RESEARCH FACILITIES

The Institute includes five research facilities. This section describes their latest equipment and activities. For further information please refer to previous IMS Annual Review issues (1978–2015).

UVSOR Facility

KOSUGI, Nobuhiro	Director
KATOH, Masahiro	Professor
SHIGEMASA, Eiji	Associate Professor
TANAKA, Kiyohisa	Associate Professor
IWAYAMA, Hiroshi	Assistant Professor
OHIGASHI, Takuji	Assistant Professor
IDETA, Shin-ichiro	Assistant Professor
FUJIMOTO, Masaki	Assistant Professor
HASUMOTO, Masami	Technical Associate
YAMAZAKI, Jun-ichiro	Technical Associate
HAYASHI, Kenji	Technical Associate
KONDO, Naonori	Technical Associate
SAKAI, Masahiro	Technical Associate
TESHIMA, Fumitsuna	Technical Associate
NAKAMURA, Eiken	Technical Assosiate
YANO, Takayuki	Technical Associate
HORIGOME, Toshio	Administrative Associate
INAGAKI, Yuichi	Specially Appointed Technical Associate
TOKUSHI, Tetsujou	Technical Fellow
HAYASHI, Ken-ichi	Technical Fellow
MINAKUCHI, Aki	Technical Fellow
HAGIWARA, Hisayo	Secretary

Outline of UVSOR Synchrotron

Since the first light in 1983, UVSOR Synchrotron has been successfully operated as one of the major synchrotron light sources in Japan. After the major upgrade of the accelerators in 2003, UVSOR was renamed to UVSOR-II and became one of the world brightest low energy synchrotron light sources. In 2012, it was upgraded again and has been renamed to UVSOR-III. The brightness of the electron beam was increased further. Totally, six undulators were installed. The storage ring is operated fully in the top-up mode, in which the electron beam intensity is kept almost constant.

The UVSOR accelerator complex consists of a 15 MeV injector linac, a 0.75 GeV booster synchrotron, and a 0.75 GeV storage ring. The magnet lattice of the storage ring consists of four extended double-bend cells with distributed dispersion function. The storage ring is normally operated under multi-bunch mode with partial filling. The single bunch top-up operation is also conducted for about two weeks per year, which provides pulsed synchrotron radiation (SR) for time-resolved experiments.

Eight bending magnets and six undulators are available for providing SR. The bending magnet with its radius of 2.2 m provides SR with the critical energy of 425 eV. There are eight bending magnet beamlines (BL1B–BL7B, BL2A). Three of the six undulators are in-vacuum soft X-ray linear-polarized undulators (BL3U, BL4U, BL6U) and the other three are VUV circular-polarized undulators (BL1U, BL5U, BL7U). Totally, fourteen beamlines (= fourteen endstations) are now operational in two categories: eleven of them are so-called "public beamlines," which are open to scientists from universities, governmental research institutes, and public and private enterprises, and also to overseas scientists; the other three beamlines are so-called "in-house beamlines," which are dedicated to some strategic projects conducted by a few IMS groups in tight collaboration with external and overseas scientists. From the viewpoint of photon energies, we have 1 soft X-rays (SX) station equipped with a double-crystal monochromator, 7 SX stations with a grazing incidence monochromator, 3 VUV stations with a normal incidence monochromator, 2 infrared/tera Hz station equipped with FT interferometers and 1 beamline for light source development without monochromator.

Figure 1. UVSOR electron storage ring and synchrotron radiation beamlines.

Collaborations at UVSOR Synchrotron

A variety of molecular science and related subjects have been carried out at UVSOR Synchrotron by IMS and external/overseas researchers. The number of visiting researchers per year tops > 1,200, whose come from > 60 different institutes. International collaboration is also pursued actively and the number of visiting foreign researchers reaches > 100 from >10 countries. UVSOR Synchrotron invites new/continuing research proposals twice a year. The proposals both for academic and public research (charge-free) and for private enterprises (charged) are acceptable. The fruits of the research activities using UVSOR Synchrotron are published as the UVSOR ACTIVITY REPORT annually.

Recent Developments

BL7U, a high energy resolution ARPES beamline, is one of the most popular beamlines in UVSOR and it has been hard to get beamtime these days. For users who need sample surface preparation such as annealing, Ar-sputtering, deposition and so on, one or two week beamtime is not enough to prepare samples. To make the beamtime efficiently, "Offline-ARPES system" with helium discharge lamp at IMS (Nanotechnology Platform Japan program) has been open for users who requested. Three user groups used the offline-ARPES system before their beamtime to prepare sample in 2015.

The construction of a new soft X-ray beamline BL5U began in January 2014. The beamline performance had been once tested and it had been confirmed that the resolving power and photon intensity were very close to the expected values. However, in December 2014, it was found that the photons below 30 eV hit the grating mount and could not reach the endstation. The grating mount has been taken out, modified and attached again in March 2015. During the second beamline performance test, we found that the first mirror and probably the grating surfaces were covered by the carbon contamination, which made the photon intensity one order of magnitude smaller than the first test. The *in situ* cleaning method, which was used at BL4U, has been applied and photon flux has recovered to a half of the first test level. BL5U will be officially open for users from 2016.

Reserch Highlight

Microbial bioleaching of metal sulfides has been used as a low-cost engineering process for extracting metals from sulfidic ores due to its fast dissolution rate. The microbial bioleaching of metal sulfide also contributes to formation of environmentally detrimental acid mine drainage (AMD), whose acidic nature and heavy-metal constituents cause serious contamination of soil and groundwater in the world. Thus, a better understanding of the mechanisms is of crucial importance for improvement of both industrial bioleaching and AMD formation. Mitsunobu, *et al.* investigated the mechanisms of the bioleaching process in bacterial pyrite leaching by leaching bacteria (*Acidithiobacillus ferrooxidans*) by scanning transmission X-ray microscopy (STXM) based C and Fe near edge X-ray absorption fine structure (NEXAFS) analyses at UVSOR BL4U.[1)]

Carbon NEXAFS analysis directly showed that attached *A. ferrooxidans* produces polysaccharide-abundant extracellular polymeric substances (EPS) at the cell-pyrite interface. Figure 2 shows the STXM-based merged Fe/C image and Fe 4p NEXAFS of bacteria cells attached to pyrite particles in 2 weeks incubation. The image in Figure 2a shows that Fe was localized around the surface of the bacteria cells. Considering that C NEXAFS demonstrated the appearance of a polysaccharide-rich EPS layer at the cell-pyrite interface, this suggests that Fe had accumulated in this polysaccharide layer. In the Fe NEXAFS spectra, both the spectra of whole cell and cell-pyrite interface (interface 1 and 2 in Figure 1b) consist of Fe(II) and Fe(III) peaks. Thus, the Fe species in both cell and cell-pyrite interface were Fe(II) addition to Fe(III). The Fe(II) detected by direct STXM based NEXAFS analyses in this study is a first direct evidence supporting the oxidative attack by the Fe(III) in EPS.

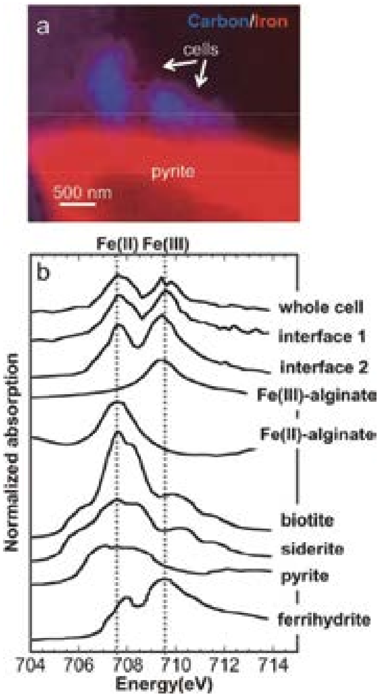


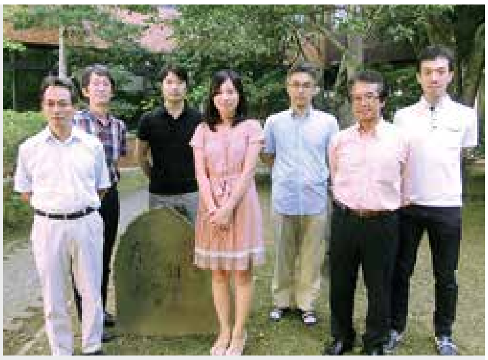
Figure 2. STXM-based C and Fe images (a) and Fe 4p NEXAFS spectra (b).

Reference

1) S. Mitsunobu, M. Zhu, Y. Takeichi, T. Ohigashi, H. Suga, M. Jinno, H. Makita, M. Sakata, K. Ono, K. Mase and Y. Takahashi, *Microbes Environ.* **31**, 63–69 (2016).

Laser Research Center for Molecular Science

OKAMOTO, Hiromi	Director, Professor
KATOH, Masahiro	Professor
OHMORI, Kenji	Professor
TAIRA, Takunori	Associate Professor
FUJI, Takao	Associate Professor
ISHIZUKI, Hideki	Assistant Professor
NOMURA, Yutaka	Assistant Professor
SHIRAI, Hideto	IMS Research Assistant Professor
OKANO, Yasuaki	Technical Associate
MASUDA, Michiko	Secretary



The Center aims to develop new experimental apparatus and methods to open groundbreaking research fields in molecular science, in collaboration with the Department of Photo-Molecular Science. Those new apparatus and methods will be served as key resources in advanced collaborations with the researchers from the community of molecular science. The main targets are (1) advanced photon sources covering wide energy ranges from terahertz to soft X-day regions; (2) novel quantum-control schemes based on intense and ultrafast lasers; and (3) high-resolution optical imaging and nanometric microscopy. The center also serves as the core of the joint research project "Extreme Photonics" between IMS and RIKEN.

Two of full-time associate professors and their research groups belong to the Center. The groups promote research projects targeting mainly on developments of novel laser light sources for molecular science. The Center also possesses several general-purpose instruments for laser-related measurements, and lends them to researchers in IMS who conduct laser-based studies, so as to support and contribute to their advanced researches.

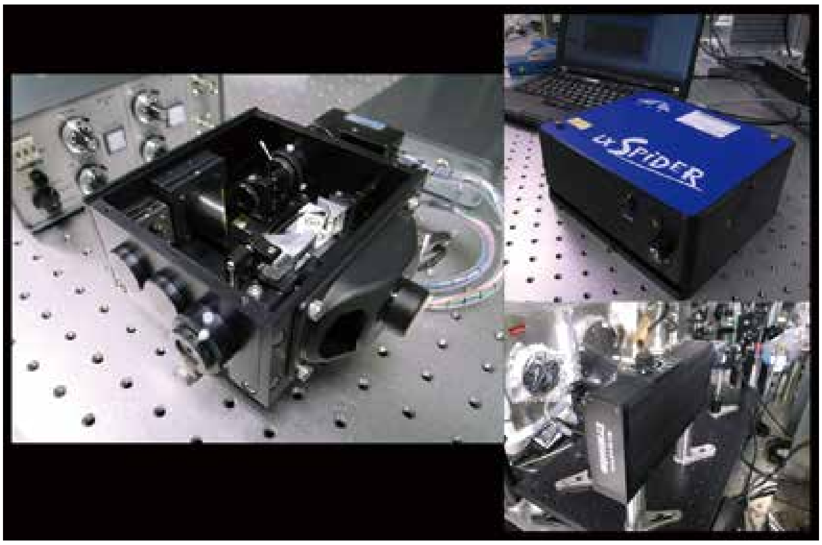


Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose ultrashort pulse characterization.

Instrument Center

KERA, Satoshi	Director, Professor
YOKOYAMA, Toshihiko	Professor
TAKAYAMA, Takashi	Technical Associate
FUJIWARA, Motoyasu	Technical Associate
OKANO, Yoshinori	Technical Associate
MIZUKAWA, Tetsunori	Technical Associate
MAKITA, Seiji	Technical Associate
UEDA, Tadashi	Technical Associate
OHARA, Mika	Nano. Platform Manager
NODA, Ippei	Nano. Platform Coordinator
NAKAO, Satoru	Post-Doctoral Fellow
NAGAO, Haruyo	Technical Fellow
IKI, Shinako	Technical Fellow
OTA, Akiyo	Secretary
NAKAGAWA, Nobuyo	Secretary
YOKOTA, Mitsuyo	Secretary
FUNAKI, Yumiko	Secretary
HYODO, Yumiko	Secretary
TOYAMA, Yu	Secretary
SAKURAI, Kumiko	Secretary

Instrument Center was organized in April of 2007 by integrating the general-purpose and state-of-the-art facilities of Research Center for Molecular Scale Nanoscience and Laser Research Center for Molecular Science. The mission of Instrument Center is to support the in-house and external researchers in the field of molecular science, who intend to conduct their researches by utilizing general-purpose and state-of-the-art instruments. The staffs of Instrument Center maintain the best conditions of the machines, and provide consultation for how to use them. The main instruments the Center now maintains in Yamate campus are: Nuclear magnetic resonance (NMR) spectrometers (JEOL JNM-ECA 920 for solutions and solids, JNM-ECA 600 for solutions, JNM-ECS400 for solutions and Bruker AVANCE800 Cryoprobe for solutions), matrix assisted laser desorption/ionization time-of-flight (MALDI TOF) mass spectrometer (Voyager DESTR), powder X-ray diffractometer (Rigaku RINT-Ultima III), circular dichroism (CD) spectrometer (JASCO JW-720WI), differential scanning calorimeter (MicroCal VP-DSC), and isothermal titration calorimeter (MicroCal iTC200), scanning electron microscope (SEM; JEOL JEM-6700F), focused ion beam (FIB) processing machine (JEOL JEM-9310FIB), and elemental analyzer (J-Science Lab Micro Corder JM10). In the Myodaiji campus, the following instruments are installed: Electron spin resonance (ESR) spectrometers (Bruker E680, E500, EMX Plus), NMR spectrometer (Bruker AVANCE600 for solids), superconducting quantum interference devices (SQUID; Quantum Design MPMS-7 and MPMS-XL7), solution X-ray diffractometer (Rigaku NANO-Viewer), single-crystal X-ray diffractometers (Rigaku Mercury CCD-1, CCD-2, RAXIS IV, and 4176F07), thermal analysis instruments (TA TGA2950, DSC2920, and SDT2960), fluorescence spectrometer (SPEX Fluorolog2), X-ray fluorescence spectrometer (JEOL JSX-3400RII), UV-VIS-NIR spectrometer (Hitachi U-3500), Raman microscope (Renishaw INVIA REFLEX532), nanosecond excimer/dye laser system (Lambda Physics LPX105i/LPD3002), Nd:YAG pumped OPO laser (Spectra Physics GCR-250/Lambda Physics Scanmate OPPO), fluorinated excimer laser (Lambda Physics Complex 110F), picosecond tunable laser system (Spectra Physics Tsunami/Quantronix Titan/Light Conversion TOPAS), low vacuum analytical SEM (Hitachi SU6600), electron spectrometers for chemical analysis (ESCA) (Omicron EA-125), angle resolved ultraviolet photoelectron spectroscopy (ARUPS) for functional band structures (VG-Scienta DA30), and FTIR spectrometer (Bruker IFS 66v/S). In the fiscal year of 2015, Instrument Center accepted 141 applications from institutions outside IMS and the total user time including in-house use amounted 3,539 days/36 equipments. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (58,240 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (33,164 L/year). The staffs of Instrument Center provide consultation for how to treat liquid helium, and provide various parts necessary for low-temperature experiments.

Instrument Center organizes the Inter-University Network for Common Utilization of Research Equipments and the Molecule and Material Synthesis Platform in the Nanotechnology Platform Program supported by Ministry of Education, Culture, Sports, Science and Technology. These special programs are described in the other chapter of the booklet.

Equipment Development Center

YAMAMOTO, Hiroshi	Director
MIZUTANI, Nobuo	Technical Associate
AOYAMA, Masaki	Technical Associate
YANO, Takayuki	Technical Associate
KONDOU, Takuhiko	Technical Associate
YOSHIDA, Hisashi	Technical Associate
TOYODA, Tomonori	Technical Associate
TAKADA, Noriko	Technical Associate
NAKANO, Michiko	Technical Associate
KIMURA, Sachiyo	Specially Appointed Technical Associate
KOSUGI, Yuta	Specially Appointed Technical Associate
TANAKA,Takashi	Technical Fellow
SAWADA, Toshihiro	Technical Fellow
URANO, Hiroko	Secretary

Researches and developments of novel instruments demanded in the forefront of molecular science, including their design and fabrication, are the missions of this center. Technical staffs in the two work sections, mechanics and electronics, are engaged in developing state-of-the-art experimental instruments in collaboration with scientists. We expanded our service to other universities and research institutes since 2005, to contribute to the molecular science community and to improve the technology level of the center staffs. A few selected examples of our recent developments are described below.

Introduction of 3D Printer

We have introduced a fused deposition modeling (FDM) type 3D printer, and started production of molecule models, such as proteins.

The model structures are based on a PDB file which includes the coordinate data of protein atoms. We convert it to the STL file, which is the collection of triangles for 3D printer, in a careful manner so that the printer can generate the 3D structure in an appropriate precision. After printing, finishing process of the model is completed through a lot of steps such as removal of supports, surface treatments, and coloring. Now we can produce fairly large and complex models. (Figure 1)

In addition, we utilize the 3D printer in the trial of designing and manufacturing. In the design phase, we can confirm the shape and movement of a given equipment by producing a prototype model with 3D printer. Model structure provided by 3D printer is of a great help for communication with a client. Furthermore, it also provides a short cut to produce high quality equipment in fewer steps. (Figure 2)

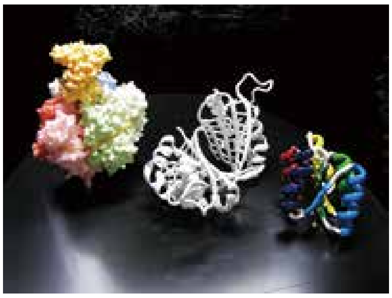


Figure 1. Structural Models of proteins.

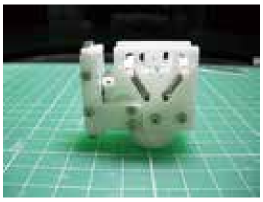


Figure 2. Prototype model of the equipment for crystal bending generated by 3D printer.

CPLD and ARM-Microcontroller-Based TTL Level Double Pulse Generator

In the analyses of chemical reaction processes using irradiation of a laser to molecules, we need to control the measurement apparatus and to open its gate in a short period of time whose duration is defined by predetermined delay time and pulse width, with synchronization to the pump laser. We have developed the TTL level double pulse generator (Figure 3) for this purpose. The main specification of this generator is shown in Table 1. This generator is made of CPLD (Complex Programmable Logic Device; EPM570T100C5N by Altera) and ARM® microcontroller (LPC1114FBD48/302 by NXP).

CPLD generates the delay pulse synchronized to trigger input. Then it generates logical disjunction of the delay pulse and the trigger pulse, with an interface operated by ARM microcontroller. More precisely, CPLD measures a delay time when trigger pulse is inputted. Then CPLD sets the delay pulse to 'H' level and measures a pulse width. ARM microcontroller operates the adjustments of delay and pulse width, and transfers the data back to CPLD.

Figure 3. TTL level double pulse generator.

Table 1. Main specification of TTL level double pulse generator.

Trigger input	TTL level, 1 kHz (typ.)
Output 1	Delay time: 500 μs ~ 2 sec Pulse width: 1 μs ~ 200 μs Time resolution: 100 ns
Output 2	Logical OR of Trigger input and Output 1

Research Center for Computational Science

SAITO, Shinji	Director, Professor
EHARA, Masahiro	Professor
OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Assistant Professor
ISHIDA, Tateki	Assistant Professor
FUKUDA, Ryoichi	Assistant Professor
ITOH, Satoru G.	Assistant Professor
MIZUTANI, Fumiyasu	Technical Associate
NAITO, Shigeki	Technical Associate
SAWA, Masataka	Technical Associate
IWAHASHI, Kensuke	Technical Associate
MATSUO, Jun-ichi	Technical Associate
NAGAYA, Takakazu	Technical Associate
TOYA, Akiko	Secretary
ISHIHARA, Mayumi	Secretary

Research Center for Computational Science provides state-of-the-art computational resources to academic researchers in molecular science and related fields, *e.g.* quantum chemistry, molecular simulations, and solid state physics. The computer systems consist of Fujitsu PRIMERGY RX300, PRIME HPC FX10 and PRIMERGY CX2550, SGI UV2000. The systems have been used by 758 people in 217 research groups in 2015. Large scale calculations, for example accurate electronic structure calculations of molecular systems and conformation searches using non-Boltzmann ensemble methods, have been performed with the systems. The Center also provides a number of application programs, for example Gaussian 09, GAMESS, Molpro, AMBER, and NAMD. The Center offers the Quantum Chemistry Literature Database, which has been developed by the Quantum Chemistry Database Group in collaboration with members of the Center. The latest release, QCLDB II Release 2015, contains 136,758 data of quantum chemical studies. Detailed information on the hardware and software is available on the web site (http://ccportal.ims.ac.jp/).

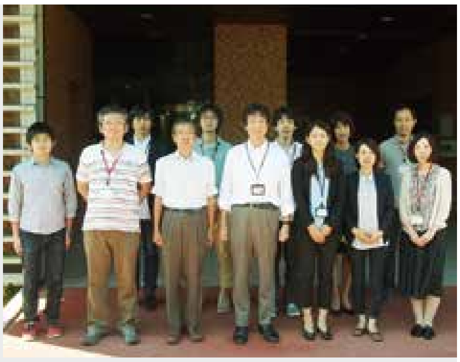
In addition to the provision of computational resources to individual academic researchers in Japan, the Center contributes up to 20% of the computational resources to the Post-K Supercomputer Priority Researches 5 and 7 and the Professional development Consortium for Computational Materials Scientists.

Figure 1. Fujitsu PRIMERGY CX2550.

Figure 2. SGI UV2000.

Okazaki Institute for Integrative Bioscience

AONO, Shigetoshi	Professor
KATO, Koichi	Professor
IINO, Ryota	Professor
KURIHARA, Kensuke	Research Associate Professor
KURAHASHI, Takuya	Assistant Professor
YOSHIOKA, Shiro	Assistant Professor
YAMAGUCHI, Takumi	Assistant Professor
NAKAMURA, Akihiko	Assistant Professor
MURAKI, Norifumi	Assistant Professor
YAGI-UTSUMI, Maho	Assistant Professor
YANAKA, Saeko	IMS Research Assistant Professor
TANAKA, Kei	Secretary
NAKANE, Kaori	Secretary



The main purpose of Okazaki Institute for Integrative Bioscience (OIIB) is to conduct interdisciplinary, molecular research on various biological phenomena such as signal transduction, differentiation and environmental response. OIIB, founded in April 2000, introduces cutting edge methodology from the physical and chemical disciplines to foster new trends in bioscience research. OIIB is a center shared by and benefited from all three institutes in Okazaki, thus encouraging innovative researches adequately in advance of academic and social demands. OIIB has started the research programs, "Okazaki ORION Project" and "BioNEXT Program" from 2014. The research groups of three full professors and one associate professor who have the position in IMS join OIIB to be involved in these research projects. The research activities of these groups are as follows.

Aono group is studying the bioinorganic chemistry of metalloproteins that show a novel function. Their research interests are focused on the structure and function relationships of transcriptional regulators and metal transport proteins that are responsible for metal homeostasis, especially iron and/or heme homeostasis, in bacteria. They are also working on a novel photosensor protein that adopts vitamin B_{12} (adenosylcobalamin) as the active site for photosensing, which is a transcriptional factor regulating gene expression in response to visible ligth. In this year, they successfully determined the crystal structures of HtaA and HtaB that are heme-binding and heme-transport proteins responsible for heme uptake reaction in *Croynebacterium glutamicum*. They also determined the crystal structure of a novel photosensor protein CarH from *Thermus thermophilus*, which uses adenosylcobalamin as a photoreceptor. Iino group is studying operation and design principles of molecular machines using single-molecule analysis, structural analysis, and protein engineering. Especially, they focus on rotary and linear molecular motors. In this year, they have succeeded in direct observation of intermediate states during the stepping motion of a linear molecular motor kinesin-1. They also have succeeded in direct imaging of binding, dissociation, and processive movement of a linear molecular motor Trichoderma reesei Cel6A and its domains on crystalline cellulose. Kato group is studying structure, dynamics, and interactions of biological macromolecules using nuclear magnetic resonance (NMR) spectroscopy, X-ray crystallography, and other biophysical methods. In particular, they conducted studies aimed at elucidating the dynamic structures of glycoconjugates and proteins for integrative understanding of the mechanisms underlying their biological functions. In this year, they successfully characterized dynamic processes of protein assembly and disassembly involved in the intracellular protein transport and the proteasome formation by native mass spectrometry and also the drug-induced conformational change of HIV-1 reverse transcriptase by NMR spectroscopy. Kurihara group is studying artificial cells based on molecular assemblies from chemical approach. Their goal is to create artificial cells which have three main elements, *i.e.* information, compartment and metabolism. In this year, they studied catalyst-producing vesicular system: A vesicle is reproduced by the catalyst which was synthesized in the vesicle. In this system, they observed the interaction between the production of compartment membrane molecule and the production of catalyst. In addition, they constructed the self-reproducing oil droplet system, which lead to the formation of giant vesicles.

Safety Office

UOZUMI, Yasuhiro	Director
TOMURA, Masaaki	Assistant Professor
TANAKA, Shoji	Assistant Professor
SUZUI, Mitsukazu	Technical Associate
UEDA, Tadashi	Technical Associate
TAKAYAMA, Takashi	Technical Associate
SAKAI, Masahiro	Technical Associate
MAKITA, Seiji	Technical Associate
KONDO, Naonori	Technical Associate
MIZUTANI, Nobuo	Technical Associate
ONITAKE, Naoko	Secretary
TSURUTA, Yumiko	Secretary
KAMO, Kyoko	Secretary

The Safety Office was established in April 2004. The mission of the Office is to play a principal role in the institute to secure the safety and health of the staffs by achieving a comfortable workplace environment, and improvement of the working conditions. In concrete terms, it carries out planning, work instructions, fact-findings, and other services for safety and health in the institute. The Office is comprised of the following staffs: The Director of the Office, Safety-and-Health Administrators, Safety Office Personnel, Operational Chiefs and other staff members appointed by the Director General.

The Safety-and-Health Administrators patrol the laboratories in the institute once every week, and check whether the laboratory condition is kept sufficiently safe and comfortable to conduct researches. The Office also edits the safety manuals and gives safety training courses, for Japanese and foreign researchers.