

Cooperation between Industry, Academia and Government

--- Guest Research Scientists and Researchers from Joint Research companies ---

We have had numerous inquiries regarding joint research ventures or technical training from companies and universities. Our human resources, cutting-edge computing facilities and equipment and environment may have attracted them. To meet these demands, we have received guest research scientists and trainees (graduate school students) from universities and researchers from joint research companies. This cooperative and stimulating network between industry, academia and government has formed the basis of our research and will lead to social benefits as well as paper publications and patent applications.

Here to share in their experience at the CBRC are two such researchers.

Glycobiology: elucidation of the structure of oligosaccharides on the surface of proteins has recently received considerable attention in post-genome science.

Dr. Yamagaki has worked on structural analysis of oligosaccharides using mass spectrometry. The demand currently exists for a technique that is capable of analyzing the precise structure of oligosaccharides, particularly since their structure is known to exhibit divergence and numerous constitutional isomers and types of bonds. A collaborative effort directed at the development of a new technique with which to analyze oligosaccharides is currently underway within our Cellular Informatics Team (Leader,



FT-ICR mass spectrometer and the tunable laser

Tohru Yamagaki
Assistant Professor, Department of Chemistry, School of Science, The Univ. of Tokyo

Katsutoshi Takahashi). The technique employs separation by the latest FT-ICR mass spectrometer and tunable (variable frequency) lasers.

Research on elucidating oligosaccharide structure has lagged behind research efforts into proteins and peptides. Oligosaccharide research also requires high-performance computing resources for accurate predictions of structure and these requirements are being met by collaboration with our High Performance Computing Team (Kazuhiko Fukui, Research Scientist). The technique involves prediction of MS/MS spectra by simulating fragmentation reactions in a mass spectrometer and then to use that data for the analysis of oligosaccharide structure for entities the structures for which are still unknown.

“When we could develop this technique, *it will be possible to assess person’s physical condition from a drop of their blood*”, Dr. Yamagaki expects.

Yoshikazu Mori

Pharmacognosy & Medical Resources Research Dept., R&D Division, Tsumura & Co.

Mr. Mori looks back at his time spent undertaking joint research, “I learned a lot, particularly about molecular modeling and design (MMD) techniques, the importance of bioinformatics, the way these techniques can be applied and other potential applications.”

This joint research exercise between Tsumura & Co. and our Molecular Modeling & Design Team (Leader, Takatsugu Hirokawa) started in June 2004. The aim of the work was to rationalize, through bioinformatics, new methods of drug discovery research based on their unique herbal medicine knowledge. The research is concerned with the identification of basic pharmaceutical lead compounds using MMD, as well as acquiring the latest MMD skills and the techniques developed by CBRC. The research has entered a more concrete phase

involving the modeling of three drug target proteins related to inflammatory disease and calculating their dockings with chemical compounds.



Mr. Mori and Hirokawa

Mr. Mori gave us a strong impression of his determination when asked about the next objective,

“I will try to develop a more rationalized and accurate system for searching for lead compounds, as well as becoming more involved in the screening system of ligand modeling currently possible using CoLBA.”

◆ Collaboration between Industry, Academia and Government ◆

| | 2001 | 2002 | 2003 | 2004 |
|-----------------------|------|------|------|------|
| Commissioned Research | 3 | 4 | 7 | 8 |
| Joint Research | 1 | 5 | 6 | 13 |
| Technical Training | 20 | 20 | 25 | 28 |
| Patent Applications | 3 | 23 | 7 | 6 |
| IPR Utilization | 1 | 2 | 6 | 0 |

* As of the end of March, 2005

◆ Belongings ◆

| Guest Research Scientist | Joint Research Scientist |
|---|---------------------------------------|
| Osaka Univ. 2 | Cyber Laser Inc. 1 |
| Kanazawa Institute of Technology . . . 1 | Tsumura & Co. 1 |
| Kyoto Univ. 1 | Fujitsu Laboratories 1 |
| The Univ. of Tokyo 2 | JST 2 |
| Ritsumeikan Univ. 1 | |
| Technical Trainee (from University) | Technical Trainee (from Company) |
| The Univ. of Tokyo 6 | Intec W&G Informatics Corp. 1 |
| Tokyo Institute of Technology 1 | NEC Soft, Ltd. 1 |
| Tokyo Univ. of Agriculture and Technology . 1 | IMS Lab. Inc. 7 |
| Nara Institute of Science and Technology . 5 | Best Systems Inc. 1 |
| Waseda Univ. 3 | Fujitsu FIP Corp. 1 |
| Univ. of Southern California 1 | Ryoka Systems Inc. 1 |