IWBSB 2009 (Boston) Participation Report

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Participation summary[1]

For myself, IWBSB 2009 was a great success. Along with a number of interesting presentations and social activities prepared by BU, the following were the main accomplishments pertaining to my Ph.D. thesis.

1. Meeting with Professor Ernst Walter-Knapp of the Free University of Berlin and his students. Professor Knapp will be my advisor during my visit to his laboratory from September 2nd - October 15th, 2009. The visit will be funded by the International Training Program (ITP).

2. After the poster session and discussions with Professor Knapp, the following research projects will be undertaken during my stay in Berlin:

   - A further generalization of the chiral tree-pattern graph kernel method developed (JCIM, 2009, revisions under review). The revision is to include electronegativity and electrostatic potential information in the kernel calculation. An example of two compounds with identical connectivity yet different electrostatic potential is shown in Figure 1.
   - Participation in a collaborative project suggested by Professor Knapp. His laboratory is largely invovled in protein docking, protein structure prediction, and chemoinformatics, in most cases via a physical chemistry approach. Therefore, this project will be complementary to the first project.

3. Establishment of a connection with BU Bioinformatics program director Scott Mohr of Boston University. Professor Mohr's background is in chemistry, and he will assist in the search for drug datasets that contain large numbers of valence group substitutions, e.g., $CH_4 \rightarrow SiH_4$. Ths purpose of the datasets is to demonstrate the necessity and effeciency of the electrostatic/electronegative graph kernel proposed.

4. As a corollary of the first and third items, my final Ph.D. topic will be a collaborative effort between Kyoto University, the Free University of Berlin, and Boston University.

Discussions with a number of students from BU and Berlin were also fruitful. After a busy poster session where the chiral tree-pattern graph kernel drew much attention, students provided some feedback on ways to improve the robustness of the system. Several students who had just joined their respective bioinformatics programs expressed interest in chemoinformatics as a result of my work.

[1] Abbreviations used - BU: Boston University; JCIM: Journal of Computer Information and Modelling

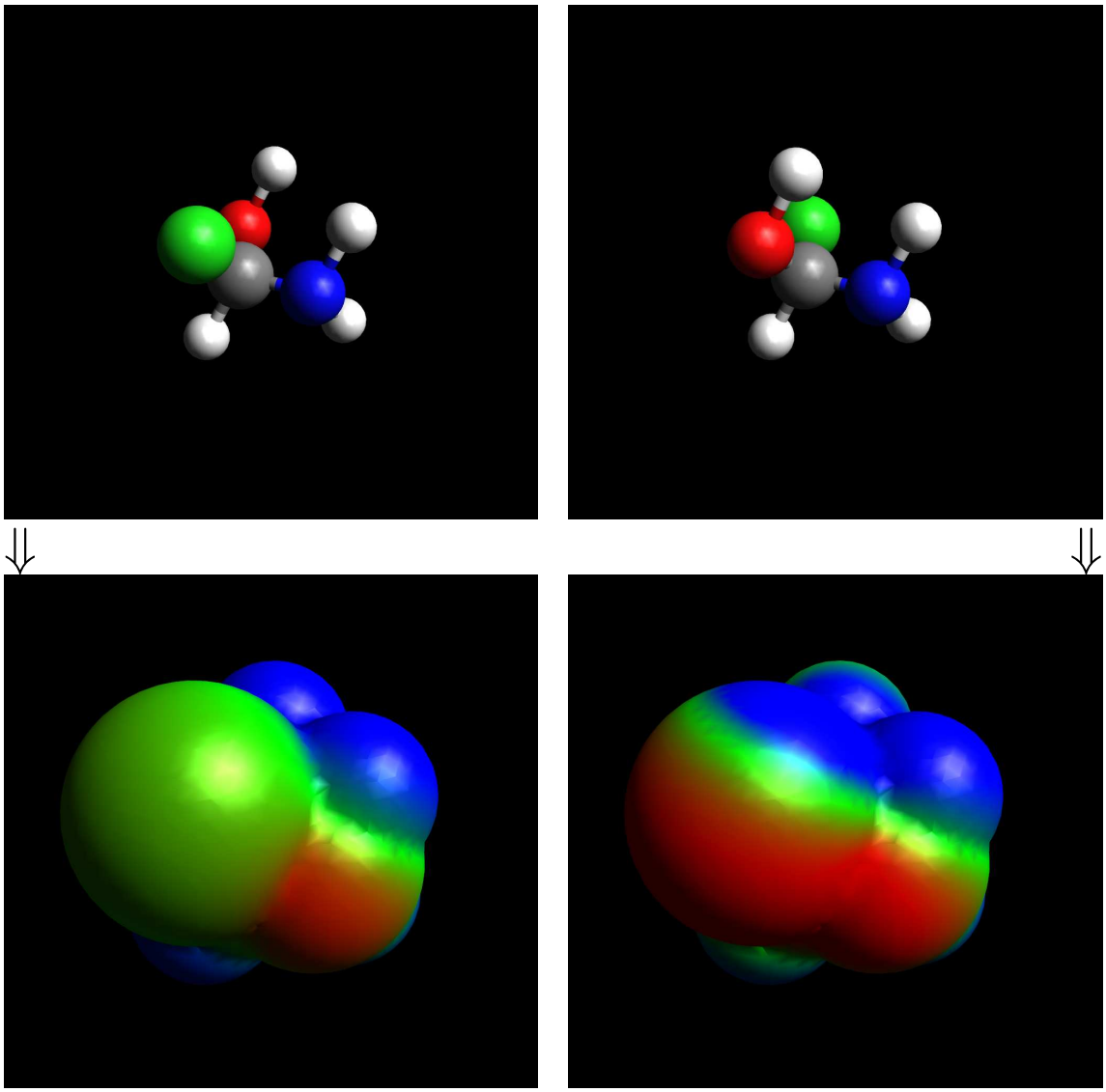

Figure 1: R- and S- forms of aminochloromethanol [CH(OH)(NH2)] (top), and their resulting electrostatic potential maps. The ESP maps are different, which can be used for detecting differences in the compounds. Using only topology, this would not be possible.