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 (1978–2014).

UVSOR Facility

KOSUGI, Nobuhiro	Director
KATOH, Masahiro	Professor
SHIGEMASA, Eiji	Associate Professor
TANAKA, Kiyohisa	Associate Professor
IWAYAMA, Hiroshi	Assistant Professor
MATSUNAMI, Masaharu	Assistant Professor
OHIGASHI, Takuji	Assistant Professor
KONOMI, Taro	Assistant Professor
IDETA, Shin-ichiro	Assistant Professor
HORIGOME, Toshio	Technical Associate
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 Associate
IIZUKA, Takuya	Research Fellow
TOKUSHI, Tetsunari	Technical Fellow
INAGAKI, Yuichi	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 > 1200, 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

BL8B for photoemission study of organic thin films was shut down in 2015 after operating for more than 30 years from the beginning of UVSOR (1983). Instead of BL8B, BL2B was reorganized for photoemission study of organic thin films in 2013, which has been conducted as one of the long-term project proposals for 2013–2015. As an endstation of BL2B, an experimental setup for angle-resolved photoelectron spectroscopy (ARPES) was brought from Chiba University. Commissioning and performance tests were started in September 2014. During commissioning, the vacuum pressure rises at the first mirror chamber were frequently observed due to a leak in the water-cooling system for the first mirror. We have decided to continue the operation of BL2B without the water-cooling system. Now it takes about 20 minutes to stabilize the beam position on the entrance slit but then the beam is stabilized in the top-up mode.

Reserch Highlight

Free University of Berlin and IMS have an international collaboration program in molecular science. One of the collaboration projects is application of our scanning transmission X-ray microscope (STXM) at the BL4U to the drug delivery from human skin. Advantages of this technique are not only high spatial resolution but also label-free approach. Dexamethasone is a widely used for the treatment of inflammatory skin diseases such as atopic dermatitis. It is aimed to study the depth profile of dexamethasone, so that specific information on the uptake process is derived. Dexamethasone was dissolved in ethanol and this 0.5% solution was applied onto the skin sample for 4 h. Subsequently, the sample was fixed and sliced into 350 nm thick sections. The skin samples were placed on silicon nitride membranes with thickness of 100 nm. Chemical selectivity is obtained from excitation at the O 1s-edge (525–560 eV). Figure 2 shows a comparison of the O 1s-absoption of fixed human skin and dexamethasone. Both spectra are similar in shape, showing an intense O 1s → π* resonance dominating the pre-edge regime. This resonance occurs at slightly lower energy in dexamethasone (E = 530.5 eV) than in skin (E = 532.2 eV), providing chemical selectivity for probing the drug uptake into skin.

Figure 3 shows a comparison of a skin sample exposed to dexamethasone probed by optical microscopy and soft X-ray microscopy. Figure 3(a) clearly shows the layered structure of the stratum corneum, the outermost skin layer, probed by optical microscopy. It is followed by the viable epidermis and the dermis. Figure 3(b) shows for the same section of the skin sample the spatial distribution of absorption, which is obtained from a difference image in X-ray absorption measured at 528 eV (pre-edge regime) and on the O 1s → π*-transition (530.5 eV) of dexamethasone (cf. Figure 2) providing chemical selectivity. The spatially resolved results indicate that highest absorption contrast is found in the stratum corneum, as indicated by red color. In contrast, lower concentration is observed in the viable epidermis and no change in absorption contrast occurs in the dermis. It is also evident that the cells nuclei in the viable epidermis (circular structures in Figure 3(a)) do not show any evidence for drug uptake.

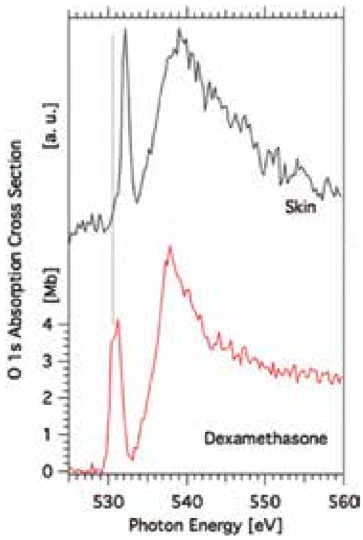

Figure 2. X-ray absorption cross section of human skin and dexamethasone at the O K-edge.

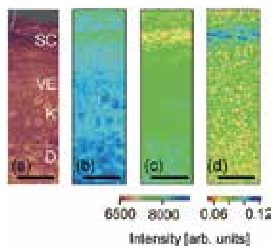

Figure 3. Uptake of dexamethasone into human skin (SC, stratum corneum; VE, viable epidermis; K, nuclei of keratinocytes; D, dermis): (a) optical micrograph of a vertical skin section, (b) absorption of the same skin section shown in (a) at 528.0 eV (pre-edge regime), (c) absorption of the same skin section shown in (a) at 530.6 eV (O 1s → π* resonance) and (d) optical density of taken up dexamethasone as a function of depth. The scale bar corresponds to 20 μm.

Reference

1) K. Yamamoto, *et al.*, *Anal. Chem.* **87**, 6173–6179 (2015).

Laser Research Center for Molecular Science

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OHMORI, Kenji	Professor
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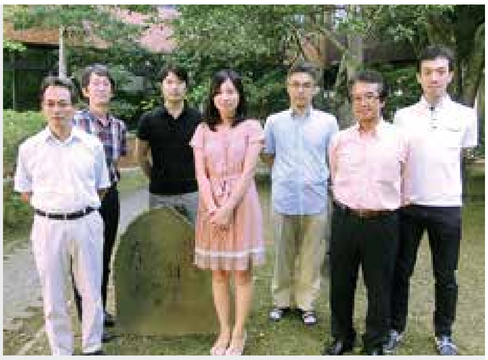
FUJI, Takao	Associate Professor
ISHIZUKI, Hideki	Assistant Professor
NOMURA, Yutaka	Assistant Professor
SHIRAI, Hideto	IMS Research Assistant Professor
OKANO, Yasuaki	Technical Associate
MASUDA, Michiko	Secretary



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.

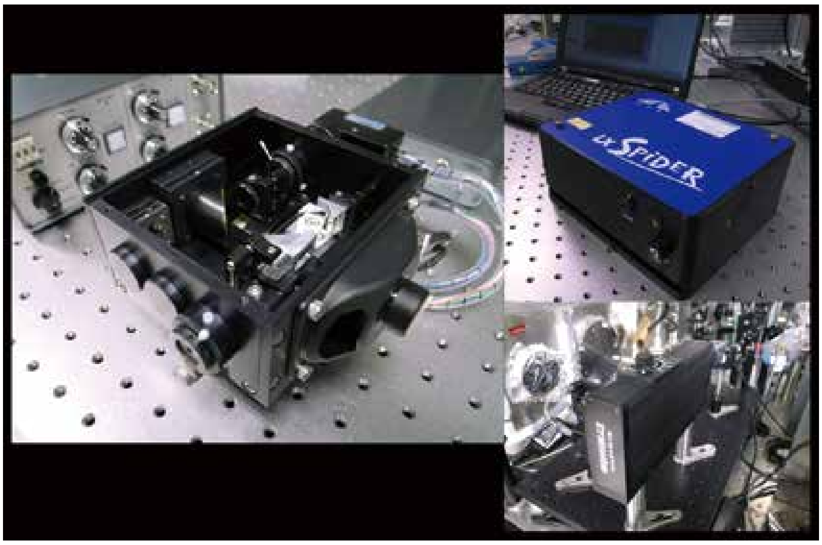


Figure 1. (left) A Fringe-Resolved Autocorrelation (FRAC) apparatus for sub-10 fs pulse characterization designed in the Center. (upper right) Spectral Phase Interferometry for Direct Electric-Field Reconstruction (SPIDER) and (lower right) Frequency-Resolved Optical Gating (FROG) apparatuses for general-purpose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

Instrument Center

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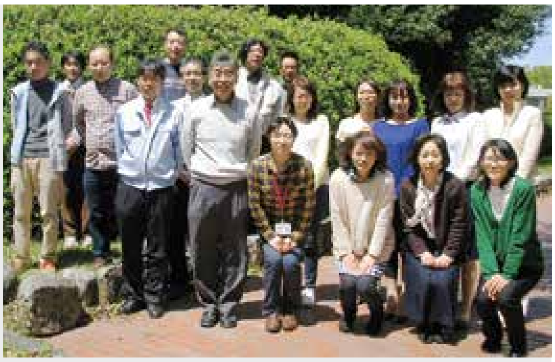
FUJIWARA, Motoyasu	Technical Associate
OKANO, Yoshinori	Technical Associate
MIZUKAWA, Tetsunori	Technical Associate
MAKITA, Seiji	Technical Associate
UEDA, Tadashi	Technical Associate
KANEKO, Yasushi	Nano. Platform Manager
INOUE, Mika	Nano. Platform Manager
NAKAO, Satoru	Post-Doctoral Fellow
OKUSHITA, Keiko	Post-Doctoral Fellow
NAGAO, Haruyo	Technical Fellow
IKI, Shinako	Technical Fellow
OTA, Akiyo	Secretary
NAKAGAWA, Nobuyo	Secretary
YOKOTA, Mitsuyo	Secretary
FUNAKI, Yumiko	Secretary
AOKI, Junko	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; JNM-LA500 shutdown in March 2015), 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) high-resolution transmission electron microscope (TEM; JEOL JEM-3100FEF), and FTIR spectrometer (Bruker IFS 66v/S). In the fiscal year of 2014, Instrument Center accepted 204 applications from institutions outside IMS and the total user time including in-house use amounted 3883 days/38 equipments. Instrument Center also maintains helium liquefiers in the both campus and provides liquid helium to users (56,221 L/year). Liquid nitrogen is also provided as general coolants used in many laboratories in the Institute (48,402 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

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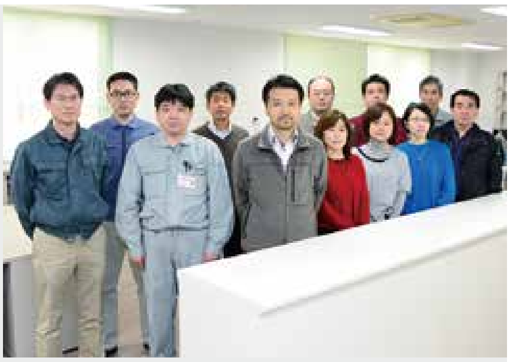
KONDOU, Takuhiko	Technical Associate
YOSHIDA, Hisashi	Technical Associate
TOYODA, Tomonori	Technical Associate
TAKADA, Noriko	Technical Associate
NAKANO, Michiko	Technical Associate
SUGITO,Shouji	Technical Fellow
TANAKA,Takashi	Technical Fellow
URANO, Hiroko	Secretary



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.

Fabrication of an Electric Probe with Substrate Bending Mechanism

In Research Center of Integrative Molecular Systems, a research on an organic field-effect transistor (FET) that shows switching of superconducting phase at low temperature is ongoing in order to obtain fundamental knowledge about interacting electrons in a molecular solid. The organic FET fabricated on a plastic substrate can be bended to result in a tensile strain at its convex surface, so that fine tuning of the electrons' kinetic energy is possible through the expansion of the lattice. In order to expand this method to FETs with much harder substrates such as $SrTiO_3$, a novel electrical probe (Figure 1) that can be used with Physical Properties Measurement System has been designed and fabricated.

Figure 1. Schematic of the probe.

ARM Microcontroller-Based Magnetic Field Measuring Instrument

In high-precision spectroscopies and controls, we need measure the environmental magnetic field to evaluate the noise signal from the environment. In this work, we have developed 3-axis magnetic-field measuring instrument. This is made by the commercial compass module and the Acorn reduced instruction set computing machine (ARM) microcontroller. (Figure 2)

This device consists of one micro USB connector for the power supply and communication, one rotary encoder for the operation, two switches for selecting and canceling, and one liquid crystal display with 16 characters and 4 lines. The compass module HMC5883L by Honeywell is connected to 4 core cables. All of these are controlled by the ARM microcontroller LPC1114FBD48/302 by NXP. The measured 3-axis magnetic fields are output as digital data with 12-bit resolution and the 8-levels measurement range from ±0.88 gauss to ±8.1 gauss. The ARM microcontroller reads by Inter Integrated Circuit (I^2C) and converts, formats separated by commas, and displays the measured data on liquid crystal display. These data can be recorded in a built-in 256 kbit EEPROM by selecting the measurement mode. In addition, we have added the functions of transferring the real-time measured data and the stored one on EEPROM to PC. To utilize these communications, we have developed an interface tool by Visual Basic 2015. (Figure 3).

Figure 2. Magnetic field measurement instrument.

Figure 3. Measuring magnetic field using communication application.

Research Center for Computational Science

SAITO, Shinji	Director, Professor
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OKUMURA, Hisashi	Associate Professor
OONO, Hitoshi	Assistant Professor
ISHIDA, Tateki	Assistant Professor
FUKUDA, Ryoichi	Assistant Professor
ITOH, G. Satoru	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

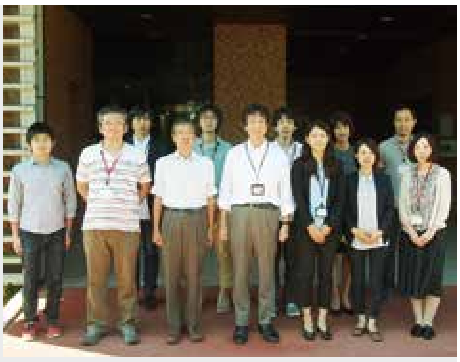
Research Center for Computational Science provides state-of-the-art computational resources to academic researchers in molecular science and related fields, *e.g.* quantum chemistry, molecular simulations, and solid state physics. The computer systems consist of Fujitsu PRIMERGY RX300, PRIME HPC FX10 and PRIMERGY CX2550, SGI UV2000. The systems have been used by 756 people in 199 research groups in 2014. 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 2014, contains 131,771 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, the Center contributes to the so-called next-generation supercomputer project which is conducted by the government. In 2010, Computational Material Science Initiative (CMSI) was established for the research fields consisting of molecular science, solid state physics, and material science, in which scientific breakthroughs are expected by using the next-generation supercomputer. The Center contributes to CMSI by providing up to 20% of its computational resource.

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	IMS Research Assistant Professor
YANAKA, Saeko	IMS Research Assistant Professor
YAGI-UTSUMI, Maho	OIIB 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. Iino group is studying operation mechanism of molecular machines using single-molecule techniques based on optical microscopy. Especially they focus on rotary and linear molecular motors. In this year, they have succeeded in generation of a rotary molecular motor F_1-ATPase with an unnatural amino acid, and determined key chemical factors of arginine finger catalysis. They also developed high-speed angle-resolved imaging of single gold nanorod with microsecond temporal resolution and one-degree angle precision, and successfully applied to probe rotation of F_1-ATPase at 3.3 µs temporal resolution. 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 conformational ensembles of high-mannose-type oligosaccharides by NMR-validated simulation and determined several crystal structures of proteins involved in protein-fate determination in cells, including putative substrate-binding domains of UGGT and protein disulfide isomerase. Kurihara group is studying an artificial cell based on a giant vesicle constructed from organic chemical approach. Their goal is to realize an artificial cell which has 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 catalyst.

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

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.