

# World Premier International Research Center Initiative (WPI)

## FY 2017 WPI Project Progress Report

Host Institution	Nagoya University	Host Institution Head	Seiichi Matsuo
Research Center	Institute of Transformative Bio-Molecules	Center Director	Kenichiro Itami

Common instructions:

\* Unless otherwise specified, prepare this report from the timeline of 31 March 2018.

\* So as to base this fiscal year's follow-up review on the "last" center project, please prepare this report from the perspective of the latest project plan.

\* Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.

\* Please prepare this report within 10-20 pages (excluding the appendices, and including Summary of State of WPI Center Project Progress (within 2 pages)).

### Summary of State of WPI Center Project Progress (write within 2 pages)

#### 1. Research Progress

The Institute of Transformative Bio-Molecules (ITbM) at Nagoya University (NU) defined its three flagship research areas as: (1) **plant chemical biology**, (2) **chemical chronobiology**; and (3) **chemistry-enabled live imaging**, and has been conducting interdisciplinary research in these areas. Main research achievements in these flagship areas are summarized below.

##### (1) Plant chemical biology

- Development of a potent *Striga* germinator "Super Strigolactone (SL)", which effectively induces suicide germination without any influence on host plant growth.
- Development of molecules that significantly increase the number of stomata in plant leaves without causing damage to plant growth. One of these new molecules also promoted root growth of several plants.
- Development of a new stomatal closing molecule, which suppresses leaf withering upon spraying of its solution on leaves.
- Identification of the co-crystal structure of a pollen tube attractant peptide (LURE) with its receptor PRK6 and the amino acids involved in the binding.

##### (2) Chemical chronobiology

- Discovery of molecules regulating the circadian rhythm in mammals by drug repurposing. Dietary administration of one of the molecules, an anti-ageing supplement, to mice significantly improved their recovery from jet lag.
- Discovery of dynamic seasonal changes in color perception of medaka fish.
- Development of a molecule that changes the flowering time of plants.

##### (3) Chemistry-enabled live imaging

- Development of a super-photostable dye PhoxBright 430 (PB430), which was resistant to photo-irradiation under the STED conditions and can be used to label proteins.
- Development of new phospho-fluorescein molecules, which exhibit significantly red-shifted emission compared to classical fluorescein-type molecules. Phospha-fluorescein works as a scaffold to produce various metal ion probes, such as calcium ions, Ca<sup>2+</sup>.
- Development of a phosphorus-containing rhodamine derivative PREX710 as a new NIR emissive fluorophore with extremely high photostability. Silica nanoparticles encapsulating PREX710 were applicable for *in vivo* visualization of tumors in tumor-bearing mice.

#### Summary of Activities in FY2017

Journal publications (Jan 2017 – Dec 2017): 156 peer-reviewed papers (36 papers = IF>10; 53 papers = IF>7; 7 Highly cited papers; 2 Hot papers)

Patent filings: 23 (14 cases co-filed among several PI groups)

Commercialization of molecules/catalysts: 3

Awards and honors: 42

Research funds: 1,098 million yen (Overseas PIs also obtained KAKENHI grants).

## 2. Advancing fusion of various research fields

ITbM's interdisciplinary research has been making significant progress under the "Mix" concept, and the center's initiatives to promote interdisciplinary research have been effective so far. The **ITbM Research Award**, established to foster interdisciplinary collaboration among young researchers and students, was granted to 4 new projects in FY2017. The **ITbM Workshop** and **Tea break Meeting** are also providing opportunities to find new partners and seeds for collaboration.

These initiatives are organized by the **Administrative Department** of ITbM, in which the **Research Promotion Division (RPD)** and the **Strategic Planning Division (SPD)** are playing key roles. In FY2017, ITbM decided to allocate additional staff to both RPD and SPD to further strengthen and expand their functions, thus promoting the "Mix" within ITbM.

ITbM's **4 supporting centers** (Molecular Structure Center, Live Imaging Center, Chemical Library Center, and Peptide Protein Center) are also making a major contribution to the promotion of ITbM's interdisciplinary research through their technical support. Due to an increase in various tasks, additional technical staff were allocated to the centers.

In 2017, ITbM has published 10 joint publications among the following research groups: Itami/Higashiyama (2), Irle/Torii (1), Itami/Irle (3), Crudden/Taki (Yamaguchi Group) (1), Higashiyama/Yamaguchi (1), Itami/Torii (1), Itami/Kinoshita (1). Research accomplishments arising from these joint papers include synthesis of molecules for plant growth and fertilization, bioimaging, as well as computational studies on molecules.

ITbM has been strategically expanding its domestic and international collaborating networks, which provides further opportunities to promote interdisciplinary collaborations.

## 3. Measures taken to globalize the institute

Organization of ITbM's annual international symposia (ISTbM-5) and hosting of 3 international awards in chemistry and biology (23rd Nagoya Medal Award of Organic Chemistry, 13th Hirata Award, and 3rd Tsuneko & Reiji Okazaki Award).

- Wolf Frommer (Düsseldorf University) joined as the fifth overseas PI at ITbM and his new group members were assembled. Exchange of researchers with Düsseldorf University will start under the Agreement of tuition-free student exchange.
- As part of the collaboration with international partner institutions, several activities were organized, including the 2nd joint workshop of ITbM, IoC, and IPMB of Academia Sinica, and the 1st international symposium at Freiburg organized by ITbM and the University of Freiburg.
- A staff member was hired in RPD, who is mainly responsible for providing local support to foreign researchers and their families staying in Japan.
- In terms of international brain circulation, 7 researchers joined ITbM from overseas institutions, and 4 foreign researchers working at ITbM have been promoted to other institutions.

## 4. Implementing organizational reforms

Under President Matsuo's Initiatives for Reform, Autonomy and Innovation 2020 (NU MIRAI 2020), NU has been carrying out extensive system reform to become a world-class research university. In the initiative, ITbM is positioned as a core research center of Nagoya University, and thus the basic policy and the measures of system reform have been established to match ITbM's needs. ITbM's Director and core members have been holding regular meetings with the President once a month to discuss any issues related to the management of ITbM. New ripple effects originating from ITbM are included in: "Designated National University" appointed to NU, Basic Agreement of NU with RIKEN, and the application to the "Takuetsu Graduate School Program" with ITbM as the core.

## 5. Efforts to secure the center's future development

ITbM will take appropriate actions to secure the necessary funds to operate ITbM, which includes building strategies to collect donations. Nevertheless, NU's strong support is crucial to sustain ITbM at the current level. NU is conducting system reform of the university to ensure that ITbM is maintained. Representative efforts in FY2017 are listed below.

- Additional staff will be appointed to the SPD to extend its activities.
- ITbM Consortium was launched as a membership-based discussion forum.
- NU will make an application for the "Takuetsu Graduate School Program" that places ITbM at the core. Accordingly, more students will be allocated to ITbM, and ITbM will be extensively involved in the education of graduate students.

- \* Please describe clearly and concisely the progress being made by the WPI center project from the viewpoints below.
- In addressing the below-listed 1-6 criteria, please place emphasis on the following:
- (1) Whether research is being carried out at a top world-level (including whether research advances are being made by fusing fields).
  - (2) Whether a proactive effort continues to be made to establish itself as a "truly" world premier international research center.
  - (3) Whether a steadfast effort is being made to secure the center's future development over the mid- to long-term.

## 1. Conducting research of the highest world level

\* Regarding the criteria used when evaluating the world level of center, please note any updated results using your previous evaluation criteria and methods or any improvements you have made to those criteria and methods.

ITbM has defined its three flagship research areas as: (1) plant chemical biology, (2) chemical chronobiology, and (3) chemistry-enabled live imaging in late FY2015, and has been continuing its efforts to develop "transformative bio-molecules" that can enhance biotic productivity and quality, along with applications in innovative bioimaging. To ensure that these targets are achieved, ITbM is developing catalysts that enable on demand synthesis in an efficient manner.

While a number of collaborative researches are ongoing, ITbM decided to place high priority on the project "Combating *Striga*" taking into account its expected impact to the global society. In 2016, the "*Striga* team" was established, consisting of researchers working on the *Striga* project along with staff of the RPD/SPD, headed by the Center Director.

### (1) Research progress

#### (a) Plant chemical biology

**Molecules to combat *Striga*** (Kinoshita Group, Ooi Group, Itami Group, Theoretical Chemistry Group, Molecular Structure Center, Chemical Library Center)

With the aim to reduce crop damage caused by the parasitic plant *Striga*, ITbM continues its effort to develop molecules to combat *Striga* via control of *Striga* seed germination.

Previously, Tsuchiya (Kinoshita group) and Uraguchi (Ooi group) had developed a strigolactone (SL) mimicking molecule, "super SL (SAMR690)" that displays remarkably high agonistic activity and selectivity towards the SL receptor ShHTL7 among isoforms of 11 SL receptors (ShHTLs). During 2017, they demonstrated that SAMR690 effectively induced suicide germination of *Striga* seeds without any influence on growth of the host plant AM-fungi even *in vivo* (manuscript to be submitted).

The team has also tried to increase the germination rate of *Striga* using molecules. The germination rate of *Striga* has never reached 100% (usually 50% in maxima) regardless of the concentration or types of germination inducers. They hypothesized that the low germination rate could be genetically installed to avoid total eradication of *Striga*, and be controlled by a network of 11 ShHTLs. Screening of the ITbM chemical library identified a series of small molecules that break the upper limit of the *Striga* germination rate. Structure-activity relationship studies and subsequent structural modification of the synthetic molecules by the Ooi group led to the development of a new class of *Striga* germination inducers, which are expected to contribute to the elucidation of the ShHTLs network.

In addition, the team identified a new structurally diverse set of antagonists, which selectively compete with either SAMR690 (selective agonist to ShHTL7), T-010 (a known agonist selective to ShHTL11) or with both. These selective antagonists will be useful to investigate the functions of redundant ShHTL signaling cascades.

They also conducted a study that focused on another type of strigolactone receptor DWARF14 (D14), which plays a central role in suppression of shoot branching, and therefore has potential in increasing crop production and biomass. Through a high-throughput chemical screening using the ITbM's fluorescence probe Yoshimulactone Green (YLG), which turns on strong fluorescence upon binding to the D14-type strigolactone receptors, Hagihara (Itami group) identified a novel small molecule DL1 as a potent inhibitor of D14. DL1 competes with endogenous strigolactones, thereby increasing the number of shoot branching in a model plant *Arabidopsis thaliana* as well as in rice. Thus, DL1 is expected to be a potent agrochemical to improve crop yield (ACS Central Sci. 2018).

#### **Molecular control of stomatal development** (Torii-Uchida Group, Itami Group)

Torii-Uchida and Itami groups have developed small molecules CL1 and CL2 that increase the number of stomata. However, these molecules were found to cause severe and undesirable plant growth inhibition (smaller seedlings with chlorosis). Thus, they synthesized a series of CL1 and

CL2 derivatives, and obtained a new small molecule ZA144 that significantly increases the number of stomata on plant leaves without causing damage to plant growth (Chem. Commun. 2017).

Torii and Uchida also identified a synthetic molecule kC9 that leads to a threefold increase in the number of stomata, along with promotion of root growth in the model plant *Arabidopsis thaliana* and in other several edible plants, such as lettuce and cucumber (PCT/JP2017/024778). They have also identified molecules that remarkably enhance both longitudinal growth and radial growth of *Arabidopsis* hypocotyls.

#### **Synthetic peptide control of plant growth** (Torii-Uchida Group, Quantum Chemistry Group)

Through structure-activity relationship studies among CLE peptides, Torii and Uchida developed a synthetic peptide that exerts two different CLE activities. In collaboration with the Quantum Chemistry group, molecular dynamics (MD) analysis between the peptide and its receptor was carried out to support the findings from a theoretical viewpoint. The design principle of synthetic hybrid peptides may be expanded to other peptide families or generalized to protein-protein interactions to understand and manipulate plant development and behavior (Nature Commun. 2017)

#### **Molecular control of stomatal movement** (Kinoshita Group, Itami Group, Chemical Library Center)

The Kinoshita group has been working on elucidation of stomata movement. In FY2017, they identified a new protein kinase as a blue light-signaling component, named **BLUE LIGHT-DEPENDENT H<sup>+</sup>-ATPASE PHOSPHORYLATION (BHP)**, in stomatal guard cells by using a combination of chemical screening of a kinase inhibitor library and reverse genetics (Sci. Rep. 2017).

Kinoshita and the Chemical Library Center have been collaborating to develop new molecules affecting stomatal movements. Among over 25,000 molecules, they identified 9 molecules (**stomata closing compounds, SCL1-SCL9**) that suppress light-induced stomatal opening. Further investigations revealed that SCL1 and SCL2 suppressed light-induced stomatal opening by inhibiting blue light-induced activation of plasma membrane (PM) H<sup>+</sup>-ATPase, but not by the abscisic acid-signaling pathway (Plant Cell Physiol. 2018). Notably, spraying of SCL1 onto dicot and monocot leaves suppressed leaf withering, indicating that inhibition of stomatal opening by these compounds confers tolerance to drought stress in plants (PCT/JP2017/34287).

#### **Enhancement of photosynthesis by overexpression of PM H<sup>+</sup>-ATPase** (Kinoshita Group)

Kinoshita demonstrated that overexpression of PM H<sup>+</sup>-ATPase is useful for the enhancement of plant growth for rice and poplar through enhancing light-induced stomatal opening, photosynthesis, ammonium uptake in roots, and biomass in hydroponic culture (manuscripts to be submitted). These modified plants were named as "PUMP" plants (**promotion and up-regulation of the plasma membrane H<sup>+</sup> (proton)-ATPase**). Application of this technology to other plants is highly anticipated.

#### **Molecules to overcome species barrier** (Higashiyama Group, Itami Group, Bode Group, Molecular Structure Center)

In their study of the pollen tube attractant peptide LURE, the Higashiyama group analyzed the co-crystal structure of LURE1-PRK6 of the model plant *Arabidopsis thaliana*, and demonstrated that PRK6 is the receptor of the pollen tube attractant peptide LURE1 (Nature Commun. 2017). In collaboration with the Tama group, the tertiary structure of LURE1-PRK6 from different plant species was calculated by *ab initio* structural modeling, and the amino acids essential to the specific interaction were identified. This modeling approach provides clues towards the design of chimeric LURE peptides of *Arabidopsis* and *Torenia* in collaboration with the Bode group.

The Higashiyama group reported the study of AMOR saccharide (4-Me-GlcA- $\beta$ -(1,6)-Gal), which enhances the competency of pollen tubes to react to LURE peptides (Plant Physiol. 2017, AMOR is now commercially available). The structure-activity relationship (SAR) studies revealed that the terminal sugar structure, 4-*O*-methyl glucuronic acid, as well as the  $\beta$ -bonding with the next residue were crucial for AMOR's activity, but the structure of the second sugar, galactose, was not so critical. Thus, AMOR derivatives including those having fluorescent units at the second sugar unit have been developed to help understand the molecular mechanism of AMOR.

### **Other main achievements**

- Ueda (Higashiyama Group) discovered for the first time on how factors arising from the mother and father in flowering plants cooperate to develop the shape of their child (*Genes & Dev.* 2017).
- Higashiyama reported a new tool, pKAMA-ITACHI vector, for highly efficient genome editing in a model plant *Arabidopsis thaliana* (*Plant Cell Physiol.* 2017, PCT/JP2017/030010). This series of vectors have been distributed through Addgene (non-profit plasmid repository, Cambridge, USA).

### **(b) Chemical chronobiology**

**Molecular control of animal circadian rhythms at cellular level** (Kay-Hirota Group, Itami Group, Ooi Group, Bode Group, Tama Group, Quantum Chemistry Group, Molecular Structure Center, Chemical Library Center, Peptide Protein Center)

Kay and Hirota previously developed a molecule KL001 that lengthens the circadian period by stabilizing the core clock proteins CRY1 and CRY2, through binding to both proteins (*Science* 2012). By conducting high-throughput chemical screen in collaboration with the Chemical Library Center, they have now discovered first-in-class selective stabilizers for CRY1 or CRY2. Optimization studies are ongoing through extensive collaboration with the Itami group (SAR study) and the Tama group (molecular dynamics (MD) simulation). Further modification of these molecules will enable specific regulation of CRY1 and CRY2.

Kay and Hirota have previously discovered a molecule GO289 as a circadian period-lengthening compound in mammals. They have elucidated the mechanism of selectivity towards protein kinase CK2 $\alpha$  through MD simulation with the Tama group using a high-resolution X-ray crystal structure of the CK2 $\alpha$ -GO289 complex (manuscript in preparation).

**Molecular control of animal circadian rhythms in vivo** (Yoshimura Group, Itami Group, Ooi Group, Crudden Group, Tama Group, Quantum Chemistry Group, Molecular Structure Center, Chemical Library Center)

The Yoshimura group has identified dehydroepiandrosterone (DHEA), also known as an anti-aging supplement, as a period-shortening compound through high-throughput chemical screening of existing drugs (drug repurposing) in collaboration with the Chemical Library Center. Dietary administration of DHEA to mice shortened free-running circadian period and accelerated re-entrainment to advanced light-dark (LD) cycles, thereby reducing jet lag. Their drug repurposing-based chemical screening also revealed the involvement of tyrosine kinases, ABL1 and ABL2, and the BCR serine/threonine kinase in regulating the circadian period. (*EMBO Mol. Med.* 2018).

Yoshimura's group focuses on the organism's physiological adaptation mechanism to cope with seasonal changes. In FY2017, they found that dynamic plasticity in phototransduction regulates seasonal changes in color perception in medaka fish. Medaka are active and exhibit clear phototaxis in summer conditions, but remain at the bottom of the tank and fail to exhibit phototaxis in winter conditions. Also, medaka are more attracted to orange-red-colored model fish in the summer than in the winter according to mate preference tests. Transcriptome analysis of the eye reveals dynamic seasonal changes in the expression of genes encoding photopigments, and their downstream pathways and behavioral analysis of photopigment-null fish shows significant differences from the wild type, suggesting that plasticity in color perception is crucial for the emergence of seasonally regulated behaviors (*Nature Commun.* 2017).

**Plant chronobiology** (Itami Group, Molecular Structure Center, Chemical Library Center)

Nakamichi (Kinoshita group) discovered that treatment of the plant with the period-shortening molecule PAC4, results in elevated expression of *FT*, encoding florigen, which triggers flowering meristem formation. PAC4 treatment caused early flowering in *Arabidopsis* grown on soil. PAC4 did not show any obvious toxicity in plants (*Arabidopsis*, bean) and in animal cell lines (U2OS). As the circadian clock is a fundamental system for photoperiodic flowering time in many plants, PAC4 was also applied to other plants. Treatment of a monocot plant with PAC4 (50  $\mu$ M solution, once per week) resulted in 5 to 10 weeks earlier flowering than in control plants (manuscript in preparation).

Nakamichi has been conducting biology/chemical biology research on the elucidation of the transcription network and its downstream signal transduction for plant circadian clocks. Their group has established a high throughput DNA sequencing (ChIP-seq) method for plants and

elucidated clock-associated transcription factors such as PRR5 and CCA1. This technology was applied to reveal that the transcription factor LNK1 was associated with some evening-phase genes and potentially activates these gene expressions. Through the project, the team expects that the entire genetic network for clock control in plants will be uncovered.

They also found the molecule PAC2 as an inhibitor for the phosphorylation of PRR5 and TOC1 through chemical screening. PAC2 showed a period lengthening effect in an *in vivo* experiment of the *ztl* mutant, in which PRR5 and TOC1 accumulated more than the wild type. This result strongly suggests that control of degradation of these biomolecules is closely related to the period lengthening effect (manuscript in preparation).

### **(c) Chemistry-enabled live imaging** (Yamaguchi Group, Higashiyama Group, Itami Group, Live Imaging Center)

The Yamaguchi group has been conducting research to develop useful fluorescent molecules. In particular, taking the structural change in the excited state, they have characterized various types of intriguing fluorophores, such as the near infrared (NIR)-emissive tropylium ions (Angew. Chem. Int. Ed. 2017). Their most important achievement was the development of phosphorus-containing fluorescent probes applicable to bioimaging. With an electron-withdrawing phosphine oxide (P=O) moiety incorporated into the  $\pi$ -skeleton of fluorescein, phospho-fluoresceins (Chem. Commun. 2017) exhibit significantly red-shifted emission compared to classical molecules related to fluorescein, and therefore can be utilized as a useful scaffold to produce various metal ion probes, such as calcium ions,  $\text{Ca}^{2+}$  (Chem. Commun. 2018).

By incorporation of the P=O group into the xanthene skeleton, phospho-rhodol exhibited large solvatochromism of absorption and showed intense emission in the NIR region, which should be beneficial to use for fluorescent imaging (Chem. Eur. J. 2017).

Silicon-bridged benzophosphole *P*-oxide having improved photostability was also developed (Inorg. Chem. 2017), which was further modified into the practically useful super-photostable dye PhoxBright 430 (PB430) through structure screening of the phosphole skeleton (J. Am. Chem. Soc. 2017). Due to its high solubility in water, PB430 is capable of labeling proteins while maintaining high fluorescence quantum yields. PB430 also exhibited outstanding resistance to photo-irradiation even under stimulated emission depletion (STED) conditions and allows continuous acquisition of STED images. By using a PB430-conjugated antibody, 3D super-resolution STED images, as well as photostability-based multicolor STED imaging of fluorescently labeled cytoskeletal structures, were acquired.

Yamaguchi and Taki developed a phosphorus-containing rhodamine derivative PREX710, as a new NIR emissive fluorophore with extremely high photostability under physiological conditions. Silica nanoparticles encapsulating PREX710 was applicable for *in vivo* visualization of tumors in tumor-bearing mice.

The Itami group developed unsymmetrical cyanine dyes in collaboration with the Higashiyama group and the Live Imaging Center. The dyes play a critical role in fluorescence enhancement. One of those cyanine dyes has unique properties. Although the negligible intrinsic fluorescence was detected in the free state, very strong fluorescence was observed upon binding to double-stranded DNA (dsDNA), which is 2 to 3 times higher in quantum yield compared to other cyanine dyes (Chem. Asian. J. 2017; most accessed article in Jan, Feb, and Mar in 2017).

Itami's group also synthesized a water-soluble warped nanographene (WNG). The modified water-soluble WNG was internalized into HeLa cells and promoted photo-induced cell death (Angew. Chem. Int. Ed. 2018). The result indicates that nanographenes are applicable to biological research such as bioimaging, cancer therapies and drug delivery.

### **(d) Other main research progress**

#### **Molecular synthesis**

Itami and his group have been developing a variety of catalysts and reactions that enable rapid molecular syntheses. With these catalysts, a variety of nanocarbons were synthesized. Based on their synthesis of cycloparaphenylene (carbon nanoring, Nature Chem. 2013) and warped nanographene (WNG, Nature Chem. 2013), the group succeeded in the synthesis of a carbon nanobelt (Science 2017), as well as the water soluble WNG (Angew. Chem. Int. Ed. 2018). The carbon nanobelt has been synthesized for the first time since the proposal of its structure more than 60 years ago, and serves a potential template for the preparation of structurally well-defined carbon nanotubes. These nanocarbon molecules are expected to have applications in various

unexplored research fields.

The Itami group also developed an efficient one-step **annulative  $\pi$ -extension** reaction (APEX) and demonstrated that a variety of polycyclic aromatic hydrocarbons and nanographenes were synthesized in a single step from structurally simpler aromatic hydrocarbons, such as diaryl acetylenes (Angew. Chem. Int. Ed. 2017) and benzo[b]thiophenes, dibenzofurans and carbazoles (Org. Lett. 2017), and nanographenes and fused heteroaromatics (Angew. Chem. Int. Ed. 2017). Murakami (Itami group) developed a single-step synthesis of small graphene nanoribbons through the palladium-catalyzed double C-H bond activation (Science 2018).

Murakami and Itami have reported a ruthenium-catalyzed equimolar C-H/N-H dehydrogenative aromatic imidation (Chem 2017).

The Yamaguchi group is conducting research on the syntheses and characterization of structurally novel compounds incorporating heteroatoms such as boron, phosphorus, and silicon. They have synthesized boron-stabilized carbon-radical compounds, which show outstanding thermal stability and resistance toward atmospheric conditions due to substantial spin delocalization through the vacant p orbital of the boron atom (J. Am. Chem. Soc. 2017). They have also developed a new photochemical reaction using the vacant p orbital of boron. Photoirradiation of dimesitylboryl-substituted (hetero)arenes produced spirocyclic boraindanes via a [1,6]-sigmatropic rearrangement (Angew. Chem. Int. Ed. 2017). A highly Lewis acidic and antiaromatic dibora-heterocycle was also developed, which activated molecular hydrogen without catalysis (Chem. Lett. 2017).

The Ooi group has developed a new catalytic system that enables highly stereoselective synthesis of amino acid derivatives. A slight structural change in this amino acid-derived organic catalyst leads to pinpoint inversion of stereochemistry. This strategy is expected to become a powerful tool to synthesize various molecules that contain multiple stereocenters in high selectivity and efficiency (Nature Commun. 2017). In addition, they have demonstrated the ability of a chiral aminophosphonium enolate, to simultaneously recognize the direction and distance of an electrophilic carbon center from a carbonyl group in alkenyl dienyl ketones, which facilitates a highly regio-, diastereo-, and enantioselective Michael reaction to give stereochemically defined functionalized enones (Chem. Commun. 2017). Moreover, they succeeded in the achievement of a site-divergent, highly diastereo- and enantioselective Michael addition to afford stereochemically defined functionalized alkynes and conjugated dienes (Angew. Chem. Int. Ed. 2018).

Crudden and Nambo have developed a synthetic route for a new class of molecules, tetraarylmethanes, which can be applied for biological and physicochemical purposes. Tetraarylmethanes were obtained by triflic acid-promoted dehydrogenative modular cross coupling of triarylmethanes and arenes. This straightforward method allows access to a series of structurally diverse tetraarylmethanes (Synlett 2017, selected to the SYNLETT Best Paper Award 2017). They have also found a synthetic method of multiply arylated methanes by nickel-catalyzed desulfonylative cross-coupling reactions of tertiary sulfones and organoboron compounds (J. Am. Chem. Soc. 2018).

Crudden and Nambo have established a simple and direct method to form self-assembled *N*-heterocyclic carbene (NHC) monolayers on gold (Au), and have prepared functionally modified Au nanoparticles (Angew. Chem. Int. Ed. 2017, J. Am. Chem. Soc. 2018).

The Bode group is promoting ITbM's interdisciplinary research through the development of effective methods for the chemical synthesis of proteins. Using a powerful chemoselective amide-forming reaction known as  $\alpha$ -ketoacid-hydroxylamine (KAHA) ligation, the antiviral membrane-associated protein IFITM3 and its modified variants (Angew. Chem. Int. Ed. 2017) and homocysteine mutant of the antibacterial cyclic protein AS48 (Chem. Sci. 2017) were synthesized. They have developed a flow-based system that enables practical parallel kinetic resolution of saturated *N*-heterocycles to provide access to both enantiomers of the starting material in good yield and high enantioselectivity (Nature Chem. 2017). They have also developed photocatalytic coupling reactions of aldehydes and silicon amine protocol (SLAP) reagents for scalable syntheses of substituted morpholines, oxazepanes, thiomorpholines, and thiazepanes under continuous flow conditions (Org. Lett. 2017, highlighted in Org. Process Res. Dev. 2017).

### Theoretical science

The Tama group started collaborations with ITbM's biologists (Higashiyama, Torii, Kinoshita, Kay-Hirota, Frommer-Nakamura Groups) to investigate the properties of biological molecules (mainly

proteins) and bioactive small molecules using its advanced computer simulation techniques. In collaboration with the Kay-Hirota group, Tama performed long time scale MD simulations of protein kinase CK2 $\alpha$  complex with different inhibitors and compared the dynamics of Apo CK2 $\alpha$  as well as the dynamics of the CK2 $\alpha$ -CX4945 complex (Protein 2017). They also revealed the molecular mechanism of the potency and the selectivity of the circadian period-lengthening molecule GO289 (manuscript in preparation). MD simulations were also applied to CRY1 and CRY2 proteins in complex with several CRY1-specific and CRY2-specific circadian clock regulators to understand the molecular mechanism for the selectivity of molecules toward CRY1/CRY2. In addition, they have performed molecular docking and field-based QSAR calculations to assess the quantitative structure-activity relationship (QSAR) of the molecules with respect to their potencies and selectivities.

In collaboration with plant biologists, the tertiary structure of the LURE peptide in *Arabidopsis thaliana* (Higashiyama) and a plausible structural model of MPK6-SCRM interaction (Torii) were calculated. MD simulations of *Striga* receptors ShHTL5 and ShHTL7 (Tsuchiya) provided insights into the protein promiscuity and ligand selectivity (manuscript in preparation).

Yokogawa (Quantum Chemistry group) developed a new method by combining their solvation theory with a high accurate quantum chemical method (DMRG) for the accurate prediction of NIR dyes (with the Yanai group at the Institute for Molecular Science, manuscript in preparation).

Hijikata (Quantum Chemistry group) revealed the selectivity of *Striga* germinators (SAM derivatives) on the ShHTL7 receptor and demonstrated that the dynamics of the entrance in the binding site of ShHTL7 was larger than in ShHTL5, based on homology modelling and MD simulations with Tsuchiya (Kinoshita group) (manuscript to be submitted). Chemogenomic active learning of small molecules to predict active molecules was carried out for chronobiology studies (Yoshimura group) and for the *Striga* project (Kinoshita group). In a collaboration with the Itami group, the dynamic state of electrically-conductive and white light-emitting iodine-cycloparaphenylene (CPP) complex was elucidated computationally (Angew. Chem. Int. Ed. 2018).

#### **Four supporting center's activities**

The Live Imaging Center, headed by Y. Sato, is involved in the majority of ITbM's research projects and has been publishing a number of journal articles. In FY2017, the center continuously covered a wide variety of biological samples (bacteria, fungi, green algae, plants, animals), supported over 200 users (from Apr. 2013), and published 47 papers in which almost half of them were published in high impact journals (Impact factor > 7, Nature, Science, PNAS, JACS, etc.). The center has been supported by the Grant-in-Aid for Scientific Research on Innovative Areas, "The Birth of New Plant Species" (Higashiyama) and "Integrative System of Autonomous Environmental Signal Recognition and Memorization for Plant Plasticity" (Kinoshita).

The Chemical Library Center, led by A. Sato, has distributed over 830,992 molecules to 56 collaborators (As of March 2018). The center has been strongly promoting collaborative research through providing small molecules that modulates specific phenotypes of their interest and supports ITbM's chemical biology research. The center has applied for 7 joint patents (including 2 PCTs) and has over 30 collaborations including 2 projects with companies. The center also established a scheme to distribute library compounds to industries and overseas collaborators under legal compliance, and has contributed to strengthening the network of the chemical library center in RIKEN (NP Depo). The center identified the first small molecules that strongly inhibited class B metallo- $\beta$ -lactamase (IMP) in collaboration with Prof. Arakawa (Medical School, NU) in the Japan Initiative for Global Research Network on Infectious Diseases (J-GRID), AMED, and contributed to the "Promotion of Photosynthesis and Plant Productivity by Controlling Stomatal Aperture (JST ALCA)" project to discover molecules that modulate stomatal movement.

The Molecular Structure Center, led by Kuwata, has established the proteomics system and has been playing a key role in identifying target proteins by installing biochemical protocols, such as immunoprecipitation, stable isotope labeling of amino acids in cell culture (SILAC), phosphoproteomics, and mass spectrometry (MS) imaging. The center actively works in response to various researchers' demands of structural identification (proteome, metabolome, imaging-MS, native-MS, HRMS, etc.), and thus the center has had 64 collaborators (since April 2013) including with companies. The center has been supported by the Grant-in-Aid for Scientific Research on Innovative Areas "Integrative system of autonomous environmental signal recognition and



memorization for plant plasticity" (Kinoshita).

The Peptide Protein Center, led by Oishi, is actively expanding its network of research with the research groups at ITbM (Itami, Yamaguchi, Kinoshita, Frommer-Nakamura, Torii-Uchida, Kay-Hirota, and Higashiyama Groups) and has distributed over 100 peptides/proteins for 16 collaborators. The center is also developing an original peptide library consisting of >100 structurally unique cyclic peptides named CycLaMEN synthesized by KAHA ligation, which contributes to the development of bioactive molecules. The center has started contract research with a global pharmaceutical company and seeks further opportunities of collaboration with industry. The center has started the preparation of a spin-off company, and was successfully funded for early stage support of startups under the strong support of the SPD.

#### **Frommer group's activity**

Wolf Frommer (Univ. Düsseldorf, Max Plank Institute) joined ITbM as the fifth overseas PI in 2016 (see Section 3-(2)). With Masayoshi Nakamura as a Co-PI (Designated Lecturer) along with postdoctoral researchers and lab technicians, the group started its research in early FY2017. Nakamura received the Career Development Award of the HFSP (Human Frontier Science Program). Frommer and the Chemical Library Center have screened 1680 chemicals using Frommer's unique SWEET transporter activity screening system, and in a year, 60 candidates have been discovered as potent SWEET transporter inhibitors. Frommer has also started collaborative research on the basis of this screening system with the Molecular Structure Center, Yamaguchi group, and plant biologists of the Graduate School of Science in NU.

#### **Development of Target ID**

In these 5 years, ITbM has identified over 200 hit compounds from more than 50 phenotypes, and their target protein identification (target ID) has been indispensable to elucidate the molecular mechanisms of biological functions and to develop transformative bio-molecules. Since FY2015, ITbM has been establishing the target ID platform for several cases. The Molecular Structure Center plays a central role, and has established omics research applicable to identify target proteins by installation of immunoprecipitation, stable isotope labeling of amino acids in cell culture (SILAC), phosphoproteomics, and mass spectrometry imaging. In collaboration with other institutions, such as the IoC of Academia Sinica and RIKEN CSRS, ITbM is planning to set up a wide range of target identification methods. The Chemical Library Center is working actively to launch a research consortium of target IDs with RIKEN CSRS. ITbM has also started a collaboration with a bio-informatician (Prof. Shimamura) from the Division of System Biology in the Medical School of NU to accelerate omics research.

#### **Application of artificial intelligence (AI) technology**

ITbM has installed a chemogenomic active learning system in order to predict promising small molecules applicable for research on animal chronobiology and the parasitic plant *Striga*. Rakers (Tama Group) and Hijikata (Quantum Chemistry Group) collaborated with the Yoshimura group and Dr. Brown of Kyoto University to build an active learning system to conduct virtual screening *in silico*.

Toda (Kinoshita Group, JST PRESTO) developed an automated quantification system of stomata aperture in combination of AI technology and machine learning of a series of data of chemical structure-activities. By this system, several molecules were predicted to show stomata-opening activity, and they indeed showed potent activity by subsequent screening.

### **(2) Journal publications, press releases, media coverage, international conferences, and awards**

In FY2017, 156 papers (WPI papers: 132 papers) were published in peer-reviewed journals (including 36 papers (WPI: 27 papers) published in journals with an Impact Factor (2016) > 10, 53 papers (WPI: 39 papers) published in journals with an Impact Factor (2015) > 7, 2 Hot Papers and 7 Highly Cited Papers). From January to April 2018, 37 papers have already been published in peer-reviewed journals.

ITbM has held 7 press conferences and has distributed 14 national/international press releases on its research achievements. In addition, ITbM's research and researchers have been featured nearly 600 times in a range of national and international media, including newspapers, TV programs,

magazines, and internet sites.

ITbM's PIs and researchers have presented their research in a total of 59 international conferences and 116 academic meetings. In FY2017, Itami was invited as a panelist to the "Nobel Prize Dialogue Tokyo 2018: The Future of Food" organized by the Nobel Media AB and JSPS.

A total of 42 awards and honors have been granted to the researchers at ITbM. During FY2017, 3 ITbM PIs, Frommer, Itami and Kay, have been recognized by Clarivate Analytics as the 2017 Highly Cited Researchers. ITbM's Associate Professors Ohmatsu and Nakamichi, have been awarded the MEXT Minister's Young Scientist Award for their research.

### **(3) Research funds**

The record of competitive research funds is a benchmark of ITbM's activity. In FY2017, the total amount of research funding granted to ITbM researchers was 1,098 million yen. Representative grants are JST-ERATO (1 project), JST-CREST (1 project), JST-PRESTO (4 projects), JST-ALCA (1 project), JST-ACCEL-FS (1 project), Grant-in-Aid for Scientific Research on Innovative Areas (2 projects as Area Representative, 1 project as Planned Research), Grant-in-Aid for Specially Promoted Research (1 project).

It is noteworthy that the overseas PIs have also been successful in obtaining KAKENHI (Grant-in-Aid for Scientific Research) from FY2014; in FY2017, Grant-in-Aid for a "Scientific Research (A)" granted to Bode, a "Scientific Research (B)" and a "Challenging Exploratory Research" granted to Crudden, and three of "Scientific Research on Innovative Areas" granted to Torii.

ITbM is also hosting JSPS Postdoctoral Fellowships for Research in Japan; 8 as Standard, 2 as a Summer Program in FY2017.

### **(4) Patent, technology transfer, and commercialization**

Patent applications in FY2017 include 7 domestic and 16 PCT filings, of which 14 filings were based on inventions that were arising from the interdisciplinary research between biology and chemistry. Technology transfer activities led to the conclusion of a total of 6 agreements on patent licensing or assignment, one of which became a core technology asset of a biotech start-up that conducts research and development of new breeding technologies to bring innovation in the crop science industry.

In addition to patent licensing, efforts have been made to expand the academia-industry partnership across industries ranging from agrochemical, pharmaceutical, seed and seedling, lab reagents, etc. In FY2017, ITbM had joint research activities with a total of 24 companies, 8 of which became a partner of ITbM for the first time since the launch of ITbM.

As for the commercialization of research outputs from ITbM, a total of 3 laboratory reagents, AMOR, C-Naphox and the carbon nanobelt, were introduced to the market in FY2017. While the commercialization of C-Naphox and AMOR were based on research outputs in FY2015 and FY2016, respectively, the carbon nanobelt was made commercially available very rapidly relative to the other molecules developed at ITbM. The carbon nanobelt took only 10 months after its journal publication in May 2017 for licensing, product development and manufacture of carbon nanobelt for laboratory use. ITbM considers that such rapid commercialization represents a high expectation for the molecule. ITbM intends to continuously deliver such molecules and research outputs of high impact.

## **2. Advancing fusion of various research fields**

ITbM's interdisciplinary research has been making notable progress under the concept of "Mix". Many collaborative projects have been emerged in a bottom-up manner, and significant progress has been made in a number of projects (see Section 1). ITbM has been implementing various initiatives to promote interdisciplinary research by: (1) **Mix Lab Seminar**, which allows newly arrived researchers to introduce their research background and initiate collaborative research projects with ITbM's members; (2) **ITbM Research Award**, which supports bottom-up interdisciplinary research proposed by young researchers at ITbM; and (3) **ITbM Workshop**, which is held in conjunction with the annual ITbM international symposium, and works as a platform for reporting progress on joint research and proposing new joint research projects to call for potential collaborators.

These initiatives are organized by **Administrative Department** of ITbM, in which the **Research Promotion Division (RPD)** and the **Strategic Planning Division (SPD)** are the key players.

The RPD has been assuming the role to find inventions and scientific discoveries from each research group at an early stage, the SPD was established in FY2016 to socially implement ITbM's research outcomes. In FY2017, ITbM decided to allocate additional staff to RPD and SPD to further strengthen and expand their functions, leading to the promotion of the "Mix" concept.

As presented in the research progress denoted in Section 1, ITbM's **4 supporting centers** (Molecular Structure Center, Live Imaging Center, Chemical Library Center, and Peptide Protein Center) have been making a major contribution to the promotion of ITbM's interdisciplinary research. Due to the increase in various tasks, additional technical staff were allocated to the centers.

### **Interdisciplinary research projects selected to ITbM research awards 2017**

Among the initiatives listed above, the ITbM Research Award has been playing a significant role to motivate all ITbM members, especially of its younger generation. The awarded projects are officially approved as ITbM's new projects and receive financial support.

During the past 3 years, 10 projects had been selected. Among them, the project to develop molecules for plant cell division inhibition by Nambo (Crudden Group) and Ueda (Higashiyama Group) led to a joint paper. Exploration of small molecules that modulate flowering time led by Nakamichi (Kinoshita Group) resulted in the discovery of a molecule that accelerates flowering time of plants, and this outcome was filed for patents. The development of fluorogenic probes for strigolactone receptors has led to the discovery of agonist/antagonist molecules selective for *Striga* receptor isoforms.

In FY2017, the following 4 challenging projects were newly selected to receive the ITbM Research Award. Of those 4 projects, 2 projects consisted of teams composed only of postdoctoral researchers and students. This clearly indicates that the Mix concept has been spreading throughout ITbM, and that the collaborations are naturally occurring on a daily basis.

- "Plant Cell Wall Localizing Group Enable Live-imaging for Extracellular Dynamic Movement of Proton", Hiroaki Ogasawara, Takuya Nagae, Kazuki Motomura, Hiromasa Shikata, Yuki Hayashi
- "Accelerating target identification for leading small compounds by combining diversity-oriented synthesis and label-free target identification technique", Rika Kato, Mizuki Murao, Hitoshi Endo
- "Identification of cell polarity determinant in plants", Akira Yoshinari, Masayoshi Nakamura, Shunsuke Oishi, Subramanian Govindan, Kumar Reddy Nandarapu
- "A Molecular-based Toolbox for Optophysiology: Analysis of long-distance signaling in animals and plants", Yuuki Kato, Riho Hosokawa, Yuichiro Tsuchiya, Masayoshi Nakamura, Taeko Ohkawa, Masakazu Nambo, Masayasu Taki

### **Joint publications and patent applications**

In 2017, ITbM has published 10 joint publications among the following research groups: Itami/Higashiyama (2), Irle/Torii (1), Itami/Irle (3), Crudden/Taki (Yamaguchi) (1), Higashiyama/Yamaguchi (1), Itami/Torii (1), Itami/Kinoshita (1). Research accomplishments arising from these joint papers include synthesis of molecules for plant growth and fertilization, bioimaging, as well as computational studies on molecules. The number of joint publications in ITbM is increasing on an annual basis and a total of 38 publications have been reported through collaborative research at ITbM.

Among the patent filings in FY2017, 14 patent applications were based on the inventions arising from interdisciplinary research between biology and chemistry, which are more than half of the applications filed in FY2017.

### **Collaboration with national/international institutions**

ITbM has been strategically extending its collaborating network. As stated in Section 3-(6), international collaboration has been considerably enhancing the ITbM's internationalization and international visibility. Meanwhile, the collaborations have been largely contributing to the promotion of interdisciplinary research. For example, ITbM's target ID platform is being developed through a collaboration with RIKEN CSRS and IoC of Academia Sinica. Research collaborations with other partner institutions such as the NSF Center for Selective C-H Functionalization (USA) and the University of Freiburg (Germany) have already started.

ITbM and RIKEN CSRS have been annually holding a joint workshop to find seeds of collaboration on the basis of a collaboration agreement concluded in January 2015. In FY2017, this framework was further expanded by incorporation of the Kihara Institute for Biological Research in Yokohama City University. Accordingly, the workshop in FY2017 was titled the "4th CSRS-ITbM Joint Workshop

with Kihara", and was held on January 2018, in order to provide further opportunities to develop new seeds for collaboration.

### 3. Establishing international research environment

\* Describe what's been accomplished in the efforts to raise the center's recognition as a genuine globally visible research institute, along with innovative efforts proactively being taken in accordance with the development stage of the center, including the following points, for example:

- Efforts being developed based on the analysis of number and state of world-leading, frontline researchers; number and state of visiting researchers; exchanges with overseas entities
- Proactive efforts to raise the level of the center's international recognition
- Efforts to make the center into one that attracts excellent young researchers from around the world (such as efforts fostering young researchers and contributing to advancing their career paths)

#### (1) ITbM international symposia/awards and a series of ITbM Seminars

ITbM's symposia and awards have been contributing to expand ITbM's international network and provide opportunities to attract overseas researchers.

ITbM has organized its fifth annual international symposium (ISTbM-5) in November 2017 at NU. The lectures were delivered by 2 ITbM researchers (Kinoshita and Itami) along with 7 invited speakers (Professors Paul Wender (Stanford University, USA), Julian Schroeder (University of California San Diego, USA), John Hogenesch (Cincinnati Children's Hospital Medical Center, USA), Jenny Russinova (Ghent University, Netherlands), Katsunori Tanaka (RIKEN), Kazunari Yoshizawa (Kyushu University), Masaki Kita (NU)), who are all world-leading international researchers in fields strongly related to ITbM's research.

ITbM also organized the 13th Hirata Award and the 3rd Tsuneko & Reiji Okazaki Award at the same time as ISTbM-5. The 13th Hirata Award was presented to Professor David Nicewicz (University of North Carolina Chapel Hill, USA), in recognition of his achievement that paves a new way toward synthesis via organic photoredox catalysis. The 3rd Tsuneko & Reiji Okazaki Award was presented to Professor Maria Barna (Stanford University, USA) for her research on ribosome heterogeneity in translating the genetic code. The symposium and the award lectures ended in great success with about 450 participants.

In December 2017, ITbM organized the 23rd Nagoya Medal Award of Organic Chemistry. The Nagoya Medal is becoming internationally recognized, with 2 of the 3 recipients of the 2016 Nobel Prize in Chemistry being previous winners of the Nagoya Medal. This year, the Gold Medal was awarded to Professor Bert Meijer of the Eindhoven University of Technology (Netherlands) and the Silver Medal to Professor Hiroaki Suga of the University of Tokyo. Nearly 400 students and researchers across Japan and other international institutes attended the award lectures, including Professor Ryoji Noyori of Nagoya University/JST and Professor Hisashi Yamamoto of Chubu University/University of Chicago (USA), who presented the medals to the winners.

ITbM has been holding a series of ITbM Seminars inviting researchers from related fields. In FY2017, ITbM had invited 7 top scientists as lecturers.

#### (2) ITbM Researchers from overseas countries

In 2016, Wolf Frommer joined ITbM as the fifth overseas PI, and accordingly ITbM hired Nakamura as a Co-PI of the Frommer group (Designated lecturer) in April 2017. Nakamura was a HFSP researcher at the Carnegie Institution for Science. In late 2016, Frommer was awarded the Humboldt Professorship, and moved to Germany as a full professor of the University of Düsseldorf and the Max Planck Institute for Breeding Research in April 2017. Frommer was also appointed to a professor of the Cluster of Excellence on Plant Sciences (CEPLAS). CEPLAS is a joint initiative of Heinrich Heine University Düsseldorf (HHU), University of Cologne (UoC), Max Planck Institute for Plant Breeding Research Cologne (MIPZ) and Forschungszentrum Jülich (FZJ), which is the only plant research center selected as the Cluster of Excellence supported by the German Research Excellence Initiative, and a world-leading institute of plant science. HHU has shown a large interest in ITbM as a collaborating partner and concluded the MOU to appoint Frommer as an overseas PI at ITbM as of April 2017. The Agreements for research collaboration and tuition-free student exchange will also be concluded in early FY2018.

In addition to the overseas PIs, many postdoctoral researchers from overseas countries have been employed. The ratio of non-Japanese researchers is 33% as of March 31, 2018.

ITbM also accepted 2 PhD students from the University of Freiburg as part of the research collaboration.

### **(3) Bilingual Operation**

The Administrative Department, composed of the Administrative Director, the Management Division, the Research Promotion Division (RPD), and the Strategic Planning Division (SPD), consists of personnel who are able to conduct various administrative and research support tasks in both English and Japanese. The ITbM's regular meetings such as the Steering Committee meetings and the PI meetings are conducted in English. Most of ITbM's secretaries of the PIs and the supporting centers are capable of conducting duties in both English and Japanese and are playing important roles for the operation of ITbM.

In FY2017, the RPD employed a female foreign researcher as an Assistant Professor (PhD in synthetic chemistry) in order to reinforce international outreach activities. In October, an administrative staff to support of overseas researchers and their families were employed (see below). The RPD also appointed an Assistant Professor (PhD in design and architecture, and biomedical engineering) with prior experience in the field of human-computer interaction and a good fluency in English as a science designer as of April 2018.

### **(4) Local Support**

A staff member in ITbM's Research Promotion Division (RPD) is mainly responsible for providing local support to ITbM's foreign researchers and their families staying in Japan. The main purpose of this role is to offer a comfortable environment to ITbM's researchers coming from abroad, so that they are able to fully concentrate on their research activities. Many foreign researchers who come to work in Japan experience the language barrier, as almost all the procedures at local government offices and medical centers are carried out in Japanese.

The role of the Local Support Officer is to provide on-scene support to foreign researchers at ward offices, including help with national health insurance and the pension system, as well as assistance in immigration affairs and other matters that may arise in their daily lives.

In order to provide more useful information, some beneficial services from the International Education & Exchange Center (IEEC) in Nagoya University are being shared with ITbM's foreign researchers. The IEEC mainly provides assistance for international students, but in recent years, the ITbM has started expanding their services to support foreign faculty members as well. Services include: seminars on tax adjustment, orientation for renting an apartment in Japan, health consultations, and information on cultural events such as Japanese flower arranging (Kado) and Origami lessons.

In addition to the above-mentioned duties, weekly Tea Break Meetings are being organized by the RPD. These are held to promote communication and to provide an opportunity to build networks among ITbM's researchers who come from various disciplines and backgrounds.

Matters that require specific care, such as child welfare and marriages between foreign nationals are expected to arise in the coming years. Gathering and providing appropriate information in a timely manner is essential to support foreign researchers and their family members.

As for medical support of foreign researchers and their families, ITbM has signed a contract with International SOS Japan Ltd. starting from 2016, to provide advanced medical service information 24 hours a day.

### **(5) International public relations and outreach activities**

In order to disseminate ITbM's interdisciplinary research activities and accomplishments to the global audience, ITbM has been constantly releasing international press releases on research accomplishments, international awards/events and other information. The releases are presented in a way that complex scientific results are conceivable to people in different fields and that the excitement from the research can be shared with the readers. As ITbM is carrying out interdisciplinary research, emphasis is also being put into conveying the joy and challenges of conducting research between different disciplines. ITbM has been highlighted in various national/international media and is receiving recognition by the international community, including journalists, researchers and companies.

ITbM has also been hosting and exhibiting at international events, including BioJapan, Science Agora and the AAAS Annual Meeting, to present its research activities, establish networks and nurture the next generation of scientists. These endeavors are envisaged to increase the international recognition of ITbM and attract prominent researchers and industrial partners from abroad.

## **(6) International collaboration**

**Overseas PIs' host institutions** are important partners of ITbM; ETH-Zürich (Switzerland), Queen's University (Canada), University of Washington (USA), and the University of Southern California (USA). In May 2017, the University of Düsseldorf (Germany) became a partner of ITbM, following Frommer's transfer from the Carnegie Institution for Science. ITbM is extensively collaborating with these partner institutions through researcher/student exchange. For example, the Bode group members in ITbM visit ETH every summer to share their research progress, and several PhD students from ETH come at a regular basis to work at ITbM.

ITbM has been collaborating with the **NSF Center for Selective C-H Functionalization (USA)** and **the Institute for Basic Science (IBS, KAIST, Korea)**. In FY2017, ITbM accepted 2 PhD students from CCHF (Pennsylvania State University and Emory University).

**The Institute of Chemistry (IoC), Academia Sinica (Taiwan)** became a partner of ITbM in 2016. Following the first ITbM-IoC joint workshop at ITbM in 2016, IoC hosted the 2nd workshop at Taipei. Researchers from the **Institute of Plant and Microbial Biology (IPMB) of Academia Sinica** were also invited, and the workshop was titled the "IoC-IPMB-ITbM Joint Symposium on New Frontiers by Fusing Chemistry and Biology". In addition to the ITbM researchers, the administrative staff joined the symposium, and had extensive discussions on establishing partnerships and collaborations between the institutions.

ITbM also started a collaboration with the **University of Freiburg (UoF, Germany)**. Based on the agreement between NU and UoF, the Institute of Advanced Research (IAR) of NU and Freiburg Institute for Advanced Studies (FRIAS) of UoF jointly launched a "Joint Freiburg-Nagoya Project Group" and a call for collaborative research in 2015. A joint proposal organized by the Ooi and Itami groups of ITbM and Professor Breit in UoF, titled "Multicomponent Supramolecular Catalysts for Sustainable Chemical Synthesis" was selected, and collaborative research in synthetic chemistry was launched in FY2016. The groups have exchanged researchers, and a joint symposium "1st International Symposium on Catalysis for Sustainable Chemical Synthesis" was organized at UoF in September 2017, inviting 8 world-leading synthetic chemists.

In November 2017, NU and UoF hosted the 2nd JANET Forum in Freiburg in collaboration with JSPS-Bonn (JANET: Japan Academic Northern Europe Network), where ITbM entered the session "Research Collaboration: How is it promoted and supported by the University?" and ITbM's activities were presented to organizations in northern Europe.

## **(7) Promotion of ITbM's researchers**

The international visibility of ITbM is indicated by how ITbM is involved in international brain circulation. In FY2017, 7 researchers joined ITbM from overseas institutions, and 4 overseas researchers working at ITbM have been promoted to the other institutions. The records are listed in Appendix 3-1.

## **(8) Visitors from overseas institutions**

ITbM actively hosts visitors from overseas institutions as an endeavor to improve its international visibility. In FY2017, ITbM hosted a visit of high school students from the Bard High School Early College. In addition, officials of overseas universities and governments have visited ITbM; North Carolina State University (USA), University of Malaya (Malaysia), Royal University of Fine Arts (Cambodia), Institute of Technology of Cambodia (Cambodia), University of Health Science (Cambodia), Sungkyunkwan University (South Korea), National University of Singapore (Singapore), the Swedish Foundation for International Cooperation in Research and Higher Education (STINT, Sweden).

## **4. Reforming the research organization**

\* If innovated system reforms generated by the center have had a ripple effect on other departments of the host institutions or on other research institutions, clearly describe in what ways.

\* Please describe the center's operation and the host institution's commitment to the system reforms.

### **(1) Innovative system reform of ITbM**

#### **(a) Decision making system**

According to NU's commitment stated in the Research Center Project, the Director has the authority to make final decisions over all matters concerning the operation and management of ITbM, such

as the appointment of personnel, the Center's budget and research priorities. The role of the President of NU is limited to the appointment of the Director according to the suggestion by the WPI program committee.

(b) Evaluation system and incentives

ITbM had established a system to provide incentives to the Director, the Vice Director, PIs, and the Administrative Director based on evaluation of their performance and responsibilities. In FY2017, their full amounts were provided in reference to their remarkable records of achievements and valuable contributions to achieve the high activity of ITbM. Evaluation was carried out based on an annual report submitted in March regarding their research activity. The evaluation of Co-PIs and postdoctoral researchers were carried out by each PI, followed by a secondary evaluation by the Director, which was reflected in the renewal of their contract.

**(2) Ripple effect to NU**

Under the President Matsuo's Initiatives for Reform, Autonomy and Innovation 2020 (NU MIRAI 2020), NU has been carrying out extensive system reform to become a world-class research university. In the initiative, ITbM is positioned as a core research center of Nagoya University, and thus the basic policy and the measures of system reform have been established to match ITbM's needs. ITbM's Director and core members have been holding regular meetings with the President once a month to discuss issues related to the management of ITbM.

(a) NU appointed as "Designated National University" by MEXT

NU was recognized for its abilities to develop world-leading education and research activities and was selected as a "Designated National University" as of March 20, 2018. Based on the concept of NU MIRAI 2020, the goal has been set. NU will make all efforts to become an international leading university and play a leading role in the reform of national universities by actively disseminating the concrete results of their influence and efforts that have contributed to the development of the society and economy. In the plan, NU has identified four key research areas, in which the first area is "interdisciplinary research in chemistry and biology led by the WPI center". The plan clearly states that NU will invest human and financial resources intensively into the key areas, and following the president's initiative, ITbM is positioned to be a core research center of NU for the future. ITbM and NU will cooperate and devise various tasks to achieve this goal.

(b) Conclusion of a Basic Agreement of NU with RIKEN

NU concluded a basic agreement on June 13, 2017 with RIKEN regarding the promotion of their partnership and cooperation to begin anew their inter-institutional partnership and produce world-class, top-level research achievements and innovation. In the past, ITbM and the Graduate School of Bioagricultural Sciences have both collaborated separately with the RIKEN Center for Sustainable Resource Science (CSRS). As other collaborative researches are projected between the two institutions, the agreement between the two institutions was considered to be very comprehensive, aiming for cooperation in all fields in which collaboration is possible.

(c) Application to the "Takuetsu Graduate School Program" with ITbM as a core

At ITbM, interdisciplinary research collaboration promoted by the "Mix" concept has been the key to bring about the marked research outcomes that are recognized worldwide. NU also recognizes the significance of the "Mix" concept and plans to extensively involve ITbM into the education of graduate schools. Thus, NU and ITbM draw up a concept for the "Takuetsu Graduate School Program" that will start its call in FY2018. In this concept, ITbM is positioned as a hub for promoting interdisciplinary research in the field of natural sciences. The role of the program involves collaboration with RIKEN, which entered a comprehensive agreement with NU in 2017, and other related institutes in order to nurture young researchers and open a new avenue in interdisciplinary research fields.

(d) "WPI-next" and related research support programs at NU

In 2014, NU launched the "WPI-next" program to support world-leading sciences of NU, which referred to ITbM's unique personnel structure, such as the Co-PI system. This program was renamed as the "Cutting-edge International Research Units" program, and two more programs: "Research Units Geared toward Young International Researchers" and "Young Researcher Units for the

Advancement of New and Undeveloped Fields" were launched in the framework of the Program for Promoting the Enhancement of Research Universities.

(e) Department for "Academic Research & Industry-Academia-Government Collaboration"

In order to promote technology transfer of intellectual properties and research outcomes from ITbM and other NU's institutes, NU conducted organizational reform of research supporting units to establish the department in 2015. In the course, the URA system that started in 2013 was also reviewed extensively with respect to the role of the RPD at ITbM. The URA was categorized into 5 groups and their functions were defined as follows: "Planning & Strategy Group", "Regional Collaboration & Communication Group", "Project Promotion Group", "Intellectual Property & Technology Transfer Group", and "International Industry-Academia-Collaboration & Human Resource Development Group". Through cooperation with these groups, ITbM's collaboration network with industries has largely expanded.

(f) International Public Relations

ITbM has been sharing its expertise and experience on international public relations to the Academic Research and Industry-Academia-Government Collaboration Department at NU. A taskforce was organized to establish international public relations strategies at NU, and members of the RPD have been involved as advisors to promote these activities and the internationalization of the university. As a result, the Department has started to distribute international press releases on research accomplishments for the entire university. Coordination is ongoing between the Department and NU's public relations office so that the public relations office can carry out international public relations.

(g) Venture business support

In 2016, NU launched a "Venture Fund of Nagoya University and Tokai Area's Universities". Establishment of these systems strongly supports ITbM's activity. ITbM's peptide protein center is planning the establishment of a start-up company that provides services and products related to its peptide synthesis technologies. The proposal of its business plan based on its core technology was selected to receive this fund in late FY2017.

(h) Information distributed in English

With respect to the English e-mail distribution by ITbM, NU started to circulate information of grants, funding and other information in both English and Japanese from the end of FY2013.

## 5. Efforts to secure the center's future development over the mid- to long-term

\* Please address the following items, which are essential to mid- to long-term center development:

- Future Prospects with regard to the research plan, research organization and PI composition; prospects for the fostering and securing of next-generation researchers
- Prospects for securing resources such as permanent positions and revenues; plan and/or implementation for defining the center's role and/or positioning the center within the host institution's institutional structure
- Measures to sustain the center as a world premier international research center after program funding ends
- Host institution's organizational reforms carried out for the Center's autonomous administration simultaneously with the creation of the Center.

ITbM will take appropriate actions stated below to secure the funds to operate ITbM. The SPD will cooperate with NU to acquire intellectual property rights and conduct business matching with companies for beneficial outcomes. ITbM will devise strategies to collect donations. Nevertheless, NU's strong support is crucial to sustain ITbM at the current level. As denoted in Section 4-(2), ITbM is positioned as a core research center at NU, and the university will invest human and financial resources intensively for the further development of ITbM. While the WPI program financially supports ITbM, NU conducts system reform of the university to ensure that ITbM is maintained. NU will include ITbM as part of the Institute of Advanced Research to secure the employment of ITbM's faculties and staffs by providing the necessary financial support.

### (1) Strengthening of the Strategic Planning Division (SPD)

The SPD was launched in 2016 to promote social implementation of the research outcomes. Its activity will be the key to ITbM's sustainability. As ITbM expands its activities, the SPD's tasks have been increasing, such as strengthening academia-industry partnerships, creation of venture start-ups, translational research utilizing outsourcing, etc. ITbM has conducted recruiting activities in



FY2017 and has appointed an experienced candidate, who will join ITbM in May 2018. The SPD has been building strong ties with the Academic Research & Industry–Academia–Government Collaboration Department of NU. This has been highly effective to expand and strengthen the collaborations with industries (see also Section 4-(2)(e)).

## **(2) Promoting Collaborative Research with Industries**

The SPD is taking initiatives to promote collaborative research with industries. 3 Major strategic actions were taken to increase the opportunities for communication on research outputs of ITbM: (a) utilization of open innovation programs supported by companies, (b) exhibitions at technology matching events; and (c) creation of ITbM's own forum, or "ITbM consortium".

### **(a) Open innovation programs**

Recently, an increasing number of pharmaceutical companies have launched their own open innovation public offering programs, where each company discloses its areas/technologies of interest to call for applications from academia. Such a wish list can be a comprehensive guide for ITbM's researchers and the SPD to search for and identify potential partners. Taking advantages of the opportunities, 2 collaborative research projects related to the regulation of circadian clocks were carried out with major pharmaceutical companies in Japan.

### **(b) Exhibitions at technology matching events**

Attending exhibitions (e.g. BioJapan) to present ITbM's research outcomes has been quite effective for establishing a connection with companies that ITbM has never been able to reach before. In FY2017, ITbM exhibited its research outputs at a total of 5 conventions/meetings (Biotech 2017, BioJapan 2017, Agribusiness Fair Tokai, DSANJ Business Meeting and 17<sup>th</sup> congress of the Japanese society for regenerative medicine). As a result of these exhibitions, Nakamichi's early flowering technology attracted significant attention, leading to media coverage, material transfer agreements for technical evaluation, and collaborative research.

### **(c) ITbM Consortium**

ITbM has launched a membership-based discussion forum, or ITbM Consortium, to promote in-depth discussion towards co-creation of values in interdisciplinary research between ITbM and industries. At the ITbM Consortium, a wide range of industrial partners can join and have access to ITbM's science, technology and people. In turn, ITbM's researchers can receive information on social needs that need to be addressed by new technologies. The pre-meeting was held in October 2017, which collected 51 attendees from 23 firms of a variety of business fields such as crop science, pharmaceuticals, functional materials, and automobiles. ITbM expects to have 15-17 members in the ITbM Consortium at the start of FY2018.

## **(3) Designated Fund for ITbM (Nagoya University Foundation)**

ITbM acknowledges that the diversification of financial resources is crucial for sustainable growth after the WPI funding ends. As part of the financial resource options, ITbM has set up a designated fund for supporting ITbM, or the ITbM support program, within the Nagoya University Foundation Program in September 2017, so that it can accept donations from public sectors including foundations, citizens, alumni, charitable persons, etc.

## **(4) "Takuetsu Graduate School Program" with ITbM as a Core**

As stated in Section 4-(2)(c), NU will apply for the "Takuetsu Graduate School Program" that places ITbM at the core. Accordingly, the students will be allocated to the center's designated faculties, and ITbM will be extensively involved in the education of students.

## **(5) Strategic collaboration with Domestic/International institutions**

While ITbM's international collaborating network has been largely improving its internationalization and international visibility, domestic institutions are also important as ITbM's partners. As stated in Section 2, the collaboration with RIKEN CSRS has been largely promoting ITbM's research activity, and the conclusion of the university-wide Basic Agreement with RIKEN will promote mutual collaboration. Hagihara (Associate Professor of Itami group) will move to RIKEN CSRS as a team leader in April 2018. He will continue his activities as a collaborative researcher of ITbM, and thus interaction between ITbM and CSRS will be further extended and will promote ITbM's activity.

## **(6) Mentoring of young researchers**

Fostering young researchers is a key mission of ITbM. In order to foster internationally competitive talents, ITbM has prepared a program and has continued to exchange faculties and PhD students with collaborating overseas institutions. ITbM is also utilizing the international programs run by NU for researcher exchange and collaboration.

Mix Labs and Mix Offices, which have been established to promote interdisciplinary research, are serving as places for young researchers to learn about other research fields. Since 2016, ITbM has been giving a lecture course series on chemical biology to establish the education system for students to conduct interdisciplinary research in chemistry and biology.

In 2015, ITbM started a program that supports the organization of student-initiated symposia. The students from several PI groups form a team and organize small events. While the program provides an opportunity to experience a series of tasks needed for event organization, it also allows the students to become visible to academic researchers. In December 2017, a student team organized a two-day workshop titled the "ITbM/IGER Chemistry Workshop 2017", inviting 6 researchers from a variety of fields in chemistry. In addition to the invited lectures, a half-day free discussion among the lecturers and students was carried out, which largely motivated the students.

## **6. Others**

\* In addition to the above 1-5 evaluation items, only if there is anything else that deserves mention regarding the center project's progress, please note it.

### **(1) Appointment of a new PI (theoretical science)**

As of the end of March 2017, Dr. Stephan Irle transferred to Oak Ridge National Laboratory (USA) as a Senior Research Leader, and resigned from both of his positions at NU (PI of ITbM and Professor of the Graduate School of Science of NU). ITbM started to seek for a new PI through open international recruitment with the Graduate School of Science of NU to succeed Prof. Irle's post. After strict evaluation and careful consideration, Dr. Takeshi Yanai (Associate Professor, Institute for Molecular Science, National Institute of Natural Science) was selected as a new PI. Dr. Yanai is one of the leading researchers in the field of quantum chemistry research, and is expected to largely contribute to ITbM's interdisciplinary research. He will be employed at NU as a PI of ITbM as well as a professor at the Department of Chemistry in the Graduate School of Science of NU, starting from April 1, 2018.

### **(2) Outreach activities headed by Research Promotion Division (RPD)**

The Research Promotion Division has also been involved in various outreach activities, including science education and experiment for high school students, and has been carrying out science demonstrations for the general public, including the Science Agora at the Telecom Center in Tokyo. Lab tours and seminars to introduce ITbM have been also held for students and teachers from local and overseas high schools as well as for other visitors. ITbM's activities are also introduced to the academic community by means of booth exhibitions at international events, including the AAAS Annual Meetings (USA) to the public, Super Science High School Presentation (Kobe) and the WPI Science Symposium.

Many of the PIs, staff and RPD members are also involved in holding public lectures to high school students and to adults interested in science. In FY2017, ITbM's research activities were presented to over 5,000 high school students and the general public, and the RPD held many outreach events (over 50 outreach events). This not only is effective for fostering future scientists (high school students) but is effective for the younger generation (elementary school students), including their parents to develop a curiosity towards molecules, which led to the establishment of the "MoleQrious!" project. The final goal of this campaign is to create a society in which molecules are recognized at the same level as common scientific words, such as the "genome".

The 5-year-educational campaign has had a substantial payoff in the form of collaboration with one of the oldest department stores, Matsuzakaya. This is the first attempt to receive private financial support for management of the event and is considered a good strategy towards sustainable management of the center. The 5-year networking with high school teachers is leading to a joint event that includes the annual WPI science symposium and Kagaku-zanmai, the largest science event in the Tokai area.

### **(3) Concern for the environment and safety**

ITbM had set up the Environment and Safety Committee so that researchers at ITbM are constantly aware of the appropriate issues when conducting their research. The 5th annual meeting was held in February 2018. The recent progress of ITbM's research projects, safety management of the molecules synthesized/discovered in ITbM, development of control environment for legal compliance, and far-sighted activities of science communication to the society were discussed.

### **7. Center's response to the follow up results in last year**

\* Transcribe the item from the "Advice/ recommendations" section in the site visit report and "Actions required and recommendations" in the Follow-up report, then note how the center has responded to them.

\* For the center launched in FY 2017, please describe the status of response to the pointed items in "Major points that need to be improved" of "The screening result for WPI centers launched in FY 2017."

\* However, if you have already provided this information, please indicate where in the report.

### **Comments in the Follow-up Report & the Site Visit Report**

**Comment 1:** ITbM should have a vision for the long-term, including a plan for after the support from the WPI program ends. It will be important to maintain strategic focus on basic science after the establishment of the ITbM Consortium, an association of potential external partners for applied aspects.

#### **<Action of ITbM>**

**Long-term perspective:** NU has identified four key research areas in the concept for "Designated National University", in which one of them is "interdisciplinary research in chemistry and biology led by the WPI center". The concept clearly states that the university will invest human and financial resources intensively into the key areas, and following the president's initiative, ITbM is positioned to be a core research center of NU for the future. ITbM's research goals will remain unchanged for the time being and will continue its activities to conduct cutting-edge research in chemistry and biology. Measures may be taken to respond to changes over time, including reordering of PIs.

ITbM plans to be extensively involved in the education of graduate schools. ITbM's faculties are already giving chemical biology lectures in the School of Science. In addition to this, NU is drawing up a concept for the "Takuetsu Graduate School Program" that places ITbM at the core. In this concept, ITbM is positioned as a hub for promoting interdisciplinary research in the field of natural sciences. The role of the program involves collaboration with RIKEN, which entered a comprehensive agreement with NU in 2017, and other related institutes in order to nurture young researchers that will carry out next-generation interdisciplinary cutting edge research. Measures to ensure sustainable employment of faculty are also under consideration.

**Promotion of basic research:** As stated in the post-interim center project progress report, ITbM's research principle is curiosity-driven innovative basic research, which may be inspired by social needs, but not necessarily by corporate interests. SPD will take initiative so that ITbM's research does not lean too much towards commercial purposes, and will make appropriate decisions on which research projects to pursue with advice from experts, such as the Environmental and Safety Committee.

**Comment 2:** Strategic Planning Division (SPD), launched for promoting collaboration with industry and other research organizations, is key to ITbM's sustainability. It would be worthwhile to recruit new talent to strengthen its function.

#### **<Action of ITbM>**

ITbM has started recruitment at the end of FY2017 to soon employ two personnel for academia-industry collaborations. Since last year, the Regional Collaboration & Communication Group of NU's Academic Research & Industry-Academia-Government Collaboration Department has been cooperating with the SPD to find potential partner companies for ITbM. This has been highly effective and many companies are joining the ITbM consortium.

**Comment 3:** Development of the graduate program would reap huge benefits for ITbM. However, there are still barriers between departments, which impede recruitment of more students to ITbM. NU and ITbM should cooperate and make every effort for success in the application for the Excellent

Graduate School program, a new MEXT program to facilitate reorganization of graduate schools.

**<Action of ITbM>**

As mentioned in the response to the first comment, ITbM is applying for the "Takuetsu Graduate School Program", which will establish a graduate school with ITbM at its core, making use of ITbM's high research profile and interdisciplinary research initiatives. Discussions about the program are ongoing between faculties of related departments and schools (Science, Engineering, Bioagricultural Sciences, and Pharmaceutical Sciences), and ITbM's Mix concept is being shared amongst the members. NU's trustee for education is taking initiative for the application of the "Takuetsu Graduate School Program" and the contents are being reviewed amongst the program committee with members consisting of the head of each department/school. The committee is making arrangements so that many graduate students can be involved in ITbM's research.

## Appendix 1 FY2017 List of Center's Research Results and Main Awards

### 1. Refereed Papers

- List only the Center's papers published in 2017. (Note: The list should be for the calendar year, not the fiscal year.)

- (1) Divide the papers into two categories, A and B.
  - A. WPI papers  
List papers whose author(s) can be identified as affiliated with the WPI program (e.g., that state the name of his/her WPI center). (Not including papers in which the names of persons affiliated with the WPI program are contained only in acknowledgements.)
  - B. WPI-related papers  
List papers related to the WPI program but whose authors are not noted in the institutional affiliations as WPI affiliated. (Including papers whose acknowledgements contain the names of researchers affiliated with the WPI program.)

Note: On 14 December 2011, the Basic Research Promotion Division in MEXT's Research Promotion Bureau circulated an instruction requiring paper authors to include the name or abbreviation of their WPI center among their institutional affiliations. As some WPI-affiliated authors of papers published up to 2011 may not be aware of this requirement, their papers are treated as "WPI-related papers." From 2012, however, the authors' affiliations must be clearly noted and only category A papers will be basically listed.

- (2) Method of listing paper
  - List only referred papers. Divide them into categories (e.g., original articles, reviews, proceedings).
  - For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is the same. (The names of the center researchers do not need to be underlined.)
  - If a paper has many authors (say, more than 20), all of their names do not need to be listed.
  - If the papers are written in languages other than English, divide them into paper's categories when listing them.
  - Assign a serial number to each paper to be used to identify it throughout the system.
  - Order of Listing
    - A. WPI papers
      1. Original articles
      2. Review articles
      3. Proceedings
      4. Other English articles
      5. Articles written in other than English
    - B. WPI-related papers
      1. Original articles
      2. Review articles
      3. Proceedings
      4. Other English articles
      5. Articles written in other than English
- (3) Submission of electronic data
  - In addition to the above, provide a .csv file output from the Web of Science (e.g.) or other database giving the paper's raw data including Document ID. (Note: the Document ID is assigned by paper database.)
  - These files do not need to be divided into paper categories.
- (4) Use in assessments
  - The lists of papers will be used in assessing the state of WPI project's progress in FY 2017.
  - They will be used as reference in analyzing the trends and whole states of research in the said WPI center, not to evaluate individual researcher performance.
  - The special characteristics of each research domain will be considered when conducting assessments.
- (5) Additional documents
  - After all documents, including these paper listings, showing the state of research progress have been submitted, additional documents may be requested.

#### A. WPI papers (Jan 1, 2017 – Dec 31, 2017)

##### 1. Original Articles

- (1) Keishu Okada, Akiko Yagi, Yasutomo Segawa and Kenichiro Itami, Chem. Sci. 2017, 8, 661–667. "Synthesis and properties of [8]-, [10]-, [12]-, and [16]cyclo-1,4-naphthylenes" (DOI: 10.1039/C6SC04048A)
- (2) Kenta Kato, Yasutomo Segawa, Kenichiro Itami, Can. J. Chem. 2017, 95, 329–333. "Phenanthro[9,10-a]corannulene by One-step Annulative n-Extension of Corannulene" (DOI: 10.1139/cjc-2016-0467)
- (3) Brandon E. Haines, Takahiro Kawakami, Keiko Kuwata, Kei Murakami, Kenichiro Itami, Djameladdin G. Musaev, Chem. Sci. 2017, 8, 988-1001. "Cu-Catalyzed Aromatic C-H Imidation with N-Fluorobenzenesulfonimide: Mechanistic Details and Predictive Models" (DOI: 10.1039/C6SC04145K). *Highly Cited Paper.*

- (4) Yoshio Nishimoto, Stephan Irle, *Chem. Phys. Lett.* 2017, 667, 317–321. "Quantum chemical prediction of vibrational spectra of large molecular systems with radical or metallic electronic structure" (DOI: 10.1016/j.cplett.2016.11.014)
- (5) Hiroki Tsutsui and Tetsuya Higashiyama, *Plant Cell Physiol.* 2017, 58, 46–56. "pKAMA-ITACHI Vectors for Highly Efficient CRISPR/Cas9-Mediated Gene Knockout in *Arabidopsis thaliana*" (DOI: 10.1093/pcp/pcw191)
- (6) Toshimasa Okita, Kazushi Kumazawa, Ryosuke Takise, Kei Muto, Kenichiro Itami, and Junichiro Yamaguchi, *Chem. Lett.* 2017, 46, 218–220. "Palladium-catalyzed Decarbonylative Alkynylation of Aromatic Esters" (DOI: 10.1246/cl.161001). *Highly Cited Paper.*
- (7) Shuka Ikematsu, Masao Tasaka, Keiko U. Torii and Naoyuki Uchida, *New Phytologist* 2017, 213, 1697–1709. "ERECTA-family receptor kinase genes redundantly prevent premature progression of secondary growth in the *Arabidopsis hypocotyl*" (DOI: 10.1111/nph.14335)
- (8) Takashi Kanadome, Hideki Shibata, Keiko Kuwata, Terunao Takahara and Masatoshi Maki, *FEBS J.* 2017, 284, 56–76. "The calcium-binding protein ALG-2 promotes endoplasmic reticulum exit site localization and polymerization of Trk-fused gene (TFG) protein" (DOI: 10.1111/febs.13949)
- (9) Eduard Carbonell-Sanroma, Pedro Brandimarte, Richard Balog, Martina Corso, Shigeki Kawai, Aran Garcia-Lekue, Shohei Saito, Shigehiro Yamaguchi, Ernst Meyer, Daniel Sánchez-Portal, and Jose Ignacio Pascual, *Nano Lett.* 2017, 17, 50–56. "Quantum Dots Embedded in Graphene Nanoribbons by Chemical Substitution" (DOI: 10.1021/acs.nanolett.6b03148)
- (10) Jiao Jiao, Akane G. Mizukami, Subramanian Sankaranarayanan, Junichiro Yamaguchi, Kenichiro Itami, Tetsuya Higashiyama, *Plant Physiol.* 2017, 173, 354–363. "Structure-Activity Relation of AMOR Sugar Molecule that Activates Pollen-Tubes for Ovular Guidance" (DOI: 10.1104/pp.16.01655)
- (11) Masahiro Yamanaka, Ken Sakata, Ken Yoshioka, Daisuke Uraguchi, and Takashi Ooi, *J. Org. Chem.* 2017, 82, 541–548. "Origin of High Regio-, Diastereo-, and Enantioselectivities in 1,6-Addition of Azlactones to Dienyl N-Acylpyrroles: A Computational Study" (DOI: 10.1021/acs.joc.6b02572)
- (12) Valentin M. Hertz, Naoki Ando, Masato Hirai, Michael Bolte, Hans-Wolfram Lerner, Shigehiro Yamaguchi, and Matthias Wagner, *Organometallics* 2017, 36, 2512–2519. "Steric Shielding vs Structural Constraint in a Boron-Containing Polycyclic Aromatic Hydrocarbon" (DOI: 10.1021/acs.organomet.6b00800)
- (13) Kakishi Uno, Taeko Sasaki, Nagisa Sugimoto, Hideto Ito, Taishi Nishihara, Shinya Hagihara, Tetsuya Higashiyama, Narie Sasaki, Yoshikatsu Sato, and Kenichiro Itami, *Chem. Asian J.* 2017, 12, 233–238. "Key Structural Elements of Unsymmetrical Cyanine Dyes for Highly Sensitive Fluorescence Turn-On DNA Probes" (DOI: 10.1002/asia.201601430)
- (14) Masakazu Nambo, Eric C. Keske, Jason P. G. Rygus, Jacky C.-H. Yim, and Cathleen M. Crudden, *ACS Catal.* 2017, 7, 1108–1112. "Development of Versatile Sulfone Electrophiles for Suzuki–Miyaura Cross-Coupling Reactions" (DOI: 10.1021/acscatal.6b03434)
- (15) Kyohei Ozaki, Keiichiro Murai, Wataru Matsuoka, Katsuaki Kawasumi, Hideto Ito and Kenichiro Itami, *Angew. Chem. Int. Ed.* 2017, 56, 1361–1364. "One-Step Annulative  $\pi$ -Extension of Alkynes with Dibenzosiloles or Dibenzogermoles by Palladium/o-chloranil Catalysis" (DOI: 10.1002/anie.201610374)
- (16) Hiroya Oshima, Aiko Fukazawa and Shigehiro Yamaguchi, *Angew. Chem. Int. Ed.* 2017, 56, 3270–3274. "Facile Synthesis of Polycyclic Pentalenes with Enhanced Hückel Antiaromaticity" (DOI: 10.1002/anie.201611344)
- (17) Ying Wang, Menggai Jiao, Zhijian Wu, and Stephan Irle, *J. Phys. Chem. C* 2017, 121, 2276–2284. "Theoretical Studies on Ethanol Dissociation on Iron Nanoparticles in the Early Stage of SWCNT Growth" (DOI: 10.1021/acs.jpcc.6b12207)

- (18) Chen Li, Yusuke Sako, Akihiro Imai, Tomoaki Nishiyama, Kari Thompson, Minoru Kubo, Yuji Hiwatashi, Yukiko Kabeya, Dale Karlson, Shu-Hsing Wu, Masaki Ishikawa, Takashi Murata, Philip N. Benfey, Yoshikatsu Sato, Yosuke Tamada, and Mitsuyasu Hasebe, *Nat. Commun.* 2017, 8, 14242. "A Lin28 homologue reprograms differentiated cells to stem cells in the moss *Physcomitrella patens*". (DOI: 10.1038/ncomms14242)
- (19) Masayasu Taki, Saki Azeyanagi, Kenzo Hayashi and Shigehiro Yamaguchi, *J. Mater. Chem. C* 2017, 5, 2142–2148. "Color-tunable fluorescent nanoparticles encapsulating trialkylsilyl-substituted pyrene liquids" (DOI: 10.1039/c6tc05208h)
- (20) Hirotaka Kitoh-Nishioka, Daisuke Yokogawa, and Stephan Irle, *J. Phys. Chem. C* 2017, 121, 4220–4238. "Förster Resonance Energy Transfer between Fluorescent Proteins: Efficient Transition Charge-Based Study" (DOI: 10.1021/acs.jpcc.7b00833)
- (21) Dmitry Mazunin and Jeffrey W. Bode, *Helv. Chim. Acta* 2017, 100, e1600311. "Potassium Acyltrifluoroborate (KAT) Ligations are Orthogonal to Thiol-Michael and SPAAC Reactions: Covalent Dual Immobilization of Proteins onto Synthetic PEG Hydrogels" (DOI: 10.1002/hlca.201600311)
- (22) Yuki Hirakawa, Hidefumi Shinohara, Kai Welke, Stephan Irle, Yoshikatsu Matsubayashi, Keiko U. Torii & Naoyuki Uchida, *Nature Commun.* 2017, 8, 14318. "Cryptic bioactivity capacitated by synthetic hybrid plant peptides" (DOI: 10.1038/ncomms14318)
- (23) Tetsushi Yoshidomi, Tomohiro Fukushima, Kenichiro Itami, and Yasutomo Segawa, *Chem. Lett.* 2017, 46, 587–590. "Synthesis, Structure, and Electrochemical Property of a Bimetallic Bis-2-pyridylidene" (DOI: 10.1246/cl.170091)
- (24) Yaowarat Surakhot, Viktor Laszlo, Chirawat Chitpakdee, Vinich Promarak, Taweesak Sudyoadsuk, Nawee Kungwan, Tim Kowalczyk, Stephan Irle, and Siriporn Jungsuttiwong, *J. Comput. Chem.* 2017, 38, 901–909. "Theoretical Rationalization for Reduced Charge Recombination in Bulky Carbazole-Based Sensitizers in Solar Cells" (DOI: 10.1002/jcc.24751)
- (25) Kayo Suda and Daisuke Yokogawa, *J. Phys. Chem. B* 2017, 121, 2164–2170. "Theoretical Study on Nonradiative Decay of Dimethylaminobenzonitrile through Triplet State in Gas-Phase, Nonpolar, and Polar Solutions" (DOI: 10.1021/acs.jpcc.6b11654)
- (26) Ryosuke Takise, Ryota Isshiki, Kei Muto, Kenichiro Itami, and Junichiro Yamaguchi, *J. Am. Chem. Soc.* 2017, 139, 3340–3343. "Decarbonylative Diaryl Ether Synthesis by Pd and Ni Catalysis" (DOI: 10.1021/jacs.7b00049). *Highly Cited Paper*.
- (27) Piyali Bhanja, Kousik Bhunia, Sabuj K. Das, Debabrata Pradhan, Ryuto Kimura, Yuh Hijikata, Stephan Irle and Asim Bhaumik, *ChemSusChem* 2017, 10, 921–929. "A new triazine based covalent organic framework for high-performance capacitive energy storage" (DOI: 10.1002/cssc.201601571)
- (28) Ryo Ohtani, Yuu Kitamura, Yuh Hijikata, Masaaki Nakamura, Leonard F. Lindoy and Shinya Hayami, *Dalton Trans.* 2017, 46, 3749–3754. "Flexible coordination sphere of a penta-coordinate complex: a correlation between conformation and redox potentials in the solid state" (DOI: 10.1039/C7DT00233E)
- (29) Kohsuke Ohmatsu, Yuichiro Ando, Takashi Ooi, *Synlett* 2017, 28, 1291–1294. "In Situ Electrophilic Activation of Hydrogen Peroxide for Catalytic Asymmetric  $\alpha$ -Hydroxylation of 3-Substituted Oxindoles" (DOI: 10.1055/s-0036-1558958)
- (30) Eri Ito, Tomohiro Fukushima, Takahiro Kawakami, Kei Murakami, and Kenichiro Itami, *Chem* 2017, 2, 383–392. "Catalytic Dehydrogenative C–H Imidation of Arenes Enabled by Photo-generated Hole Donation to Sulfonimide" (DOI: 10.1016/j.chempr.2017.02.006)
- (31) Xingyun Qi, Soon-Ki Han, Jonathan H. Dang, Jacqueline M. Garrick, Masaki Ito, Alex K. Hofstetter, Keiko U. Torii, *eLife* 2017, 6, e24102. "Autocrine regulation of stomatal differentiation potential by EPF1 and

ERECTA-LIKE1 ligand-receptor signaling" (DOI: 10.7554/eLife.24102)

- (32) Ryuji Kawano, Nao Horike, Yuh Hijikata, Mio Kondo, Arnau Carne-Sanchez, Patrick Larpent, Shuya Ikemura, Toshihisa Osaki, Koki Kamiya, Susumu Kitagawa, Shoji Takeuchi, and Shuhei Furukawa, *Chem* 2017, 2, 393–403. "Metal-organic cuboctahedra for synthetic ion channels with multiple conductance states" (DOI: 10.1016/j.chempr.2017.02.002)
- (33) Hiroki Iida, Kenji Ohmura, Ryuta Noda, Soichiro Iwahana, Hiroshi Katagiri, Naoki Ousaka, Taku Hayashi, Yuh Hijikata, Stephan Irle, and Eiji Yashima, *Chem. Asian J.* 2017, 12, 927–935. "Double-stranded helical oligomers covalently-bridged by rotary cyclic boronate esters" (DOI: 10.1002/asia.201700162)
- (34) Hiroki Kondo, Kenichiro Itami, and Junichiro Yamaguchi, *Chem. Sci.* 2017, 8, 3799–3803. "Rh-catalyzed regiodivergent hydrosilylation of acyl aminocyclopropanes controlled by monophosphine ligands" (DOI: 10.1039/c7sc00071e)
- (35) Daisuke Uruguchi, Masahiro Torii, and Takashi Ooi, *ACS Catal.* 2017, 7, 2765–2769. "Acridinium Betaine as a Single-Electron-Transfer Catalyst: Design and Application to Dimerization of Oxindoles" (DOI: 10.1021/acscatal.7b00265)
- (36) Daisuke Uruguchi, Masahiro Torii, Kohsuke Kato, and Takashi Ooi, *Heterocycles* 2017, 94, 441–447. "Stereoselective Aza-Henry Reaction of 3-Nitro-dihydro-2(1H)-quinolones with N-Boc-Aldimines under the Catalysis of Chiral Ammonium Betaines" (DOI: 10.3987/COM-16-13642)
- (37) Tomohiro Fukushima, Hirotohi Sakamoto, Kohei Tanaka, Yuh Hijikata, Stephan Irle, and Kenichiro Itami, *Chem. Lett.* 2017, 46, 855–857. "Polymorphism of [6]Cycloparaphenylene for Packing Structure-dependent Host-Guest Interaction" (DOI: 10.1246/cl.170210)
- (38) Daisuke Uruguchi, Ken Yoshioka & Takashi Ooi, *Nat. Commun.* 2017, 8, 14793. "Complete diastereodivergence in asymmetric 1,6-addition reactions enabled by minimal modification of a chiral catalyst" (DOI: 10.1038/ncomms14793)
- (39) Li Xia Zhao, Yuh Hijikata, Stephan Irle, *Int. J. Quantum Chem.* 2017, 117, e25371. "Structural influence of transition metal (Sc, Y, and Lu) atoms inside gold nanoparticles" (DOI: 10.1002/qua.25371)
- (40) Florian Rohrbachera, André Zwicky and Jeffrey W. Bode, *Chem. Sci.* 2017, 8, 4051–4055. "Chemical Synthesis of a Homoserine-Mutant of the Antibacterial, Head-to-Tail Cyclized Protein AS-48 by  $\alpha$ -Ketoacid–Hydroxylamine (KAHA) Ligation" (DOI: 10.1039/C7SC00789B)
- (41) Mina Ohtsu, Yoshikatsu Sato, Daisuke Kurihara, Takuya Suzaki, Masayoshi Kawaguchi, Daisuke Maruyama, Tetsuya Higashiyama, *Protoplasma* 2017, 254, 2107–2115. "Spatiotemporal deep imaging of syncytium induced by the soybean cyst nematode *Heterodera glycines*" (DOI: 10.1007/s00709-017-1105-0)
- (42) Kyohei Ozaki, Wataru Matsuoka, Hideto Ito, and Kenichiro Itami, *Org. Lett.* 2017, 19, 1930–1933. "Annulative  $\pi$ -Extension (APEX) of Heteroarenes with Dibenzosiloles and Dibenzogermoles by Palladium/*o*-Chloranil Catalysis" (DOI: 10.1021/acs.orglett.7b00684)
- (43) Maki Hayashi, Shin-ichiro Inoue, Yoshihisa Ueno & Toshinori Kinoshita, *Sci. Rep.* 2017, 7, 45586. "A Raf-like protein kinase BHP mediates blue light-dependent stomatal opening" (DOI: 10.1038/srep45586)
- (44) Osamu Miyashita, Chigusa Kobayashi, Takaharu Mori, Yuji Sugita, and Florence Tama, *J. Comput. Chem.* 2017, 38, 1447-1461. "Flexible Fitting to Cryo-EM Density Map Using Ensemble Molecular Dynamics Simulations" (DOI: 10.1002/jcc.24785)
- (45) Takashi Asako, Wakana Hayashi, Kazuma Amaike, Shin Suzuki, Kenichiro Itami, Kei Muto, Junichiro Yamaguchi, *Tetrahedron* 2017, 73, 3669–3676. "Synthesis of multiply arylated pyridines" (DOI: 10.1016/j.tet.2017.03.095)



- (46) Ayako Nakamura, Naoya Tochio, Shozo Fujioka, Shinsaku Ito, Takanori Kigawa, Yukihisa Shimada, Makoto Matsuoka, Shigeo Yoshida, Toshinori Kinoshita, Tadao Asami, Hideharu Seto, Takeshi Nakano, PLoS ONE 2017, 12, e0174015. "Molecular actions of two synthetic brassinosteroids, iso-carbaBL and 6-deoxoBL, which cause altered physiological activities between Arabidopsis and rice" (DOI: 10.1371/journal.pone.0174015)
- (47) Daisuke Uruguchi, Takaki Ito, Yuto Kimura, Yumiko Nobori, Makoto Sato, and Takashi Ooi, Bull. Chem. Soc. Jpn. 2017, 90, 546 – 555. "[5.5]-P-Spirocyclic Chiral Triaminoiminophosphorane-Catalyzed Asymmetric Hydrophosphonylation of Aldehydes and Ynones" (DOI: 10.1246/bcsj.20170040)
- (48) Yoshifumi Nishimura, Takao Tsuneda, Takeshi Sato, Michio Katouda, and Stephan Irle, J. Phys. Chem. C 2017, 121, 8999–9010. "Quantum Chemical Estimation of Acetone Physisorption on Graphene Using Combined Basis Set and Size Extrapolation Schemes" (DOI: 10.1021/acs.jpcc.6b13002)
- (49) Ying Wang, Hujun Qian, Zhijian Wu, and Stephan Irle, J. Phys. Chem. C 2017, 121, 8480–8489. "QM/MD Simulations on Graphene Hydrogenation/Deuteration: CxH/D Formation Mechanism and Isotope Effect" (DOI: 10.1021/acs.jpcc.7b01662)
- (50) Yoshio Nishimoto, Hiroki Kondo, Kazuya Yamaguchi, Daisuke Yokogawa, Junichiro Yamaguchi, Kenichiro Itami, and Stephan Irle, J. Org. Chem. 2017, 82, 4900–4906. "Theoretical Elucidation of Potential Enantioselectivity in a Pd-Catalyzed Aromatic C–H Coupling Reaction" (DOI: 10.1021/acs.joc.6b02675)
- (51) Raúl A. Adler, Chenguang Wang, Aiko Fukazawa, and Shigehiro Yamaguchi, Inorg. Chem. 2017, 56, 8718–8725. "Tuning the Photophysical Properties of Photostable Benzo[b]phosphole P-Oxide-Based Fluorophores" (DOI: 10.1021/acs.inorgchem.7b00658)
- (52) Shin-ichiro Inoue, Nozomi Iwashita, Yohei Takahashi, Eiji Gotoh, Eiji Okuma, Maki Hayashi, Ryohei Tabata, Atsushi Takemiya, Yoshiyuki Murata, Michio Doi, Toshinori Kinoshita, Ken-ichiro Shimazaki, Plant Cell Physiol. 2017, 58, 1048–1058. "Brassinosteroid Involvement in Arabidopsis thaliana Stomatal Opening" (DOI: 10.1093/pcp/pcx049)
- (53) Minako Ueda, Ernst Aichinger, Wen Gong, Edwin Groot, Inge Verstraeten, Lam Dai Vu, Ive De Smet, Tetsuya Higashiyama, Masaaki Umeda, and Thomas Laux, Genes & Dev. 2017, 31,617–627. "Transcriptional integration of paternal and maternal factors in the Arabidopsis zygote" (DOI: 10.1101/gad.292409.116)
- (54) Kirsi Salorinne, Renee W. Y. Man, Chien-Hung Li, Masayasu Taki, Masakazu Nambo and Cathleen M. Crudden, Angew. Chem. Int. Ed. 2017, 56, 6198–6202. "Water-Soluble N-Heterocyclic Carbene-Protected Gold Nanoparticles: Size-Controlled Synthesis, Stability, and Optical Properties" (DOI: 10.1002/anie.201701605)
- (55) Guillaume Povie, Yasutomo Segawa, Taishi Nishihara, Yuhei Miyauchi, Kenichiro Itami, Science 2017, 356, 172–175. "Synthesis of a carbon nanobelt" (DOI: 10.1126/science.aam8158). *Highly Cited Paper*.
- (56) Ken Yoshioka, Kohei Yamada, Daisuke Uruguchi and Takashi Ooi, Chem. Commun. 2017, 53, 5495–5498. "Unique site-selectivity control in asymmetric Michael addition of azlactone to alkenyl dienyl ketones enabled by P-spiro chiral iminophosphorane catalysis" (DOI: 10.1039/C7CC01715D)
- (57) Fei Wang, Shinpei Kusaka, Yuh Hijikata, Nobuhiko Hosono, and Susumu Kitagawa, ACS Appl. Mater. Interfaces 2017, 9, 33455–33460. "Development of a Porous Coordination Polymer with a High Gas Capacity Using a Thiophene-Based Bent Tetracarboxylate Ligand" (DOI: 10.1021/acsami.7b01568)
- (58) Daisuke Yokogawa and Arifin, Bull. Chem. Soc. Jpn. 2017, 90, 831–837. "Electrostatic Potential Charge including Spatial Electron Density Distribution (SEDD): Application to Biosystems" (DOI: 10.1246/bcsj.20170099)

- (59) Xin'AI Zhao, Jonathan Bramsiepe, Matthias Van Durme, Shinichiro Komaki, Maria Ada Prusicki, Daisuke Maruyama, Joachim Forner, Anna Medzihradzsky, Erik Wijnker, Hirofumi Harashima, You Lu, Anja Schmidt, Daniela Guthörl, Rosa Sahún Logroño, Yonsheng Guan, Gaetan Pochon, Ueli Grossniklaus, Thomas Laux, Tetsuya Higashiyama, Jan U. Lohmann, Moritz K. Nowack, Arp Schnittger, *Science* 2017, 356, 396–403. "RETINOBLASTOMA RELATED1 mediates germline entry in Arabidopsis" (DOI: 10.1126/science.aaf6532)
- (60) Yota Sakakibara, Eri Ito, Takahiro Kawakami, Shuya Yamada, Kei Murakami, and Kenichiro Itami, *Chem. Lett.* 2017, 46, 1014–1016. "Direct Coupling of Naphthalene and Sulfonimides Promoted by DDQ and Blue Light" (DOI: 10.1246/cl.170321)
- (61) Naoki Yanagisawa, Nagisa Sugimoto, Hideyuki Arata, Tetsuya Higashiyama & Yoshikatsu Sato, *Sci. Rep.* 2017, 7, 1403. "Capability of tip-growing plant cells to penetrate into extremely narrow gaps" (DOI: 10.1038/s41598-017-01610-w)
- (62) Takashi Yamada, Eri Tahara, Mai Kanke, Keiko Kuwata & Tomoko Nishiyama, *EMBO J.* 2017, 36, 1513–1527. "Drosophila Dalmatian combines sororin and shugoshin roles in establishment and protection of cohesion" (DOI: 10.15252/embj.201695607)
- (63) Kengo Asai, Aiko Fukazawa and Shigehiro Yamaguchi, *Angew. Chem. Int. Ed.* 2017, 56, 6848–6852. "A Near-Infrared Dye that Undergoes Multiple Interconversions through Acid–Base Equilibrium and Reversible Redox Processes" (DOI: 10.1002/anie.201702140)
- (64) Takao Fujikawa, Nobuhiko Mitoma, Atsushi Wakamiya, Akinori Saeki, Yasutomo Segawa and Kenichiro Itami, *Org. Biomol. Chem.* 2017, 15, 4697–4703. "Synthesis, properties, and crystal structures of *n*-extended double [6]helicenes: contorted multi-dimensional stacking lattice" (DOI: 10.1039/c7ob00987a)
- (65) Yoshikatsu Sato, Nagisa Sugimoto, Tadayoshi Hirai, Akihiro Imai, Minoru Kubo, Yuji Hiwatashi, Tomoaki Nishiyama & Mitsuyasu Hasebe, *Sci. Rep.* 2017, 7, 1909. "Cells reprogramming to stem cells inhibit the reprogramming of adjacent cells in the moss *Physcomitrella patens*" (DOI: 10.1038/s41598-017-01786-1)
- (66) Shiho Sairenji, Takashi Kikuchi, Mohamed Ahmed Abozeid, Shinobu Takizawa, Hiroaki Sasai, Yuichiro Ando, Kohsuke Ohmatsu, Takashi Ooi and Makoto Fujita, *Chem. Sci.* 2017, 8, 5132–5136. "Determination of the absolute configuration of compounds bearing chiral quaternary carbon centers using the crystalline sponge method" (DOI: 10.1039/C7SC01524K)
- (67) Ryo Takano, Ryo Shintani, Aiko Fukazawa, Shigehiro Yamaguchi, Koji Nakabayashi, Shin-ichi Ohkoshi, and Kyoko Nozaki, *Organometallics* 2017, 36, 2646–2653. "Structures and Physical Properties of Chemically Reduced Diindenolones and Their *n*-Extended Derivatives" (DOI: 10.1021/acs.organomet.7b00260)
- (68) Naoya Tanaka, Ryosuke Tsutsumi, Daisuke Uruguchi and Takashi Ooi *Chem. Commun.* 2017, 53, 6999–7002. "N-Sulfonyl  $\alpha$ -imino ester-derived chiral oxaziridines: catalytic asymmetric synthesis and application as a modular chiral organic oxidant" (DOI: 10.1039/C7CC02502E)
- (69) Ryota Kotani, Hikaru Sotome, Hajime Okajima, Soichi Yokoyama, Yumi Nakaike, Akihiro Kashiwagi, Chigusa Mori, Yuki Nakada, Shigehiro Yamaguchi, Atsuhiko Osuka, Akira Sakamoto, Hiroshi Miyasaka and Shohei Saito, *J. Mater. Chem. C* 2017, 5, 5248–5256. "Flapping Viscosity Probe That Shows Polarity-Independent Ratiometric Fluorescence" (DOI: 10.1039/C7TC01533J)
- (70) Toru Sugiyama, Genki Hasegawa, Chie Niikura, Keiko Kuwata, Yasutada Imamura, Yosuke Demizu, Masaaki Kurihara, Atsushi Kittaka, *Bioorg. Med. Chem. Lett.* 2017, 27, 3337–3341. "PNA monomers fully compatible with standard Fmoc-based solid-phase synthesis of pseudocomplementary PNA" (DOI: 10.1016/j.bmcl.2017.06.015)
- (71) Ying Wang, Wei Song, Menggai Jiao, Zhijian Wu, Stephan Irle, *Carbon* 2017, 121, 292–300.

- "Importance of oxygen in single-walled carbon nanotube growth: Insights from QM/MD simulations" (DOI: 10.1016/j.carbon.2017.06.005)
- (72) Shin-ichiro Inoue and Toshinori Kinoshita, *Plant Physiol.* 2017, 173, 531–538. "Blue Light Regulation of Stomatal Opening and the Plasma Membrane H<sup>+</sup>-ATPase" (DOI: 10.1104/pp.17.00166). *Highly Cited Paper.*
- (73) Chandra Bhushan Tripathi, Tsuyoshi Ohtani, Michael T. Corbett and Takashi Ooi, *Chem. Sci.* 2017, 8, 5622–5627. "Photoredox ketone catalysis for the direct C–H imidation and acyloxylation of arenes" (DOI: 10.1039/C7SC01700F)
- (74) Noriaki Ozaki, Hirotohi Sakamoto, Taishi Nishihara, Toshihiko Fujimori, Yuh Hijikata, Ryuto Kimura, Stephan Irle and Kenichiro Itami, *Angew. Chem. Int. Ed.* 2017, 56, 11196–11202. "Electro-Activated Conductivity and White Light Emission of a Hydrocarbon N<sup>+</sup>-anion-Iodine Assembly" (DOI: 10.1002/anie.201703648)
- (75) A. S. Hutama, Y. Hijikata, and S. Irle, *J. Phys. Chem. C* 2017, 121, 14888–14898. "Coupled Cluster and Density Functional Studies of Atomic Fluorine Chemisorption on Coronene as Model Systems for Graphene Fluorination" (DOI: 10.1021/acs.jpcc.7b03627)
- (76) Sudipta K. Kundu, Ramana Singuru, Taku Hayashi, Yuh Hijikata, Stephan Irle and John Mondal, *ChemistrySelect* 2017, 2, 4705–4716. "Constructing Sulfonic Acid Functionalized Anthracene Derived Conjugated Porous Organic Polymer for Efficient Metal-Free Catalytic Acetalization of Bio-Glycerol" (DOI: 10.1002/slct.201700901)
- (77) Miki Nakano, Osamu Miyashita, Slavica Jonic, Changyong Song, Daewoong Nam, Yasumasa Joti and Florence Tama, *J. Synchrot. Radiat.* 2017, 24. "Three-dimensional reconstruction for coherent diffraction patterns obtained by XFEL" (DOI: 10.1107/S1600577517007767)
- (78) Artur K. Kokornaczyk, Dirk Schepmann, Junichiro Yamaguchi, Kenichiro Itami, Erik Laurini, Maurizio Fermeglia, Sabrina Pricl, and Bernhard Wünsch, *ChemMedChem* 2017, 12, 1070–1080. "Thiazole-Based  $\sigma_1$  Receptor Ligands: Diversity by Late-Stage C–H Arylation of Thiazoles, Structure–Affinity and Selectivity Relationships, and Molecular Interactions" (DOI: 10.1002/cmdc.201700166)
- (79) Huapeng Liu, Xiao Cheng, Houyu Zhang, Yue Wang, Hongyu Zhang and Shigehiro Yamaguchi, *Chem. Commun.* 2017, 53, 7832–7835. "ESIPT-active organic compounds with white luminescence based on crystallization-induced keto emission (CIKE)" (DOI: 10.1039/c7cc03758a)
- (80) Jan Petersen, Shin-ichiro Inoue, Sharon M. Kelly, Stuart Sullivan, Toshinori Kinoshita, and John M. Christie, *J. Biol. Chem.* 2017, 292, 13843–13852. "Functional characterization of a constitutively active kinase variant of Arabidopsis phototropin 1" (DOI: 10.1074/jbc.M117.799643)
- (81) Jacky C.-H. Yim, Masakazu Nambo, and Cathleen M. Crudden, *Org. Lett.* 2017, 19, 3715–3718. "Pd-Catalyzed Desulfonative Cross-Coupling of Benzylic Sulfone Derivatives with 1,3-Oxazole" (DOI: 10.1021/acs.orglett.7b01510)
- (82) Takao Fujikawa, Yasutomo Segawa, and Kenichiro Itami, *J. Org. Chem.* 2017, 82, 7745–7749. "Laterally  $\pi$ -Extended Dithia[6]helicenes with Heptagons: Saddle-Helix Hybrid Molecules" (DOI: 10.1021/acs.joc.7b01540)
- (83) Aiko Fukazawa, Junichi Usuba, Raúl A. Adler and Shigehiro Yamaguchi, *Chem. Commun.* 2017, 53, 8565–8568. "Synthesis of seminaphtho-phospha-fluorescein dyes based on the consecutive arylation of aryldichlorophosphines" (DOI: 10.1039/c7cc04323f)
- (84) Hirotaka Kitoh-Nishioka, Kai Welke, Yoshio Nishimoto, Dmitri G. Fedorov, and Stephan Irle, *J. Phys. Chem. C* 2017, 121, 17712–17726. "Multiscale Simulations on Charge Transport in Covalent Organic Frameworks Including Dynamics of Transfer Integrals from the FMOFTB/LCMO Approach" (DOI: 10.1021/acs.jpcc.7b05779)

- (85) F. Javier Domínguez-Gutiérrez, Felipe Bedoya, Predrag S. Krstić, Jean P. Allain, Stephan Irle, Charles H. Skinner, Robert Kaita and Bruce Koel, *Nucl. Fusion* 2017, 57 086050. "Unraveling the plasma-material interface with real time diagnosis of dynamic boron conditioning in extreme tokamak plasmas" (DOI: 10.1088/1741-4326/aa7b17)
- (86) Chenguang Wang, Masayasu Taki, Yoshikatsu Sato, Aiko Fukazawa, Tetsuya Higashiyama, and Shigehiro Yamaguchi, *J. Am. Chem. Soc.* 2017, 139, 10374 – 10381. "Super-Photostable Phosphole-Based Dye for Multiple-Acquisition Stimulated Emission Depletion Imaging" (DOI: 10.1021/jacs.7b04418)
- (87) Rika Ochi, Shin-ichiro Noro, Yuh Hijikata, Kazuya Kubo, and Takayoshi Nakamura, *Eur. J. Inorg. Chem.* 2017, 4013–4019. "Structural Diversification of Light-Metal Coordination Polymers Using 4-(Methylsulfonyl)benzoate with a Charge-Polarized Neutral Methylsulfonyl Coordination Moiety" (DOI: 10.1002/ejic.201700627)
- (88) Wataru Matsuoka, Hideto Ito and Kenichiro Itami, *Angew. Chem. Int. Ed.* 2017, 56, 12224–12228. "Rapid Access to Nanographenes and Fused Heteroaromatics by Palladium-Catalyzed Annulative  $\pi$ -Extension Reaction of Unfunctionalized Aromatics with Diiodobiaryls" (DOI: 10.1002/anie.201707486)
- (89) Asraa Ziadi, Naoyuki Uchida, Hiroe Kato, Rina Hisamatsu, Ayato Sato, Shinya Hagihara, Kenichiro Itami and Keiko U. Torii, *Chem. Commun.* 2017, 53, 9632–9635. "Discovery of synthetic small molecules that enhance the number of stomata: C–H functionalization chemistry for plant biology" (DOI: 10.1039/c7cc04526c)
- (90) Thibault J Harmand, Vijaya R Pattabiraman and Jeffrey W. Bode, *Angew. Chem. Int. Ed.* 2017, 56, 12639–12643. "Chemical Synthesis of the Highly Hydrophobic Antiviral Membrane Associated Protein IFITM3 and Modified Variants" (DOI: 10.1002/anie.201707554)
- (91) Yuko Shishido, Fumiaki Tomoike, Yasuaki Kimura, Keiko Kuwata, Takato Yano, Kenji Fukui, Haruka Fujikawa, Yoshitaka Sekido, Yuko Murakami-Tonami, Tomoshi Kameda, Satoshi Shuto and Hiroshi Abe, *Chem. Commun.* 2017, 53, 11138–11141. "A covalent G-site inhibitor for glutathione S-transferase Pi (GSTP1-1)" (DOI: 10.1039/c7cc05829b)
- (92) Mari Shibata, Hideto Ito, and Kenichiro Itami, *Chem. Lett.* 2017, 46, 1701–1704. "Oxidative Homocoupling Reaction of Aryltrimethylsilanes by Pd/o-chloranil Catalysis" (DOI: 10.1246/cl.170723)
- (93) Tsuyoshi Shimmura, Tomoya Nakayama, Ai Shinomiya, Shoji Fukamachi, Masaki Yasugi, Eiji Watanabe, Takayuki Shimo, Takumi Senga, Toshiya Nishimura, Minoru Tanaka, Yasuhiro Kamei, Kiyoshi Naruse & Takashi Yoshimura, *Nature Commun.* 2017, 8, 412. "Dynamic plasticity in phototransduction regulates seasonal changes in color perception" (DOI: 10.1038/s41467-017-00432-8)
- (94) Mina Ohtsu, Daisuke Kurihara, Yoshikatsu Sato, Takuya Suzuki, Masayoshi Kawaguchi, Daisuke Maruyama, Tetsuya Higashiyama, *Cytologia* 2017, 82, 251–259. "Fluorescent labeling of the cyst nematode *Heterodera glycines* in deep-tissue live imaging" (DOI: 10.1508/cytologia.82.251)
- (95) Daisuke Kurihara, Yusuke Kimata, Tetsuya Higashiyama, Minako Ueda, *J. Vis. Exp.* 2017, 127, e55975. "In Vitro Ovule Cultivation for Live-cell Imaging of Zygote Polarization and Embryo Patterning in *Arabidopsis thaliana*" (DOI: 10.3791/55975)
- (96) Taeko Sasaki, Yoshikatsu Sato, Tetsuya Higashiyama & Narie Sasaki, *Sci. Rep.* 2017, 7, 11257. "Live imaging reveals the dynamics and regulation of mitochondrial nucleoids during the cell cycle in Fucci2-HeLa cells" (DOI: 10.1038/s41598-017-10843-8)
- (97) Takafumi Araki, Masato Hirai, Atsushi Wakamiya, Warren E. Piers, and Shigehiro Yamaguchi, *Chem. Lett.* 2017, 46, 1714–1717. "Antiaromatic Dithieno-1,2-dihydro-1,2-diborin Splits Diatomic Hydrogen" (DOI: 10.1246/cl.170812)

- (98) Marek Grzybowski, Masayasu Taki, and Shigehiro Yamaguchi, *Chem. Eur. J.* 2017, 23, 13028–13032 "Selective Conversion of P=O-Bridged Rhodamines into P=ORhodols: Solvatochromic Near-Infrared Fluorophores" (DOI: 10.1002/chem.201703456)
- (99) Naoki Ando, Aiko Fukazawa, Tomokatsu Kushida, Yoshihito Shiota, Shuhei Itoyama, Kazunari Yoshizawa, Yasunori Matsui, Yutaro Kuramoto, Hiroshi Ikeda, and Shigehiro Yamaguchi, *Angew. Chem. Int. Ed.* 2017, 56, 12210–12214. "Photochemical Intramolecular C-H Addition of Dimesityl-(hetero)arylboranes through a [1,6]-Sigmatropic Rearrangement" (DOI: 10.1002/anie.201706929)
- (100) Masakazu Nambo, Jacky C.-H. Yim, Kevin G. Fowler, Cathleen M. Crudden, *Synlett* 2017, 28, 2936–2940. "Synthesis of Tetraarylmethanes by the Triflic Acid-Promoted Formal Cross-Dehydrogenative Coupling of Triarylmethanes with Arenes" (DOI: 10.1055/s-0036-1588563)
- (101) Christian R. Larrea, Christopher J. Baddeley, Mina R. Narouz, Nicholas J. Mosey, J. Hugh Horton, and Cathleen M. Crudden, *ChemPhysChem* 2017, 18, 3536–3539. "N-Heterocyclic Carbene Self-assembled Monolayers on Copper and Gold: Dramatic Effect of Wingtip Groups on Binding, Orientation and Assembly" (DOI: 10.1002/cphc.201701045)
- (102) Shin Suzuki, Kenichiro Itami and Junichiro Yamaguchi, *Angew. Chem. Int. Ed.* 2017, 56, 15010–15013. "Synthesis of Octaaryl Naphthalenes and Anthracenes with Different Substituents" (DOI: 10.1002/anie.201709332)
- (103) Susanne Bähr, Hiroaki Ogasawara, Shigehiro Yamaguchi, and Martin Oestreich, *Organometallics* 2017, 36, 4013–4019. "An Expedient Procedure for the Synthesis of Benzo[4,5]silolo[2,3-b]thiophenes and Related Systems" (DOI: 10.1021/acs.organomet.7b00619)
- (104) Tomokatsu Kushida, Shusuke Shirai, Naoki Ando, Toshihiro Okamoto, Hiroyuki Ishii, Hiroyuki Matsui, Masakazu Yamagishi, Takafumi Uemura, Junto Tsurumi, Shun Watanabe, Jun Takeya, and Shigehiro Yamaguchi, *J. Am. Chem. Soc.* 2017, 139, 14336–14339. "Boron-Stabilized Planar Neutral  $\pi$ -Radicals with Well-Balanced Ambipolar Charge-Transport Properties" (DOI: 10.1021/jacs.7b05471)
- (105) John L. Bowman, Takayuki Kohchi, Katsuyuki T. Yamato, Jerry Jenkins, Shengqiang Shu, Kimitsune Ishizaki, Shohei Yamaoka, Ryuichi Nishihama, Yasukazu Nakamura, Frederic Berger, Catherine Adam, Shiori Sugamata Aki, Felix Althoff, Takashi Araki, Mario A. Arteaga-Vazquez, Sureshkumar Balasubramanian, Kerrie Barry, Diane Bauer, Christian R. Boehm, Liam Briginshaw, Juan Caballero-Perez, Bruno Catarino, Feng Chen, Shota Chiyoda, Mansi Chovatia, Kevin M. Davies, Mihails Delmans, Taku Demura, Tom Dierschke, Liam Dolan, Ana E. Dorantes-Acosta, D. Magnus Eklund, Stevie N. Florent, Eduardo Flores-Sandoval, Asao Fujiyama, Hideya Fukuzawa, Bence Galik, Daniel Grimanelli, Jane Grimwood, Ueli Grossniklaus, Takahiro Hamada, Jim Haseloff, Alexander J. Hetherington, Asuka Higo, Yuki Hirakawa, Hope N. Hundley, Yoko Ikeda, Keisuke Inoue, Shin-ichiro Inoue, Sakiko Ishida, Qidong Jia, Mitsuru Kakita, Takehiko Kanazawa, Yosuke Kawai, Tomokazu Kawashima, Megan Kennedy, Keita Kinose, Toshinori Kinoshita, Yuji Kohara, Eri Koide, Kenji Komatsu, Sarah Kopischke, Minoru Kubo, Junko Kyojuka, Ulf Lagercrantz, Shih-Shun Lin, Erika Lindquist, Anna M. Lipzen, Chia-Wei Lu, Efrain De Luna, Robert A. Martienssen, Naoki Minamino, Masaharu Mizutani, Miya Mizutani, Nobuyoshi Mochizuki, Isabel Monte, Rebecca Mosher, Hideki Nagasaki, Hirofumi Nakagami, Satoshi Naramoto, Kazuhiko Nishitani, Misato Ohtani, Takashi Okamoto, Masaki Okumura, Jeremy Phillips, Bernardo Pollak, Anke Reinders, Moritz Rovekamp, Ryosuke Sano, Shinichiro Sawa, Marc W. Schmid, Makoto Shirakawa, Roberto Solano, Alexander Spunde, Noriyuki Suetsugu, Sumio Sugano, Akifumi Sugiyama, Rui Sun, Yutaka Suzuki, Mizuki Takenaka, Daisuke Takezawa, Hirokazu Tomogane, Masayuki Tsuzuki, Takashi Ueda, Masaaki Umeda, John M. Ward, Yuichiro Watanabe, Kazufumi Yazaki, Ryusuke Yokoyama, Yoshihiro Yoshitake, Izumi Yotsui, Sabine Zachgo, and Jeremy Schmutz, *Cell* 2017, 171, 287–304. "Insights into Land Plant Evolution Garnered from the *Marchantia polymorpha* Genome" (DOI: 10.1016/j.cell.2017.09.030)
- (106) Yunsheng Ma, Yuki Harada, Akihiro Hori, Yuh Hijikata, Liangchun Li and Ryotaro Matsuda, *Dalton Trans.* 2017, 46, 15200–15203. "Tuning the flexibility of interpenetrated frameworks by a small difference in

the fluorene moiety" (DOI: 10.1039/c7dt03338a)

- (107) Ryota Isshiki, Ryosuke Takise, Kenichiro Itami, Kei Muto, Junichiro Yamaguchi, *Synlett* 2017, 28, 2599–2603. "Catalytic  $\alpha$ -Arylation of Ketones with Heteroaromatic Esters" (DOI: 10.1055/s-0036-1589120)
- (108) Kohsuke Ohmatsu, Yukino Furukawa, Mari Kiyokawa and Takashi Ooi, *Chem. Commun.* 2017, 53, 13113–13116. "Diastereo- and enantioselective phase-transfer alkylation of 3-substituted oxindoles with racemic secondary alkyl halides" (DOI: 10.1039/C7CC07122A)
- (109) Xiaoxiao Zhang, Weijia Liu, Takuya T. Nagae, Hidenori Takeuchi, Heqiao Zhang, Zhifu Han, Tetsuya Higashiyama & Jijie Chai, *Nature Commun.* 2017, 8, 1331. "Structural basis for receptor recognition of pollen tube attraction peptides" (DOI: 10.1038/s41467-017-01323-8)
- (110) Shintaro Inoue, Toshiki Moriya, Rihito Morita, Keiko Kuwata, Sanjog T. Thul, Bijaya K. Sarangi, Yoshiko Minami, *Plant Physiol. Biochem.* 2017, 121, 226–233. "Characterization of UDP-glucosyltransferase from *Indigofera tinctoria*" (DOI: 10.1016/j.plaphy.2017.11.002)
- (111) Zhijun Li, Kim Munro, Irakli I. Ebralize, Mina R. Narouz, J. Daniel Padmos, Hongxia Hao, Cathleen M. Crudden, and J. Hugh Horton, *Langmuir* 2017, 33, 13936–13944. "N- Heterocyclic Carbene Self-Assembled Monolayers on Gold as Surface Plasmon Resonance Biosensors" (DOI: 10.1021/acs.langmuir.7b03280)
- (112) Jason P. G. Rygus and Cathleen M. Crudden, *J. Am. Chem. Soc.* 2017, 139, 18124–18137. "Enantiospecific and Iterative Suzuki–Miyaura Cross-Couplings" (DOI: 10.1021/jacs.7b08326)
- (113) Mina R. Narouz, Chien-Hung Li, Ali Nazemi, and Cathleen M. Crudden, *Langmuir* 2017, 33, 14211–14219. "Amphiphilic N- Heterocyclic Carbene-Stabilized Gold Nanoparticles and Their Self-Assembly in Polar Solvents" (DOI: 10.1021/acs.langmuir.7b02248)
- (114) Nan Luo, An Yan, Gang Liu, Jingzhe Guo, Duoyan Rong, Masahiro M. Kanaoka, Zhen Xiao, Guanshui Xu, Tetsuya Higashiyama, Xinping Cui & Zhenbiao Yang, *Nature Commun.* 2017, 8, 1687. "Exocytosis-coordinated mechanisms for tip growth underlie pollen tube 1 growth guidance" (DOI: 10.1038/s41467-017-01452-0)
- (115) Takuya Ohzono, Kaoru Katoh, Chenguang Wang, Aiko Fukazawa, Shigehiro Yamaguchi & Jun-ichi Fukuda, *Sci. Rep.* 2017, 7, 16814. "Uncovering different states of topological defects in schlieren textures of a nematic liquid crystal" (DOI: 10.1038/s41598-017-16967-1)

## 2. Review Articles

- (1) Toshiaki Tameshige, Shuka Ikematsu, Keiko U. Torii and Naoyuki Uchida, *J. Exp. Bot.* 2017, 68, 45-53. "Stem development through vascular tissues: EPFL–ERECTA family signaling that bounces in and out of phloem" (DOI: 10.1093/jxb/erw447)
- (2) Mizuho Ichinose and Mamoru Sugita, *Genes* 2017, 8, 5. "RNA Editing and Its Molecular Mechanism in Plant Organelles" (DOI: 10.3390/genes8010005)
- (3) Tetsuya Higashiyama and Wei-cai Yang, *Plant Physiol.* 2017, 173, 112–121. "Gametophytic Pollen Tube Guidance: Attractant Peptides, Gametic Controls, and Receptors" (DOI: 10.1104/pp.16.01571). *Highly Cited Paper, Hot Paper.*
- (4) Shin Miyamura, Kenichiro Itami, Junichiro Yamaguchi, *Synthesis* 2017, 49, A–S. "Syntheses of Biologically Active 2-Arylcyclopropylamines" (DOI: 10.1055/s-0036-1588390)
- (5) Xian Qu, Kylee M. Peterson and Keiko U. Torii, *Curr. Opin. Genet. Dev.* 2017, 45, 1–9. "Stomatal development in time: the past and the future" (DOI: 10.1016/j.gde.2017.02.001)

- (6) Subramanian Sankaranarayanan, Muhammad Jamshed, Abhinandan Kumar, Logan Skori, Sabine Scandola, Tina Wang, David Spiegel and Marcus A. Samuel, *Int. J. Mol. Sci.* 2017, 18, 898. "Glyoxalase Goes Green: The Expanding Roles of Glyoxalase in Plants" (DOI: 10.3390/ijms18040898)
- (7) Kei Murakami, Shuya Yamada, Takeshi Kaneda, and Kenichiro Itami, *Chem. Rev.* 2017, 117, 9302–9332. "C–H Functionalization of Azines" (DOI: 10.1021/acs.chemrev.7b00021). *Highly Cited Paper*.
- (8) Yuki Hirakawa, Keiko U. Torii, Naoyuki Uchida, *Plant Cell Physiol.* 2017, 58, 1313–1318. "Mechanisms and Strategies Shaping Plant Peptide Hormones" (DOI: 10.1093/pcp/pcx069)
- (9) Hideto Ito, Kyohei Ozaki, and Kenichiro Itami, *Angew. Chem. Int. Ed.* 2017, 56, 11144–11164. "Annulative  $\pi$ -Extension (APEX): Rapid Access to Fused Arenes, Heteroarenes, and Nanographenes" (DOI: 10.1002/anie.201701058)
- (10) Keisuke Ikegami, Takashi Yoshimura, *Best Pract. Res. Clin. Endoc. Metab.* 2017, 31, 475–485. "The hypothalamic–pituitary–thyroid axis and biological rhythms: The discovery of TSH's unexpected role using animal models" (DOI: 10.1016/j.beem.2017.09.002)
- (11) Masahiko Yoshimura, Yuichiro Tsuchiya, Yoshikatsu Sato, Kenichiro Itami, Toshinori Kinoshita, Shinya Hagihara. *Plant Morphology* 2017, 29, 33–37. "Strigolactone receptors in *Striga hermonthica*"
3. Proceedings
4. Other English Articles
- (1) Junichiro Yamaguchi and Kenichiro Itami, *Bull. Chem. Soc. Jpn.* 2017, 90, 367–383. "Toward an Ideal Synthesis of (Bio)molecules through Direct Arene Assembling Reactions" (DOI: 10.1246/bcsj.20160365)
- (2) Shigehiro Yamaguchi, Aiko Fukazawa, and Masayasu Taki, *J. Synth. Org. Chem. Jpn.* 2017, 75, 1179–1187. "Phosphole P-Oxide-Containing  $\pi$ -Electron Materials: Synthesis and Applications in Fluorescence Imaging" (DOI: 10.5059/yukigoseikyokaishi.75.1179)
- (3) Michael R. Blatt, Tim J. Brodribb, Keiko U. Torii, *Plant Physiol.* 2017, 174, 467–469. "Small Pores with a Big Impact" (DOI: 10.1104/pp.17.00642)
- (4) P. Eisenberger and C. M. Crudden, *Dalton Trans.* 2017, 46, 4874–4887. "Borocation catalysis" (DOI: 10.1039/c6dt04232e)
- (5) Megumi Hatori, Claude Gronfier, Russell N. Van Gelder, Paul S. Bernstein, Josep Carreras, Satchidananda Panda, Frederick Marks, David Sliney, Charles E. Hunt, Tsuyoshi Hirota, Toshiharu Furukawa and Kazuo Tsubota, *NPJ Aging Mech. Dis.* 2017, 3, 9. "Global rise of potential health hazards caused by blue light-induced circadian disruption in modern aging societies" (DOI: 10.1038/s41514-017-0010-2)
- (6) Kei Murakami, Gregory J. P. Perry and Kenichiro Itami, *Org. Biomol. Chem.* 2017, 15, 6071–6075. "Aromatic C–H amination: a radical approach for adding new functions into biology- and materials-oriented aromatics" (DOI: 10.1039/c7ob00985b)
- (7) Tetsuya Higashiyama, *Science Robotics* 2017, 2, eaao1891. "Pollen tube navigation can inspire microrobot design" (DOI: 10.1126/scirobotics.aao1891)
- (8) Yin Wang and Toshinori Kinoshita, *Bio-protocol* 2017, 7, e2266. "Measurement of Stomatal Conductance in Rice" (DOI: 10.21769/BioProtoc.2226)
- (9) Toshiyuki Shimizu and Florence Tama, *Curr. Opin. Struct. Biol.* 2017, 43, 7–9. "Editorial overview: Macromolecular assemblies" (DOI: 10.1016/j.sbi.2017.04.009)

5. Articles written in other than English

- (1) Osamu Miyashita, Florence Tama, Seibutsu Butsuri 2017, 2, 90–94. "Hybrid Approach for Biological Structure Modeling: Cryo-electron Microscopy and X-ray Free Electron Laser Data" (DOI: 10.2142/biophys.57.090)

**B. WPI-related papers (Jan 1, 2017 – Dec 31, 2017)**1. Original Articles

- (1) Rico Gamuyao, Keisuke Nagai, Madoka Ayano, Yoshinao Mori, Anzu Minami, Mikiko Kojima, Takamasa Suzuki, Hitoshi Sakakibara, Tetsuya Higashiyama, Motoyuki Ashikari and Stefan Reuscher, *Plant Cell Physiol.* 2017, 58, 702–716. "Hormone Distribution and Transcriptome Profiles in Bamboo Shoots Provide Insights on Bamboo Stem Emergence and Growth" (DOI: 10.1093/pcp/pcx023)
- (2) Sunjoo Joo, Yoshiki Nishimura, Evan Cronmiller, Ran Ha Hong, Thamali Kariyawasam, Ming Hsiu Wang, Nai Chun Shao, Saif-El-Din El Akkad, Takamasa Suzuki, Tetsuya Higashiyama, Eonseon Jin, Jae-Hyeok Lee, *Plant Physiol.* 2017, 175, 314–332. "Gene Regulatory Networks for the Haploid-to-Diploid Transition of *Chlamydomonas reinhardtii*" (DOI: 10.1104/pp.17.00731)
- (3) Masaki Hada, Shohei Saito, Sei'ichi Tanaka, Ryuma Sato, Masahiko Yoshimura, Kazuhiro Mouri, Kyohei Matsuo, Shigehiro Yamaguchi, Mitsuo Hara, Yasuhiko Hayashi, Fynn Roehricht, Rainer Herges, Yasuteru Shigeta, Ken Onda, and R. J. Dwayne Miller, *J. Am. Chem. Soc.* 2017, 139, 15792–15800. "Structural monitoring of the onset of excited-state aromaticity in a liquid crystal phase" (DOI: 10.1021/jacs.7b08021)
- (4) Imants Kreituss and Jeffrey W. Bode, *Nat. Chem.* 2017, 9, 446–452. "Flow chemistry and polymer-supported pseudoenantiomeric acylating agents enable parallel kinetic resolution of chiral saturated N-heterocycles" (DOI: 10.1038/nchem.2681)
- (5) Sheng-Ying Hsieh and Jeffrey W. Bode, *ACS Cent. Sci.* 2017, 3, 66–72. "Lewis Acid Induced Toggle from Ir(II) to Ir(IV) Pathways in Photocatalytic Reactions: Synthesis of Thiomorpholines and Thiazepanes from Aldehydes and SLAP Reagents" (DOI: 10.1021/acscentsci.6b00334)
- (6) Alberto Osuna Gálvez, Cédric P. Schaack, Hidetoshi Noda, and Jeffrey W. Bode, *J. Am. Chem. Soc.* 2017, 139, 1826–1829. "Chemoselective Acylation of Primary Amines and Amides with Potassium Acyltrifluoroborates under Acidic Conditions" (DOI: 10.1021/jacs.7b00059)
- (7) Sean Oriana, Ye Cai, Jeffrey W. Bode and Yoko Yamakoshi, *Org. Biomol. Chem.* 2017, 15, 1792-1800. "Synthesis of tri-functionalized MMP2 FRET probes using a chemo-selective and late-stage modification of unprotected peptides" (DOI: 10.1039/C7OB00150A)
- (8) Fumito Saito and Jeffrey W. Bode, *Chem. Sci.* 2017, 8, 2878–2884. "Synthesis and stabilities of peptide-based [1]rotaxanes: molecular grafting onto lasso peptide scaffolds" (DOI: 10.1039/C7SC00021A)
- (9) Moritz K. Jackl, Luca Legnani, Bill Morandi, and Jeffrey W. Bode, *Org. Lett.* 2017, 19, 4696–4699. "Continuous Flow Synthesis of Morpholines and Oxazepanes with Silicon Amine Protocol (SLAP) Reagents and Lewis Acid Facilitated Photoredox Catalysis" (DOI: 10.1021/acs.orglett.7b02395)
- (10) Michael U. Luescher, Teerawat Songsichan, Sheng-Ying Hsieh, and Jeffrey W. Bode, *Helv. Chim. Acta* 2017, 100, e1700199. "Copper Promoted Oxidative Coupling of SnAP Hydrazines and Aldehydes to Form Chiral 1,4,5-Oxadiazepanes and 1,2,5-Triazepanes" (DOI: 10.1002/hlca.201700199)
- (11) Jumpei Taguchi, Toshiki Ikeda, Rina Takahashi, Ikuo Sasaki, Yasushi Ogasawara, Tohru Dairi, Naoya Kato, Yasunori Yamamoto, Jeffrey W. Bode, and Hajime Ito, *Angew. Chem. Int. Ed.* 2017, 56, 13847 – 13851. "Synthesis of Acylborons by Ozonolysis of Alkenylboronates: Preparation of an Enantioenriched Amino-Acid Acylboronate" (DOI: 10.1002/anie.201707933)



- (12) Prateek Tripathi, Marcela Carvallo, Elizabeth E. Hamilton, Sasha Preuss, and Steve A. Kay, *PNAS* 2017, 11, 172–177. "Arabidopsis B-BOX32 interacts with CONSTANS-LIKE3 to regulate flowering" (DOI: 10.1073/pnas.1616459114)
- (13) Greg Boyle, Kerstin Richter, Henry D. Priest, David Traver, Todd C. Mockler, Jeffrey T. Chang, Steve A. Kay, Ghislain Breton, *PLoS ONE* 2017, 12, e0169923. "Comparative Analysis of Vertebrate Diurnal/Circadian Transcriptomes" (DOI: 10.1371/journal.pone.0169923)
- (14) Eilon Shani, Mohammad Salehin, Yuqin Zhang, Sabrina E. Sanchez, Colleen Doherty, Renhou Wang, Cristina Castillejo Mangado, Liang Song, Iris Tal, Odelia Pisanty, Joseph R. Ecker, Steve A. Kay, Jose Pruneda-Paz, and Mark Estelle, *Curr. Biol.* 2017, 27, 437–444. "Plant Stress Tolerance Requires Auxin-Sensitive Aux/IAA Transcriptional Repressors" (DOI: 10.1016/j.cub.2016.12.016)
- (15) Akane Kubota, Shogo Ito, Jae Sung Shim, Richard S. Johnson, Yong Hun Song, Ghislain Breton, Greg S. Goralogia, Michael S. Kwon, Dianne Laboy Cintrón, Tomotsugu Koyama, Masaru Ohme-Takagi, Jose L. Pruneda-Paz, Steve A. Kay, Michael J. MacCoss, Takato Imaizumi, *PLoS Genet* 2017, 1, e1006856. "TCP4-dependent induction of CONSTANS transcription requires GIGANTEA in photoperiodic flowering in Arabidopsis" (DOI: 10.1371/journal.pgen.1006856)
- (16) Xiaobo Li, Hongbao Yang, Hao Sun, Runze Lu, Chengcheng Zhang, Na Gao, Qingtao Meng, Shenshen Wu, Susanna Wang, Michael Aschner, Jiong Wu, Boping Tang, Aihua Gu, Steve A. Kay and Rui Chen, *PNAS* 2017, 114, E9655–E9664. "Taurine ameliorates particulate matter-induced emphysema by switching on mitochondrial NADH dehydrogenase genes" (DOI: 10.1073/pnas.1712465114)
- (17) Michael E. Hughes, Katherine C. Abruzzi, Ravi Allada, Ron Anafi, Alaaddin Bulak Arpat, Gad Asher, Pierre Baldi, Charissa de Bekker, Deborah Bell-Pedersen, Justin Blau, Steve Brown, M. Fernanda Ceriani, Zheng Chen, Joanna C. Chiu, Juergen Cox, Alexander M. Crowell, Jason P. DeBruyne, Derk-Jan Dijk, Luciano DiTacchio, Francis J. Doyle, Giles E. Duffield, Jay C. Dunlap, Kristin Eckel-Mahan, Karyn A. Esser, Garret A. FitzGerald, Daniel B. Forger, Lauren J. Francey, Ying-Hui Fu, Frédéric Gachon, David Gatfield, Paul de Goede, Susan S. Golden, Carla Green, John Harer, Stacey Harmer, Jeff Haspel, Michael H. Hastings, Hanspeter Herzog, Erik D. Herzog, Christy Hoffmann, Christian Hong, Jacob J. Hughey, Jennifer M. Hurley, Horacio O. de la Iglesia, Carl Johnson, Steve A. Kay, Nobuya Koike, Karl Kornacker, Achim Kramer, Katja Lamia, Tanya Leise, Scott A. Lewis, Jiajia Li, Xiaodong Li, Andrew C. Liu, Jennifer J. Loros, Tami A. Martino, Jerome S. Menet, Martha Merrow, Andrew J. Millar, Todd Mockler, Felix Naef, Emi Nagoshi, Michael N. Nitabach, Maria Olmedo, Dmitri A. Nusinow, Louis J. Ptáček, David Rand, Akhilesh B. Reddy, Maria S. Robles, Till Roenneberg, Michael Rosbash, Marc D. Ruben, Samuel S.C. Rund, Aziz Sançar, Paolo Sassone-Corsi, Amita Sehgal, Scott Sherrill-Mix, Debra J. Skene, Kai-Florian Storch, Joseph S. Takahashi, Hiroki R. Ueda, Han Wang, Charles Weitz, Pål O. Westermarck, Herman Wijnen, Ying Xu, Gang Wu, Seung-Hee Yoo, Michael Young, Eric Erquan Zhang, Tomasz Zielinski, John B. Hogenesch, *J. Biol. Rhythm* 2017, 32, 383–390. "Guidelines for Genome-Scale Analysis of Biological Rhythms" (DOI: 10.1177/0748730417728663)
- (18) Naomi R. Latorraca, Nathan M. Fastman, A.J. Venkatakrisnan, Wolf B. Frommer, Ron O. Dror, Liang Feng, *Cell* 2017, 169, 96–107. "Mechanism of Substrate Translocation in an Alternating Access Transporter" (DOI: 10.1016/j.cell.2017.03.010)
- (19) Kevin L. Cox, Fanhong Meng, Katherine E. Wilkins, Fangjun Li, Ping Wang, Nicholas J. Booher, Sara C. D. Carpenter, Li-Qing Chen, Hui Zheng, Xiquan Gao, Yi Zheng, Zhangjun Fei, John Z. Yu, Thomas Isakeit, Terry Wheeler, Wolf B. Frommer, Ping He, Adam J. Bogdanove & Libo Shan, *Nature Commun.* 2017, 8, 15588. "TAL effector driven induction of a SWEET gene confers susceptibility to bacterial blight of cotton" (DOI: 10.1038/ncomms15588)
- (20) Cindy Ast, Jessica Foret, Luke M. Oltrogge, Roberto De Michele, Thomas J. Kleist, Cheng-Hsun Ho & Wolf B. Frommer, *Nature Commun.* 2017, 8, 431. "Ratiometric Matryoshka biosensors from a nested cassette of green- and orange-emitting fluorescent proteins" (DOI: 10.1038/s41467-017-00400-2)
- (21) Annalisa Rizza, Ankit Walia, Viviane Lanquar, Wolf B. Frommer & Alexander M. Jones, *Nat. Plants* 2017,

3, 803–817. "In vivo gibberellin gradients visualized in rapidly elongating tissues" (DOI: 10.1038/s41477-017-0021-9)

2. Review Articles

- (1) Jeffrey W. Bode, *Acc. Chem. Res.* 2017, 50, 2104–2115. "Chemical Protein Synthesis with the  $\alpha$ -Ketoacid–Hydroxylamine Ligation" (DOI: 10.1021/acs.accounts.7b00277)

3. Proceedings

N/A

4. Other English Articles

- (1) Joanna Friesner, Sarah M. Assmann, Ruth Bastow, Julia Bailey-Serres, Jim Beynon, Volker Brendel, C. Robin Buell, Alexander Bucksch, Wolfgang Busch, Taku Demura, Jose R. Dinneny, Colleen J. Doherty, Andrea L. Eveland, Pascal Falter-Braun, Malia A. Gehan, Michael Gonzales, Erich Grotewold, Rodrigo Gutierrez, Ute Kramer, Gabriel Krouk, Shisong Ma, R.J. Cody Markelz, Molly Megraw, Blake C. Meyers, James A.H. Murray, Nicholas J. Provart, Sue Rhee, Roger Smith, Edgar P. Spalding, Crispin Taylor, Tracy K. Teal, Keiko U. Torii, Chris Town, Matthew Vaughn, Richard Vierstra, Doreen Ware, Olivia Wilkins, Cranos Williams, Siobhan M. Brady, *Plant Physiol.* 2017, 175, 1499–1509. "The Next Generation of Training for Arabidopsis Researchers: Bioinformatics and Quantitative Biology" (DOI: 10.1104/pp.17.01490)
- (2) Jun Xiao, Run Jin, Xiang Yu, Max Shen, John D Wagner, Armaan Pai, Claire Song, Michael Zhuang, Samantha Klasfeld, Chongsheng He, Alexandre M Santos, Chris Helliwell, Jose L Pruneda-Paz, Steve A Kay, Xiaowei Lin, Sujuan Cui, Meilin Fernandez Garcia, Oliver Clarenz, Justin Goodrich, Xiaoyu Zhang, Ryan S Austin, Roberto Bonasio & Doris Wagner, *Nature Genet.* 2017, 49, 1546–1552. "Cis and trans determinants of epigenetic silencing by Polycomb repressive complex 2 in Arabidopsis" (DOI: 10.1038/ng.3937)
- (3) Prateek Tripathi, José L. Pruneda-Paz, Steve A. Kay, *J. Vis. Exp.* 2017, 125, e56080. "A Modified Yeast-one Hybrid System for Heteromeric Protein Complex-DNA Interaction Studies" (DOI: 10.3791/56080)

5. Articles written in other than English

N/A

## 2. Invited Lectures, Plenary Addresses (etc.) at International Conferences and International Research Meetings

- List up to 10 main presentations during FY2017 in order from most recent.
- For each, write the lecturer/presenter's name, presentation title, conference name and date(s)

- 1) Cathleen Crudden, "N-heterocyclic carbenes as ligands for metal surfaces", 255th ACS National Meeting, New Orleans, Louisiana, USA, Mar 18-22, 2018
- 2) Toshinori Kinoshita, "Blue light-signaling pathway in stomatal guard cells", Taiwan-Japan Plant Biology 2017, Academia Sinica, Taipei, Taiwan, Nov 3-6, 2017
- 3) Steve Kay, 2017 World Nobel Prize Laureate Summit, Guiyang, China, Sep 14-16, 2017
- 4) Jeffrey Bode, "Chemical Protein Synthesis with the KAHA Ligation", Chemical Protein Synthesis Symposium, Haifa, Israel, Sep 4-7, 2017
- 5) Takashi Ooi, "Catalyst-directed Multiple Selectivity Control", Joint Symposium on New Frontiers by Fusing Chemistry and Biology, Taiwan, Jul 13-14, 2017
- 6) Shigehiro Yamaguchi, "Main Group Strategy for Functional pi-Electron Materials", Gordon Research Conference 2017, Physical Organic Chemistry Symposium, Holderness, NH, USA, Jun 26-29, 2017
- 7) Kenichiro Itami, "Creation of molecular nanocarbons by metal catalysis", 19th IUPAC International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis (OMCOS19), Jun 26, 2017
- 8) Keiko Torii, "Breaking the silence: Making decisions in the world of uncertainty", ICAR2017 (International Conference of Arabidopsis Research), St Lois, MO, USA, Jun 23, 2017
- 9) Takashi Yoshimura, "Understanding the molecular basis of vertebrate seasonal adaptation", 18th International Congress of Comparative Endocrinology, Lake Louise, Canada, Jun 9, 2017
- 10) Tetsuya Higashiyama, "Cellular Signaling and Dynamics in Pollen Tube Guidance", Cold Spring Harbor Asia Conference on Plant Cell and Developmental Biology, Suzhou, China, May 22-26, 2017

## 3. Major Awards

- List up to 10 main awards received during FY2017 in order from the most recent.
- For each, write the recipient's name, name of award, and year issued.
- In case of multiple recipients, underline those affiliated with the center.

- 1) Tetsuya Higashiyama, Inoue Prize for Science, Inoue Foundation for Science, 2018
- 2) Wolf Frommer, 2017 Highly Cited Researcher, Clarivate Analytics, 2017
- 3) Kenichiro Itami, 2017 Highly Cited Researcher, Clarivate Analytics, 2017
- 4) Steve Kay, 2017 Highly Cited Researcher, Clarivate Analytics, 2017
- 5) Tetsuya Higashiyama, Kihara Foundation Award, 2017
- 6) Kenichiro Itami, 70th Chunichi Cultural Award, Chunichi Shimbun, Japan, 2017
- 7) Kenichiro Itami, 23rd Yomiuri Techno Forum Gold Medal Prize, Yomiuri Shimbun, Japan, 2017
- 8) Cathleen Crudden, R.U. Lemieux Award for Organic Chemistry, Canadian Society for Chemistry, 2017
- 9) Cathleen Crudden, The SYNLETT Best Paper Award 2017, Thieme, 2017
- 10) Takashi Ooi, The Society of Synthetic Organic Chemistry Award, 2017

## Appendix 2 FY 2017 List of Principal Investigators

## NOTE:

- Underline names of principal investigators who belong to an overseas research institution. Place an asterisk (\*) by names of investigators considered to be ranked among world's top researchers.
- In case of researchers not listed in the latest report, attach "Biographical Sketch of a New Principal Investigator".

		<Results at the end of FY2017>			Principal Investigators Total: 12		
Name	Age	Affiliation (Position title, department, organization)	Academic degree specialty	Effort (%)*	Starting date of project participation	Status of project participation (Describe in concrete terms)	Contributions by PIs from overseas research institutions
Center director Kenichiro ITAMI*	46	Director, Professor Institute of Transformative Bio-Molecules, Nagoya University	Dr.Eng <i>Specialties</i> : Organic Synthesis, Catalysis, Pharmaceutical Science, Nanocarbon Chemistry	80	from the beginning	usually stays at the center	
Tetsuya HIGASHIYAMA*	46	Vice-Director, Professor Institute of Transformative Bio-Molecules, Nagoya University	Dr.Sci <i>Specialties</i> : Live Cell Biology, Plant Reproduction, Bio-active molecules, Peptides	90	from the beginning	usually stays at the center	
<u>Jeffrey W. BODE*</u>	44	Professor of Organic Chemistry Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland	Doctoral of Natural Science <i>Specialties</i> : Organic Synthesis, Peptide and Protein Chemistry, Catalysis, Ligation and Bioconjugation reactions	21	from the beginning	Stayed at the center one week in FY2017. Connected 24 hours through iPad to the center. Holds on-line group meeting once a week. Joins PI meeting online.	
<u>Cathleen M. CRUDDEN*</u>	51	Professor Department of Chemistry, Queen's University, Canada	Ph.D <i>Specialties</i> : Catalysis, Organic Synthesis, Materials Chemistry, Chirality	21	from the beginning	Stayed at the center one month in FY2017. Holds Skype group meeting once a week. Joins PI meeting online.	
Toshinori KINOSHITA*	49	Professor Institute of Transformative Bio-Molecules, Nagoya University	Dr.Sci <i>Specialties</i> : Plant Molecular Physiology	90	from the beginning	usually stays at the center	
Takashi OOI*	52	Professor Institute of Transformative Bio-Molecules, Nagoya University	Dr. Engineering <i>Specialties</i> : Organic Synthesis, Catalysis, Molecular Recognition	90	from the beginning	usually stays at the center	

<u>Keiko TORII</u> *	52	Distinguished Professor Department of Biology, University of Washington Investigator Howard Hughes Medical Institute and Gordon and Betty Moore Foundation (HHMI-GBMF)	Ph.D. <i>Specialties</i> : Plant Development, Signal Transduction, Stem Cell Maintenance/Differentiat i-on in Plants	21	from the beginning	Stayed at the center for three weeks in FY2017. Holds on-line plant biology meeting "Mixplant meeting" once a week. Joins PI meeting online.	
Shigehiro YAMAGUCHI*	49	Vice-Director, Professor Institute of Transformative Bio-Molecules, Nagoya University	Dr. Engineering <i>Specialties</i> : Main Group Chemistry, Physical Organic Chemistry	90	from the beginning	usually stays at the center	
Takashi YOSHIMURA*	48	Professor Institute of Transformative Bio-Molecules, Nagoya University	Dr. Agriculture <i>Specialties</i> : Animal Physiology, Systems Biology, Neuroendoc- rinology	70	from the beginning	usually stays at the center	
<u>Steve A. Kay</u> *	58	Dean and Anna H. Bing Dean's Chair, Professor of Biological Sciences, Professor of Neurology, Physiology and Biophysics, Dornsife College of Letters, Arts and Sciences, University of Southern California	Ph.D. <i>Specialties</i> : Chronobiolo-gy, Genetics, Biochemistry, Systems Biology	21	from April 1st 2014	Holds on-line meeting on an as-needed basis. Joins PI meeting online.	
Florence Tama*	43	Professor Institute of Transformative Bio-Molecules / Department of Physics, Graduate School of Science, Nagoya University	Ph.D <i>Specialties</i> : computational biophysics	50	from April 1st 2016	usually stays at the center	
<u>Wolf B. Frommer</u> *	60	Staff Member and Dir. emerit., Carnegie Science, Stanford Professor (by Courtesy) Dep. Biology, Stanford University	Dr. rer. nat. <i>Specialties</i> : Biology	21	from October 16th 2016	Stayed at the center one month in FY2017. Holds on-line group meeting once a week. Joins PI meeting online.	

\*Percentage of time that the principal Investigator will devote to his/her work for the center vis-à-vis his/her total working hours (total time for whole working activities including education, medical services, and others as well as research).

**Researchers unable to participate in project in FY 2017**

Name	Affiliation (Position title, department, organization)	Starting date of project participation	Reasons	Measures taken

## Appendix 2a Biographical Sketch of Principal Investigator

(within 3 pages per person)

### Name (Age)

\* Place an asterisk (\*) by the name of the principal investigators who are considered to be ranked among the world's top researchers.

**Affiliation and position** (Position title, department, organization, etc.)

### Academic degree and specialty

**Effort** %

\* Percentage of time that the PI will devote to his/her work for the center vis-à-vis his/her total working hours (total time for whole working activities including education, medical services, and others as well as research).

### Research and education history

### Achievements and highlights of past research activities

\* Describe the PI's qualifications as a top-caliber researcher if s/he is considered to be ranked among the world's top researchers.

### Achievements

**(1) International influence** \* Describe the kind of attributes listed below.

- a) Guest speaker or chair of related international conference and/or director or honorary chairman of a major international academic society in the subject field
- b) Member of a scholarly academy in a major country
- c) Recipient of international awards
- d) Editor of an influential journal, etc.

**(2) Receipt of large-scale competitive funds (over the past 5 years)**

**(3) Article citations (Titles of major publications, number of citations)**

**(4) Others (Other achievements indicative of the PI's qualification as a top-world researcher, if any.)**

## Appendix 3-1 FY 2017 Records of Center Activities

### 1. Researchers and center staffs, satellites, partner institutions

#### 1-1. Number of researchers in the "core" established within the host institution

- Regarding the number of researchers at the Center, please fill in the table in Appendix 3-1a.

#### Special mention

- Enter matters warranting special mention, such as concrete plans for achieving the Center's goals, established schedules for employing main researchers, particularly principal investigators.

As a result of international open recruitment in FY2017, Dr. Takeshi Yanai, Associate Professor at Department of Theoretical and Computational Molecular Science, Institute for Molecular Science newly joins ITbM as a Nagoya University PI as of April 1, 2018.

- As background to how the Center is working on the global circulation of world's best brains, give good examples, if any, of how career paths are being established for the Center's researchers; that is, from which top-world research institutions do researchers come to the Center and to which research institutions do the Center's researchers go, and how long are their stays at those institutions.

Examples of researchers involved in the global brain circulation:

Position at ITbM	Period of project participation	Previous Affiliation (organization, *country)	Next Affiliation (Position title, organization, *country)
Research Fellow	3/1/2016 ~8/31/2017	—	Scientist, Central Drug Research Institute, India
Research Fellow	10/1/2016 ~10/31/2017	Free University of Berlin, Germany	Junior Associate Professor, Kyoto University, Japan
Research Fellow	1/1/2017 ~12/31/2017	University of Washington, USA	Assistant Professor, Central Drug Research Institute, India
Designated Lecturer	4/1/2017 ~Present	Carnegie Institution for Science, USA	—
Research Fellow	6/1/2017 ~Present	Academia Sinica, Taiwan	—
Research Fellow	8/1/2017 ~Present	Indian Institute of Technology Madras, India	—
Research Fellow	9/1/2017 ~Present	ENS-PARIS-SACLAY, France	—
Designated Assistant Professor	11/1/2017 ~Present	University of Washington, USA	—
Research Fellow	11/16/2017 ~Present	University of Toronto • Canada	—
Research Fellow	1/1/2018 ~1/31/2018	—	Postdoctoral Researcher, Cold Spring Harbor Laboratory, USA



## 1-2. Satellites and partner institutions

- List the satellite and partner institutions in the table below.
- Indicate newly added and deleted institutions in the "Notes" column.
- If satellite institutions have been established, describe by satellite the Center's achievements in coauthored papers and researcher exchanges in Appendix 4.

### <Satellite institutions>

Institution name	Principal Investigator(s), if any	Notes
n/a		

### < Partner institutions>

Institution name	Principal Investigator(s), if any	Notes
ETH Zurich	Jeffrey W. BODE	
Queen's University	Cathleen M. CRUDDEN	
University of Washington	Keiko TORII	
University of Southern California	Steve A. KAY	
Heinrich Heine University Düsseldorf	Wolf B. FROMMER	From FY2017
NSF Center for Selective C-H Functionalization		
University of Freiburg		
RIKEN Center for Sustainable Resource Science (CSRS)		
Institute of Chemistry (IoC), Academia Sinica		

## 2. Securing external research funding\*

External research funding secured in FY2017

Total: 1,098,108,126 yen

- Describe external funding warranting special mention. Include the name and total amount of each grant.

\* External research funding includes "Grant-in-Aid for Scientific Research," funding for "commissioned research projects," and for "joint research projects" as listed under "Research projects" in Appendix 3-2, Project Expenditures.

- Name: Strategic Basic Research Programs (ERATO), JST  
Total Amount: 293,658,000 JPY (acquired by Kenichiro Itami)
- Name: Grant-in-Aid for Specially Promoted Research, JSPS  
Total Amount: 75,140,000 JPY (acquired by Takashi Yoshimura)
- Name: Grant-in-Aid for Scientific Research on Innovative Areas (Research in a proposed research area), JSPS  
Total Amount: 39,910,000 JPY (acquired by Tetsuya Higashiyama)
- Name: Grant-in-Aid for Scientific Research on Innovative Areas (Research in a proposed research area), JSPS  
Total Amount: 43,420,000 JPY (acquired by Toshinori Kinoshita)
- Name: Grant-in-Aid for Scientific Research on Innovative Areas (Research in a proposed research area), JSPS  
Total Amount: 42,640,000 JPY (acquired by Takashi Ooi)

### 3. International research conferences or symposiums held to bring world's leading researchers together

- Indicate the number of international research conferences or symposiums held in FY2017 and give up to three examples of the most representative ones using the table below.

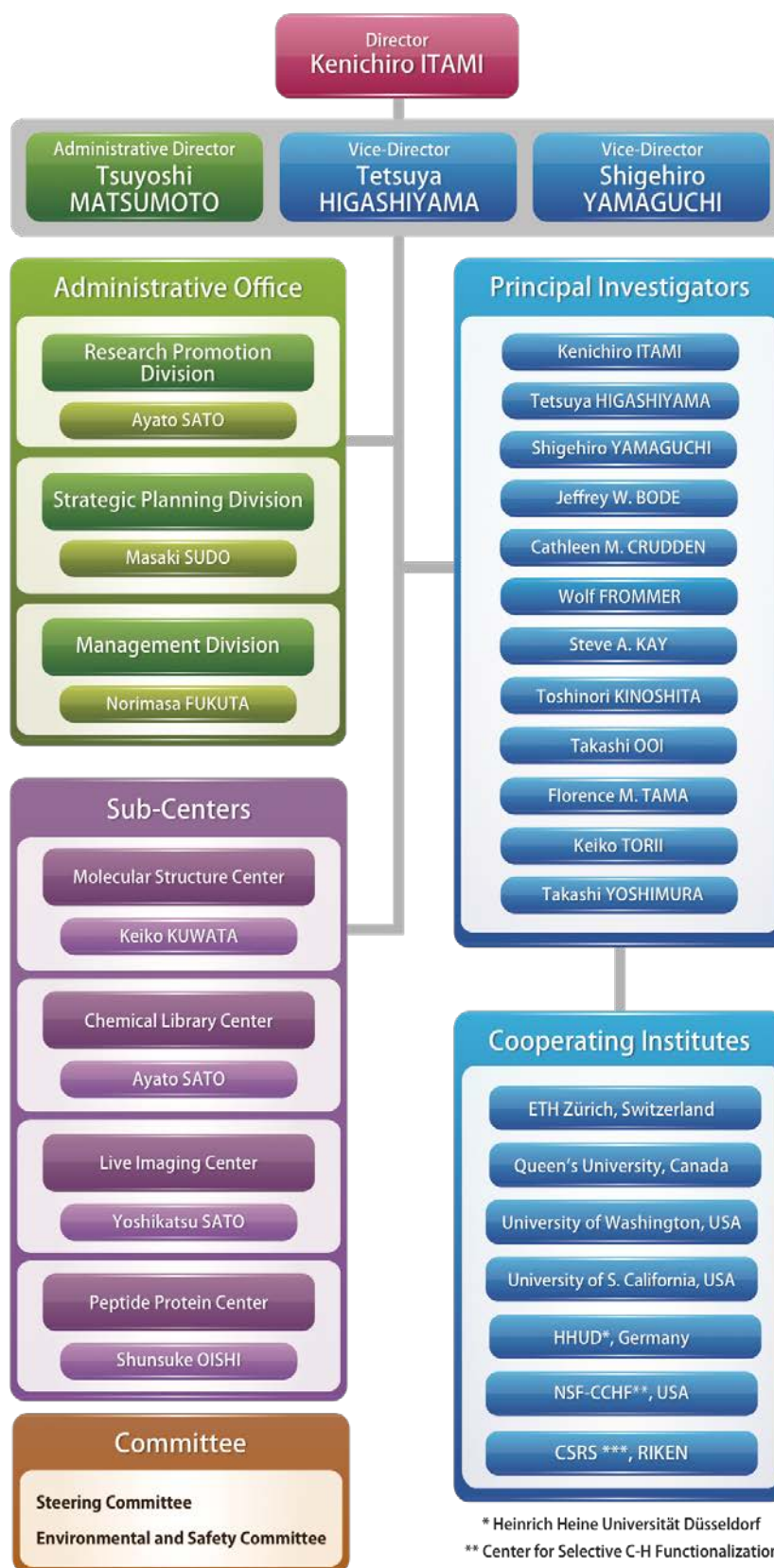
FY 2017: 2 meetings	
Major examples (meeting titles and places held)	Number of participants
The 5th International Symposium of Transformative Bio-Molecules (ISTbM-5), Hirata Award, Okazaki Award Noyori Conference Hall, Nagoya University November 20-21, 2017	From domestic institutions: 380 From overseas institutions: 20
The 23rd Nagoya Medal of Organic Chemistry Noyori Conference Hall, Nagoya University December 22, 2017	From domestic institutions: 367 From overseas institutions: 1
The 1st International Symposium on Catalysis for Sustainable Chemical Synthesis, Lecture Hall, Chemische Institute, University of Freiburg, September 25-26, 2017	From domestic institutions: 12 From overseas institutions: 73

Other events organized by ITbM's PI and ITbM:

- IoC-IPMB-ITbM Joint Symposium on New Frontiers by Fusing Chemistry and Biology, Ta-Shue Chou Lecture Hall, IoC, Academia Sinica, July 13-14, 2017
- International ERATO Itami Molecular Nanocarbon Symposium 2017, Noyori Conference Hall, Nagoya University, August 3-4, 2017
- ITbM Consortium Workshop, ITbM, Nagoya University, September 29, 2017
- The 4th CSRS-ITbM Joint Workshop with Kihara, Main Office Building Hall, RIKEN Yokohama campus, January 15, 2018.

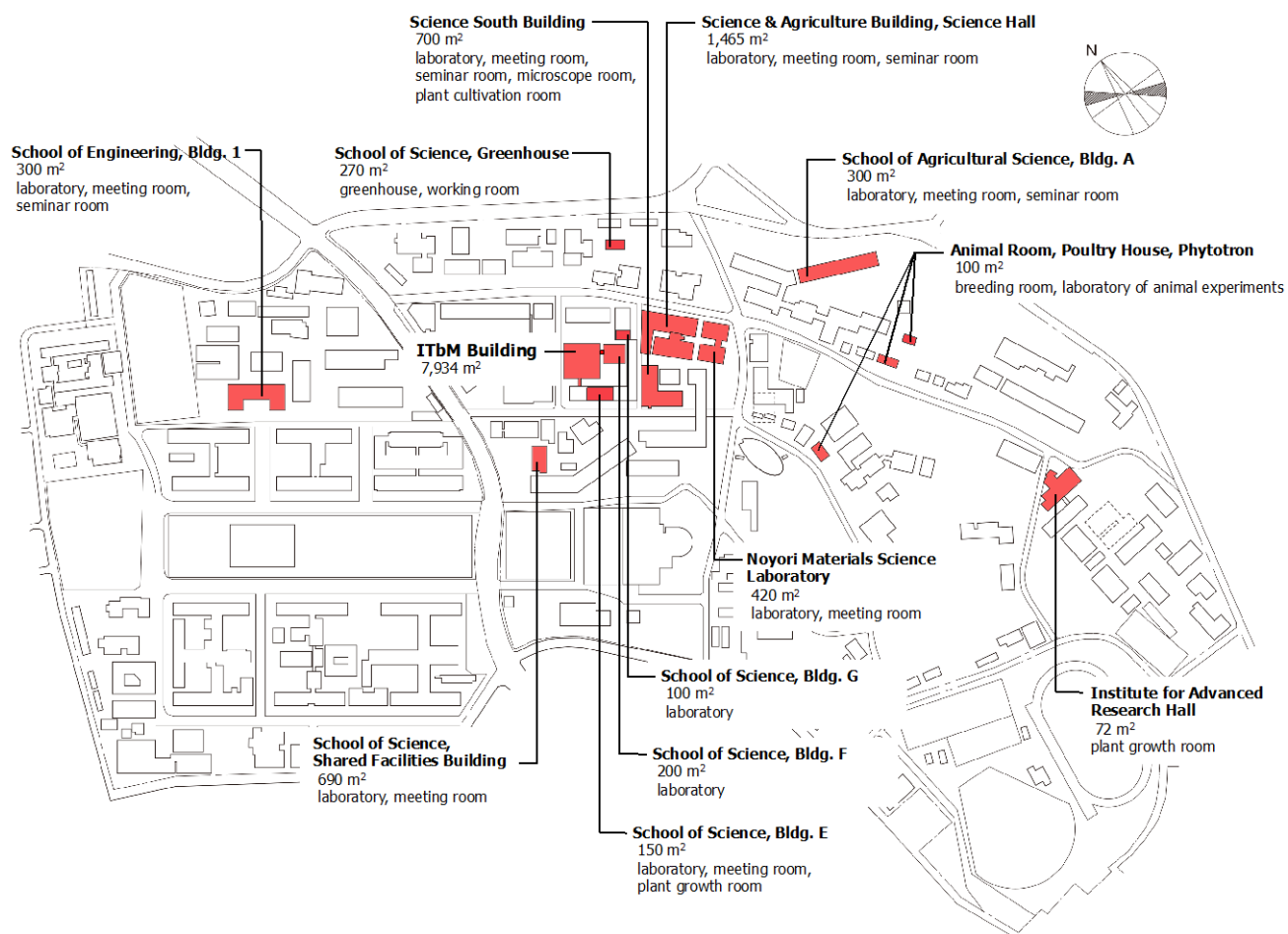
#### 4. Center's management system

- Please diagram management system in an easily understood manner.
- If any changes have been made in the management system from that in the latest "center project," please describe them. Please describe any important changes made in such as the center director, administrative director, head of host institution, and officer(s) in charge at the host institution (e.g., executive vice president for research).



## 5. Campus Map

- Please draw a simple map of the campus showing where the main office and principle investigator(s) are located.



The offices of the Center Director, All the PIs, and Administrative Department are located in the "ITbM Building"

## Appendix 3-1a FY 2017 Records of Center Activities

### 1. Researchers and other center staffs, satellites, partner institut

#### 1-1. Number of researchers and other center staffs

\* Please fill in the number of researchers and other center staffs in the table blow.

\* Please describe the final goals for achieving these numbers and dates when they will be achieved.

#### a) Principal Investigators (full professors, associate professors or other researchers of comparable standing)

(persons)

	At beginning of project	At end of FY 2017	Final goal (Date: 3, 2022)
Researches from within the host institution	7	7	8
Foreign researchers invited from abroad	3	5	5
Researchers invited from other Japanese institutions	0	0	0
Total principal investigators	10	12	13

#### b) Total members

	At beginning of project		At end of FY2017		Final goal (Date: month, year)	
	Number of persons	%	Number of persons	%	Number of persons	%
Researchers	20	/	75	/	80	/
Overseas researchers	5	25	25	33	27	34
Female researchers	4	20	22	29	21	26
Principal investigators	10	/	12	/	13	/
Overseas PIs	3	30	5	42	6	46
Female PIs	2	20	3	25	3	23
Other researchers	10	/	63	/	67	/
Overseas researchers	2	20	20	32	21	31
Female researchers	2	20	19	30	18	27
Research support staffs	10	/	47	/	50	/
Administrative staffs	10	/	13	/	12	/
Total number of people who form the "core" of the research center	40	/	135	/	142	/

## Appendix 3-2 Project Expenditures

### 1) Overall project funding

\* In the "Total Cost" column, enter the total amount of funding required to implement the project, without dividing it into funding sources.

\* In the "Amount covered by WPI funding" column, enter the amount covered by WPI within the total amount.

\* In the "Personnel," "Project activities," "Travel," and "Equipment" blocks, the items and details may be changed to coincide with the project's actual content.

(Million yens)

Costs (Million yens)

Cost Items	Details (For Personnel - Equipment please fill in the breakdown of fiscal expenditure, and the income breakdown for Research projects.)	Total Costs	Amount covered by WPI funding
Personnel	Center director and Administrative director	32	18
	Principal investigators (no. of persons):9	87	16
	Other researchers (no. of persons):50	254	205
	Research support staffs (no. of persons):29	60	60
	Administrative staffs (no. of persons):23	78	48
	Subtotal	511	347
Project activities	Gratuities and honoraria paid to invited principal investigators (no. of persons):0	0	0
	Cost of dispatching scientists (no. of persons):1	3	3
	Research startup cost (no. of persons):15	10	9
	Cost of satellite organizations (no. of satellite organizations):0	0	0
	Cost of international symposiums (no. of symposiums):6	1	1
	Rental fees for facilities	23	4
	Cost of consumables	27	27
	Cost of utilities	55	55
	Other costs	97	95
	Subtotal	216	194
Travel	Domestic travel costs	4	4
	Overseas travel costs	12	12
	Travel and accommodations cost for invited scientists (no. of domestic scientists):13 (no. of overseas scientists):6	7	7
	Travel cost for scientists on secondment (no. of domestic scientists):1 (no. of overseas scientists):5	3	3
	Subtotal	26	26
Equipment	Depreciation of buildings	54	7
	Depreciation of equipment	674	621
	Subtotal	728	628
Research projects (Detail items must be fixed)	Projects supported by other government subsidies, etc.	232	0
	Grants-in-Aid for Scientific Research, etc.	353	0
	Commissioned research projects, etc.	569	0
	Joint research projects	21	0
	Others (donations, etc.)	10	0
Subtotal	1185	0	
<b>Total</b>		<b>2666</b>	<b>1195</b>

### WPI grant in FY 2017

700

### Costs of establishing and maintaining

0

### Cost of equipment procured

132

Name of equipment:LumiCEC High Sensitivity Bioluminescence Measurement System, Number of units: 2 Set Costs paid: 11

Name of equipment:UV-NIR Absolute PL Quantum Yield Spectrometer, Number of units: 1 Set Costs paid: 10

Name of equipment:Nanosecond Time-Resolved Spectroscopy System, Number of units: 1 Set Costs paid: 11

Name of equipment:Nanoliter Dispensing System, Number of units: 1 Set Costs paid: 11

Name of equipment:All-in-one Fluorescence Microscope, Number of units: 1 Set Costs paid: 12

Name of equipment:Multimode Plate Reader Number of units: 1 Set Costs paid: 12

Name of equipment:Electric Inverted Microscope Number of units: 1 Set Costs paid: 12

Others 53

\*1. Funding sources that include government subsidies (including Enhancements promotion expenses (機能強化促進経費), National university reform reinforcement promotion subsidy (国立大学改革強化推進補助金) etc.), indirect funding, and allocations from the university's own resources.

\*2 When personnel, travel, equipment (etc.) expenses are covered by Grants-in-Aid or under commissioned research projects or joint research projects, the amounts should be entered in the "Research projects" block.

## Appendix 4 FY 2017 Status of Collaboration with Overseas Satellites

### 1. Coauthored Papers

- List the refereed papers published in FY 2017 that were coauthored between the center's researcher(s) in domestic institution(s) (include satellite institutions) and overseas satellite institution(s). List them by overseas satellite institution in the below blocks.
- Transcribe data in same format as in Appendix 1. Italicize the names of authors affiliated with overseas satellite institutions.
- For reference write the Appendix 1 item number in parentheses after the item number in the blocks below. Let it free, if the paper is published in between Jan.-Mar. 2018 and not described in Appendix 1.

#### Overseas Satellite 1    Name (Total: OO papers)

- 1)
- 2)
- 3)
- 4)

#### Overseas Satellite 2    Name (Total: OO papers)

- 1)
- 2)
- 3)
- 4)

## 2. Status of Researcher Exchanges

- Using the below tables, indicate the number and length of researcher exchanges in FY 2017. Enter by institution and length of exchange.
- Write the number of principal investigator visits in the top of each space and the number of other researchers in the bottom.

### Overseas Satellite 1:

<To satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2017					

<From satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2017					

### Overseas Satellite 2:

<To satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2017					

<From satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2017					



## Appendix 5 FY 2017 Visit Records of World Top World-level Researchers from Abroad

\* If top world-level researchers have visited/ stayed at the Center, please provide information on them in the below table.

\* To determine whether the researcher is a "top world-level researcher," please see the standard stipulated in the Application Guideline.

**Total: 26**

	Name	Age	Affiliation (Position title, department, organization)	Academic degree, specialty	Record of research activities (Awards record, etc.)	Time, duration	Summary of activities during stay at center (e.g., participation as principal investigator; short- term stay for joint research; participation in symposium)
1	Cathleen Crudden	51	Principal Investigator, ITbM / Professor, Department of Chemistry, Queens University	Ph.D. Chemistry	<ul style="list-style-type: none"> <li>The Aldrich Lecture Award</li> <li>Clara Benson Award, CSC</li> <li>Catalysis Lectureship Award, Catalysis Society</li> </ul>	1 month	<ul style="list-style-type: none"> <li>participation as principal investigator</li> </ul>
2	Keiko Torii	52	Principal Investigator, ITbM / Professor, Department of Biology, Washington University	Ph.D. Biochemistry	<ul style="list-style-type: none"> <li>JSPS Prize</li> <li>SJWS Award</li> <li>Fellow, AAAS</li> </ul>	3 weeks	<ul style="list-style-type: none"> <li>participation as principal investigator</li> </ul>
3	Jeffrey W. Bode	44	Principal Investigator, ITbM / Professor, Department of Chemistry and Applied Bioscience, ETH Zurich	Dok. Nat. Sci.	<ul style="list-style-type: none"> <li>E.J. Corey Award</li> <li>Novartis Lectureship</li> <li>Hirata Gold Award</li> </ul>	1 week	<ul style="list-style-type: none"> <li>participation as principal investigator</li> </ul>
4	Wolf B. Frommer	60	Principal Investigator, ITbM / Director, Carnegie Institution	Dr. rer. Nat	<ul style="list-style-type: none"> <li>Young investigator Award, German Federal Ministry for Science and Technology (1992)</li> <li>Gottfried-Wilhelm-Leibniz Preis, German Research Foundation (DFG) (1998)</li> <li>European Science Award, Körber Foundation (2001)</li> <li>Fellow, American Association for the Advancement of Science (2003)</li> <li>Laurence Bogorad Award for Excellence in Plant Biology Research, American Society of Plant Biology (2012)</li> <li>Member, German Academy of Sciences, Leopoldina (2015)</li> </ul>	1 month	<ul style="list-style-type: none"> <li>participation as principal investigator</li> </ul>
5	Jake Yeston	N/A	Deputy Director, Science, AAAS	Ph.D. Chemistry	<ul style="list-style-type: none"> <li>Humbolt fellowship</li> </ul>	1 day	<ul style="list-style-type: none"> <li>discussion</li> </ul>
6	Peter McBreen	N/A	Professor, Laval University	Ph.D. Surface Chemistry	N/A	3 days	<ul style="list-style-type: none"> <li>lecture @ ITbM seminar</li> <li>research discussion</li> </ul>
7	Maria Barna	N/A	Assistant Professor, Stanford University	Ph.D. Genetics, Developmental Biology	<ul style="list-style-type: none"> <li>Elizabeth Hay Award, Society of Developmental Biology (2017)</li> <li>H.W. Mossman Award in Developmental Biology, American Association of Anatomists (2017)</li> <li>Tsuneko and Reiji 'Okazaki Award', Japan (2017)</li> <li>American Society for Cell Biology Emerging Leader Prize, ASCB (2016)</li> <li>Rosalind Franklin Young Investigator Award, Gruber Foundation and Genetics Society of America (2016)</li> </ul>	6 days	<ul style="list-style-type: none"> <li>invited lecture @ 5th International Symposium on Transformative Bio-Molecules (ISTbM-5)</li> </ul>
8	Paul A. Wender	N/A	Professor, Stanford University	Ph.D. Chemistry	<ul style="list-style-type: none"> <li>2015 ACS Arthur C. Cope Award</li> <li>2013 Prelog Medal (ETH, Switzerland), 2013</li> <li>2013 Prelog Medal (ETH, Switzerland), 2013</li> <li>2010 Wilbur Lucius Cross Medal (Yale Graduate Alumni),</li> <li>2008 The Hamilton Award (U. Nebraska)</li> </ul>	6 days	<ul style="list-style-type: none"> <li>invited lecture @ 5th International Symposium on Transformative Bio-Molecules (ISTbM-5)</li> </ul>
9	David Nicewicz	N/A	Associate Professor, the University of North Carolina at Chape Hill	Ph.D. Organic Chemistry	<ul style="list-style-type: none"> <li>2017 The Hirata Award, Nagoya University</li> <li>2016 Society of Synthetic Organic Chemistry, Japan Lectureship Award</li> <li>2015 Camille Dreyfus Teacher-Scholar Award</li> <li>2015 Ruth Hettelman Prize for Artistic and Scholarly Achievement – University of North Carolina</li> <li>2015 Eli Lilly Grantee Award</li> </ul>	6 days	<ul style="list-style-type: none"> <li>invited lecture @ 5th International Symposium on Transformative Bio-Molecules (ISTbM-5)</li> </ul>
10	Jennt Russinova	N/A	Group Leader, Ghent University	Ph.D. Plant Biology	N/A	1 week	<ul style="list-style-type: none"> <li>invited lecture @ 5th International Symposium on Transformative Bio-Molecules (ISTbM-5)</li> </ul>
11	Julian I. Schroeder	N/A	Professor, University of California San Diego	Ph.D. Bioengineering	<ul style="list-style-type: none"> <li>Presidential Young Investigator Award (NSF)</li> <li>ASPB Charles Albert Shull Award (1997)</li> <li>DFG Heinz-Maier-Leibnitz Prize</li> <li>Blasker Award in Environmental Science</li> <li>top 10 breakthrough of the year selected by Science (2009)</li> </ul>	6 days	<ul style="list-style-type: none"> <li>invited lecture @ 5th International Symposium on Transformative Bio-Molecules (ISTbM-5)</li> </ul>
12	John B. Hogenesch	50	Professor, University of Cincinnati	Ph.D. Chronobiology	N/A	1 week	<ul style="list-style-type: none"> <li>invited lecture @ 5th International Symposium on Transformative Bio-Molecules (ISTbM-5)</li> </ul>
13	Egbert W. Meijer	62	Professor, Eindhoven University of Technology	Ph.D. Molecular Sciences, Organic Chemistry	<ul style="list-style-type: none"> <li>Prelog medal in 2014</li> <li>Cope Scholar Award of the ACS in 2012</li> <li>International Award of the Society of Polymer Science Japan in 2011</li> <li>AkzoNobel Science Award 2010</li> <li>ACS Award for Polymer Chemistry in 2006</li> </ul>	5 days	<ul style="list-style-type: none"> <li>invited lecture @ 23rd Nagoya Medal of Organic Chemistry</li> </ul>
14	George Shimizu	N/A	Professor, University of Calgary	Ph.D. Inorganic Chemistry	N/A	2 days	<ul style="list-style-type: none"> <li>lecture @ ITbM seminar</li> <li>research discussion</li> </ul>
15	Frederic Berger	50	Professor, Gregor Mendel Institute of Molecular Plant Biology	Ph.D. Plant Biology	N/A	1 day	<ul style="list-style-type: none"> <li>lecture @ seminar</li> </ul>
16	Grossniklaus Ueli	54	Professor, Institute of Plant Biology, University of Zürich	Ph.D. Plant Biology	N/A	1 day	<ul style="list-style-type: none"> <li>lecture @ seminar</li> </ul>
17	Ullas V. Pedmale	N/A	Principal Investigator, Cold Spring Harbor Laboratory Watson School of Biological Sciences	Ph.D. Plant Biology	N/A	1 day	<ul style="list-style-type: none"> <li>lecture @ seminar</li> </ul>
18	Guy C. Lloyd-Jones	51	Professor, University of Edinburgh	Ph.D Organic Chemistry	<ul style="list-style-type: none"> <li>University of British Columbia, The Aldrich Distinguished Organic Lecture (2016)</li> <li>Harvard University, The Bristol Myers Squibb Lecture (2014-2015)</li> <li>Royal Society of Chemistry, Tilden Prize (2014)</li> <li>Royal Society of Chemistry, Physical Organic Chemistry Prize (2013)</li> <li>GSK/AstraZeneca/Pfizer/Syngenta Process Chemistry Research Prize (2010)</li> </ul>	5 days	<ul style="list-style-type: none"> <li>lecture @ ITbM seminar</li> <li>research discussion</li> </ul>

19	Matthias Wagner	52	Professor, Goethe-Universität Frankfurt	Ph.D. Chemistry	<ul style="list-style-type: none"> <li>• Karl-Winnacker-Award of the Hoechst AG (1997)</li> <li>• Jury member: Prize for excellent teaching at universities in the state of Hesse awarded by the Hessian Ministry for Science and Culture (Since 2007)</li> <li>• Member of the Polytechnische Gesellschaft e.V. (Since 2014)</li> </ul>	3 weeks	<ul style="list-style-type: none"> <li>• JSPS invitation fellowship</li> </ul>
20	Daniel John Weix	N/A	Professor, University of Rochester	Ph.D. Chemistry	<ul style="list-style-type: none"> <li>• Green Chemistry Award, Pfizer-Groton Green Chemistry Team 2015</li> <li>• Camille Dreyfus Teacher-Scholar Award, Camille &amp; Henry Dreyfus Foundation 2014</li> <li>• Novartis Early Career Award in Organic Chemistry 2014</li> <li>• Thieme Chemistry Journal Award 2013</li> <li>• Sloan Research Fellowship, Alfred P. Sloan Foundation 2013</li> </ul>	2 days	<ul style="list-style-type: none"> <li>• lecture @ ITbM seminar</li> <li>• research discussion</li> </ul>
21	Jerome Lacour	N/A	Professor, University of Geneva	Ph.D. in Chemistry	<ul style="list-style-type: none"> <li>• Visiting Professorships: Nagoya (2018), Bordeaux (2013)</li> <li>• Taiwan Chemistry Research Promotion Center, Visiting lectureship (2014)</li> </ul>	1 day	<ul style="list-style-type: none"> <li>• research discussion</li> </ul>
22	Paolo Melchiorre	44	Professor, ICIQ	Ph.D. in Chemical Sciences	<ul style="list-style-type: none"> <li>• Prize for Scientific Excellence from the Royal Spanish Chemical Society (RSEQ) 2016</li> </ul>	14 days	<ul style="list-style-type: none"> <li>• research discussion</li> </ul>
23	Peter R. Schreiner	52	Professor, Institute of Organic Chemistry, Justus-Liebig-University	Ph.D. Computational Chemistry, Organic Chemistry	<ul style="list-style-type: none"> <li>• Adolf-von-Baeyer Memorial Medal of the GDCh (2017)</li> </ul>	1 day	<ul style="list-style-type: none"> <li>• research discussion</li> </ul>
24	Barbara Helm	N/A	Reader, University of Glasgow	Ph.D. Biology	<ul style="list-style-type: none"> <li>• 2004 Awarded "Otto-Hahn Medal"</li> <li>• 2009 Awarded "Walther-Arndt Prize"</li> </ul>	3 days	<ul style="list-style-type: none"> <li>• lecture @ seminar</li> <li>• research discussion</li> </ul>
25	Samuel Refetoff	80	Professor, University of Chicago	Ph.D. Endocrinology	<ul style="list-style-type: none"> <li>• Fred Conrad Koch Lifetime Achievement Award of the Endocrine Society (2012)</li> <li>• Rosalind Pitt-Rivers Medal of the British Thyroid Association (2011)</li> <li>• MERIT Award, National Institutes of Health (2006, 1989)</li> <li>• Thyroid Pathophysiology Award Medal, The American Thyroid Association (2005)</li> </ul>	3 weeks	<ul style="list-style-type: none"> <li>• JSPS invitation fellowship</li> </ul>
26	Daniel Philippe Matton	53	Professor, University of Montreal	Ph.D. Plant Molecular Biology	<ul style="list-style-type: none"> <li>• University of Montréal Research Chair, Univ. de Montréal, 2012-2015.</li> <li>• Canada Research Chair in Functional Genomics and Plant Signal Transduction (2002-2007; renewed 2007-2012), Canada Research Chair Program.</li> <li>• Alexander von Humboldt Research Fellowship (Munich, Germany), Alexander von Humboldt Foundation (2007).</li> <li>• C. D. Nelson Award, Canadian Society of Plant Biologists (2004).</li> <li>• Postdoctoral Fellowships (NSERC and FRQNT; 1992-94).</li> </ul>	6 months	<ul style="list-style-type: none"> <li>• JSPS invitation fellowship</li> </ul>

## Appendix 6 FY2017 State of Outreach Activities

\* Using the table below, show the achievements of the Center's outreach activities in FY2017(number of activities, times held).

\* Describe those activities that have yielded novel results or that warrant special mention in the "Special Achievements" space below.

\* In appendix 7, list and describe media coverage (e.g., articles published, programs aired) in FY2017 resulting from press releases and reporting.

Activities	FY2017 (number of activities, times held)
PR brochure, pamphlet	ITbM A4 Pamphlet, ITbM B4 Pamphlet, Asia Research News 2018 (ITbM Research), ITbM Funding Brochure, NU Topics
Lectures, seminars for general public	NU Institute for Advanced Research Lecture (Itami), Gifu University Department of Engineering Lecture (Itami), Yomiuri Techno Forum Award Lecture (Itami), Nippon Soda Lecture (Itami), Sumitomo Dainippon Pharma Lecture (Itami), Coordination Chemistry Summer School (Itami), Yomiuri Techno Forum Osaka Lecture (Itami), ITbM Consortium Workshop (Itami), NU Alumni (Itami), Arimoto Salon (Higashiyama), NU Homecoming Day (Higashiyama), NU Open Lecture (Kinoshita), NU Coop (Sato)
Teaching, experiments, training for elementary, secondary and high school students	Kanuma HS Lecture (Itami), Nambu Junior HS Lecture (Itami), Asahi Kids Newspaper Forum (Itami/Higashiyama), University of Freiburg-Strasbourg-Nagoya Interdisciplinary and International Summer School (Itami), Takamatsu Daiichi HS SSH (Itami), Handa HSI SSH (Itami), Jishukan HS SSH (Itami), NU HS SSH Lecture (Higashiyama), Zuiryo HS Science Course (Yoshimura), Handa SSH Science Communication (Yoshimura), Hamamatsu City HS (Sato), Sakuradai HS (Sato), Asahigaoka HS (Sato), Ise HS (Sato)
Science café	NU School of Science Fresher's Science Café
Open houses	NU Festival, NU Homecoming Day
Participating, exhibiting in events	NU Fresher's Training, Chemistry Gran-Prix, International Chemistry Olympiad, Super Science High School Event, BioTech, BioJapan, Science Agora, AAAS Annual Meeting, Matsuzakaya Fukubukuro Science Event, WPI Science Symposium
Press releases	14 Press releases (Itami, Ueda, Y. Sato, Yamaguchi, Yoshimura, Torii, Murakami) 7 Press conferences (Itami, Ueda, Yoshimura, Higashiyama, Torii)

### <Special Achievements>

14 International Event/Press releases

## Appendix 7 FY 2017 List of Project's Media Coverage

\* List and describe media coverage (e.g., articles published, programs aired) in FY2017 resulting from press releases and reporting.

	Date	Types of Media (e.g., newspaper, television)	Description
1	Apr 4 - Nov 1, 2017	Newspaper, Magazine, Websites (Domestic/International)	Professor Takashi Ooi's research on organocatalysts, published in Nature Communications. Featured in Chunichi Shimbun and Monthly Chemistry magazine.
2	Apr 5 - 13, 2017	Newspaper, Websites (Domestic)	Professor Toshinori Kinoshita's research on plant stomata, published in Scientific Reports. Featured in Nikkei Sangyo Shimbun, Kagaku Kogyo Nippo
3	Apr 11 - 24, 2017	Websites (International)	Professors Tetsuya Higashiyama and Shigehiro Yamaguchi's research on a fluorescent probe molecule published in Angewandte Chemie International Edition. Featured in: Science Daily, Phys.Org
4	Apr 14 - Dec 17, 2017	Newspapers, Websites, TV, Magazines (Domestic/International)	Professor Kenichiro Itami's research on the synthesis of a carbon nanobelt, published in Science. Featured in: Chunichi Shimbun, Asahi Shimbun, Mainichi Shimbun, Yomiuri Shimbun, Nikkei Shimbun, Toyo Keizai, Monthly Chemistry magazine, FNN News, CBC TV, NHK, Nagoya TV, Fuji TV, Chemistry World, Science Magazine
5	Apr 21 - Oct 31, 2017	Newspapers, Websites (Domestic/International)	Dr. Minako Ueda and Professor Tetsuya Higashiyama's research on plant cell development, published in Genes and Development. Featured in: Nikkei Biotech, Nikkei Sangyo Shimbun, Kagaku Shimbun, Science Daily, Global Plant Council, Phys.Org
6	May 1, 2017	Website, Magazine (International)	Professor Tetsuya Higashiyama's research on ClearSee, a reagent to see inside plants, published in Development. Featured in: National Geographic
7	May 3 - Jun 1, 2017	Websites, Newspapers (Domestic)	Professor Kenichiro Itami was awarded the Chunichi Cultural Award. Featured in: Chunichi Shimbun
8	Jun 1 - Sep 26, 2017	Websites, TV (Domestic)	Professors Takahashi Yoshimura (animal biology), Kenichiro Itami (synthetic chemistry), Tetsuya Higashiyama's (plant biology) research was featured in a TV program series: Kagaku Michiru.
9	Jun 7 - Aug 21, 2017	Websites, Newspapers (Domestic/International)	Professor Kenichiro Itami's research on carbon rings, published in Angewandte Chemie International Edition. Featured in: Chunichi Shimbun, Nikkan Kogyo Shimbun, Kagaku Shimbun, Science Daily.
10	Jul 6 - Aug 8, 2017	Websites (Domestic/International)	Dr. Norihito Nakamichi and Professor Toshinori Kinoshita research on the circadian clock in plants, published in the Plant Journal. Featured in: Nikkei Asian Review, Agricultural Business Magazine
11	Jul 25 - Aug 25, 2017	Websites, Newspapers (Domestic/International)	Professors Tetsuya Higashiyama and Shigehiro Yamaguchi's research on a fluorescent probe molecule published in the Journal of the American Chemical Society. Featured in: Nikkei Sangyo Shimbun, Nikkan Kogyo Shimbun, Science Daily, Phys.Org
12	Aug 2, 2017 - Mar 6, 2018	Websites (International)	Professor Takashi Yoshimura's research on the circadian clock in roosters, published in Scientific Reports and Current Biology. Featured in various languages: Italian, Spanish, Indonesian, Chinese, French
13	Sep 4 - Nov 3, 2017	Newspapers, Websites, TV, Magazines (Domestic/International)	Professor Takashi Yoshimura's research on the color perception of Medaka fish, published in Nature Communications. Featured in: Chunichi Shimbun, Asahi Shimbun, Yomiuri Shimbun, Nikkan Kogyo Shimbun, Nikkei Shimbun, NHK, Newton magazine, Science Daily, Science Magazine
14	20-Sep-17	Websites (International)	Professors Kenichiro Itami and Keiko Torii's research on plant stomata, published in Chemical Communications. Featured in: Science Daily, Phys.Org

15	Oct 1, 2017	Website, Magazine (Domestic)	Professor Kenichiro Itami's Interview. Featured in: Technologist's Magazine
16	Nov 11, 2017	Magazine (Domestic)	Professor Shigehiro Yamaguchi's interview. Featured in: Monthly Chemistry
17	Nov 13, 2017 - Jan 3, 2018	Websites, Newspapers (Domestic/International)	Professor Tetsuya Higashiyama's research on plant fertilization, published in Nature Communications. Featured in: Chunichi Shimbun, Nikkan Kogyo Shimbun, Science Daily, Phys.Org, Innovations Report
18	Jan 22 - 24, 2017	Websites, Newspapers (Domestic/International)	Professors Keiko Torii, Kenichiro Itami and Toshinori Kinoshita's research on plant hormones, published in Nature Chemical Biology. Featured in: Mainichi Shimbun, Chunichi Shimbun, Phys.Org
19	Jan 26 - Feb 19, 2017	Websites, Newspapers, TV (Domestic/International)	Professor Kenichiro Itami's research on nanographene synthesis, published in Science. Featured in: Chunichi Shimbun, Asahi Shimbun, Kagaku Shimbun, Nikkan Kogyo Shimbun, Nikkei Shimbun, NHK News, C&EN News, Science Daily, Phys. Org, Materials Today
20	Jan 31 - Feb 20, 2018	Websites (Domestic/International)	Professors Kenichiro Itami and Tetsuya Higashiyama's research on a flexible warped nanographene, published in Angewandte Chemie International Edition. Featured in: Nikkei Shimbun, Yahoo! Japan, Science Magazine, Imaging & Microscopy
21	Feb 7 - 13, 2018	Websites (International)	Professors Toshinori Kinoshita and Kenichiro Itami group's research on the parasitic plant, <i>Striga</i> , published in ACS Central Science. Featured in: C&EN News
22	Mar 22 - 29, 2018	Websites (Domestic/International)	Professor Kenichiro Itami's research on graphenes, published in Scientific Reports. Featured in: Optronics Online, Science Daily, Phys.Org, Science Magazine, Asian Scientist
23	Mar 25, 2018	Websites and Newspapers (Domestic)	Dr. Kei Murakami was awarded the Akazaki Award. Featured in: Chunichi Shimbun, Japan Press Network