COLD SPRING HARBOR ASIA CONFERENCES

Protein Structure Based Drug Design
Suzhou Dushu Lake Conference Center
September 19 - 23, 2011

The conference included twelve oral sessions and one poster session. Several topics were included to oral sessions, for example, rational drug design, structure-based drug design, predicting function from sequence, docking ligands to proteins, molecular dynamics and drug design, mechanistic-based drug design, high throughput screening and genomics. The poster session referred to the latest findings across many topics in protein structure research.

Several well-known scientists shown their latest research during the oral session, one of impressive study was about the scaffold-based drug discovery (SBDD) tool application. The researcher used the discovery and development of Vemurafenib (PLX4032) as an example to illustrate the application and impact of SBDD on the discovery of new drug candidates. As one hot spot of research, Raymond Steven's group solved several of GPCR crystal structures. It was demonstrated that β2-adrenergic receptor bound to the partial agonist carazolol and human human adenosine A2A receptor bound to the antagonist ZM241385. This information will throw light on designing novel drug targeting to the GPCR superfamily.

For the poster part, I showed the latest results of my research, which identified several small molecules binding to the MOD1 protein based on virtual screening. Four persons were interested in my project and they gave me very good advices, for instance, one audience from *Novartis International AG* suggested me to redo the virtual screening based on alternative library instead of FIMM, because it was said some databases may have specificity to certain protein. More hits should be figured out if the suitable database was chosen. One person from local pharmaceutical company showed strong enthusiasm on my study. Realizing their own shortcoming, this manager was really eager to set up connection with our group and express the ambition to cooperate.

During the conference, a lot of possibilities were given to communicate with other researchers. I discussed about molecule modeling software with one researcher from Malaysia. We compared Sybyl and Schrödinger, the experience to use the software was also shared.

After the conference I went with my supervisor to the city of Xi'an to visit the Northwestern Polytechnical University. He gave two lectures about computational drug discovery. I helped to organize his visit and participated in the discussions.

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