**Summer Project**

**Summary:**

Our objectives can be summarized into these questions:

*Is it possible to collect most of organic reaction database into the software?*

*Is it possible to input chemical structure into a* *reconcilable computer language?*

*Is it possible to predict reaction product base on reactants and condition?*

*Is it possible to make interference friendly that even my grandma can use it?*

*Is it possible to make it Wikipedia like software that people all over the world can add their reactions into the software with reference?*

*Is it possible to predict reactant only bases on product?*

……

**Goal**: Organic reaction predictor software.

Organic synthesis is a special branch of chemical synthesis and is concerned with the construction of organic compounds via organic reactions. It is the most common reaction type in the chemical industry. Each type of organic reaction will follow a certain reaction mechanism under a certain condition (side reaction might occur). So based on the reaction mechanism, people are able to predict the reaction products. It can also be described as input to output process in computer area.

**For example:**



With addition of Acid (H+), it will cause OH group leaves as H2O which will provide an empty spot, without any other addition molecule, it will cause CH3 to migrate (migration also has its own rule to follow) which leave another empty spot for OH, and it will generally make a C=O bond.

**Our goal is using Organic Textbook as database, and only focuses on the university level organic chemistry reactions.** It can be used as a study tool in chemistry.

**Major Challenge:** input chemical structure. For example, <http://www.nmrdb.org/> or UltraChemDraw. Generally, you could draw a chemical structure, and computer is able to identify the structure or the environment of the chemical (function groups). For example, as the mechanism showing above, if people drawing that structure, the software should be able to identify there are two OH groups, and this molecule is alcohol or more specifically diols (two OH-groups).

**Major Challenge:** Designing a reaction engine.

**Market Target: University students**. The software can be used as a great reference for student to use as a study tool.

**Currently existing program:**

<http://en.wikipedia.org/wiki/List_of_computer-assisted_organic_synthesis_software>

However, our goal is producing interface friendly software that even a high school student can play around, like (<http://www.nmrdb.org/>). Almost all of those programs remain unknown for almost every university student. No App was found.

**The work is voluntary, but if we can turn our program into profit, we will be able to earn some money. If not, I would consider this as a great experience that we can certainly write on our future resume.**

**Comment by other professors:**

Computational chemist: Dr. Jason Pearson:

*It is a challenging project, but I would say it’s feasible….*

Organic chemist: Dr. Nola Etkin

*I think it is a great idea…….especially in App.*

Computes science: Dr. Cezar Câmpeanu

*If you can find someone can do computer programing, bring him to me…*

If you are interested in this project, please contact Christopher for details

**Contact: syyy1213@hotmail.com**