determine their molecular structures, molecular properties, and chemical reactivity. We would like to suggest that a research field correlating them with the electronic structures using tools of Chemoinformatics should be called "Electronic-Structure Informatics (ESI)". In order to develop ESI, we are currently developing a computer system consisting of five components as shown in Fig. 1: (1) "Electronic-Structure Database", (2) the "Electronic Spectral Similarity Analysis", (3) "Electronic Shape Similarity Analysis", (4) the "Electronic-Structure Data Mining", and (5) the "Knowledge-Data Search by Text-mining". By combining these tools, we can rank, classify, analyze various aspects of functional molecules. It is also possible to suggest promising molecules having desired electronic properties. In the presentation, we will discuss the details of our system and will show several applications to drug molecules and biomolecules.

Figure 1. Components of an "Electronic-Structure Informatics" system called "Intelligent Molecular Informatics Systems (IMIS)" developed in Kumamoto University