

Date: 08/25/2019

JSPS US ALUMNI ASSOCIATION SEMINAR PROGRAM
REPORT

Organizer (Awardee)

Name: Duy H. Hua

Position & Affiliation: University Distinguished Professor, Kansas State University

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| 1. TITLE OF SEMINAR 2019 Designing Molecules Workshop and Conference |
| 2. DATE(S) August 15 – August 17, 2019 |
| 3. VENUE & CITY, STATE King Hall, Room 4, Department of Chemistry, Kansas State University, Manhattan, Kansas |
| 4. TARGETED RESEARCH AREAS (1) Nanoparticles and Application (2) Drug Discovery and Chemical Synthesis and (3) Biopolymers and Macromolecules |
| 5. NUMBERS OF PARTICIPANTS TOTAL: <u>67</u> persons including <u>1</u> US Alumni Association members -US: <u>30</u> persons -FROM OVERSEAS: <u>37</u> person(s) including <u>5</u> person(s) from Japan |

NOTES FOR REPORT

*Please be sure to include the following contents. (Maximum 5 pages)

- Executive Summary
- Topics Discussed with Outcomes & Future Challenges
- Workshop/Seminar Agenda

Executive Summary:

The 2019 Designing Molecules Conference would not be possible without the financial support from the Japan Society for Promotion of Science (JSPS) Washington Office and supplemental funding from the Department of Chemistry and Department of Grain Science and Industry at Kansas State University (KSU). The seminar program consisted of three-day events: (i) a Reception on the first evening; (ii) Presentations of ten seminars and twenty-five posters on the second date; and (iii) an excursion on the last day. The Director of JSPS Washington Office, Dr. Kohji Hirata, and International Program Associate, Mr. Hideki Kunii, provided JSPS International Program Information. In addition, ten outstanding researchers including two scientists from Japan and eight from United States were invited to present their current research results. They are (i) Professor Kiyosei Takasu from the Pharmaceutical Sciences, Kyoto University; (ii) Professor Nicolas Wallace from the Division of Biology, KSU; (iii) Professor Si Wu from the Department of Chemistry, University of Oklahoma; (iv) Professor Yonghui Li from the Department of Grain Science and Industry, KSU; (v) Professor Keiji Maruoka, Special Appointed Professor from Kyoto University; (vi) Professor Ho Leung Ng from the Department of Biochemistry and Biophysics, KSU; (vii) Professor James Takacs from the Department of Chemistry, University of Nebraska at Lincoln; (viii) Professor Shin Moteki from the Department of Chemistry, University of Missouri at Kansas City; (ix) Professor Nathan Oyler from the Department of Chemistry, University of Missouri at Kansas City; and (x) Professor Jun Li from the Department of Chemistry, KSU. Graduate students, postdoctoral fellows and faculty members have also presented their current research results in poster formats. Presenters and titles and abstracts of the seminar and poster presentations can be found in our website: www.ksu.edu/chem/dmwc2019/. Professors Takasu and Maruoka have agreed to serve as contacts for those who may need a host in Japan for collaboration in research projects for application to JSPS or postdoctoral fellowships and Visiting Professorships. Kiyosei Takasu and Duy Hua have also established collaboration on research projects in the synthesis and bio-evaluation of novel synthetic molecules. Graduate students, postdoctoral fellows and junior faculty members benefit greatly from frontier research projects from the presentations and discussions in addition to the information of JSPS-supported research programs and visiting scholarships in Japan.

Topics Discussed with Outcomes & Future Challenges:

The organizing committee was able to invite the aforementioned two faculty members from Japan and eight from the United States to present their cutting-edge research results and to attract twenty-five poster presentations on various research projects. Seminar Presentations include:

- New chemistry of four-membered carbocycles
- Human papillomavirus
- Top-down mass spectrometry for functional proteome and protein target identification
- Peptide antioxidants from grain proteins
- Organocatalysts for asymmetric catalysis
- Machine learning for drug discovery and design

- Catalytic asymmetric hydroboration
- Measurement of drug release using NMR
- Self-assembled catalytic dendrimers
- Electronic detection of protease activity for cancer diagnosis

The topics of poster presentations include drug-target identification using mass spectrometry, polystyrene-block-poly(ethylene oxide) microdomains, bacterial mutations revealing hydrogen bonds in structural heterogeneity, broad-spectrum antifungal agents based on drimenol, nanofibrillar-mediated *Streptococcus* biofilms, hyphal growth in *Candida albicans*, inhibition of drug-resistance human pathogenic fungi, functional metal-organic framework materials, synthesis and bio-evaluation of marine natural products, involvement of trioxodinitrate in formation of nitroxyl in cytochrome C oxidase, electron-transfer reaction in ferrocycytochrome C, theranostic agents based on gadolinium-based contrasting agent and their antitumor activity and drug delivery, fluorescence spectroscopy studies of silica-based heterogeneous catalysis, effective thiourea-core antibiotics, anti-methicillin-resistant staphylococcus aureus (MRSA) thiosemicarbazone complexes, dietary fiber assay for phosphorylated cross-linked starch, waxy starches for improving food storage, ring-closing reaction of isothiocyanate diselenides, mechanistic study of dye-decolorizing peroxidases, design of anti-leukemic drug 6-thiopurine, platinum-anchored vertically aligned carbon nanofibers in oxygen reduction of fuel cells, and protease profiling of breast cancers based on electrochemical biosensors.

Through presentations and discussions, we realized the importance of chemical reactions in various fundamental studies and applications including chemical and enzymatic catalysis, drug discovery, spectroscopic characterization, and development of electronic biosensors. We exchanged ideas and results and possible collaborations are developed including the use of mass spectrometry in identification of drug targets, novel drug discovery based on their unique mechanism of actions and applications in nano-delivery from specifically designed nanoparticles along with early detections of various diseases. Future challenges lie in the detailed understanding of mechanisms and targets of various chemical processes and diseases. Collaborations among different scientific disciplines may reach these goals.



Representative photos taken from the excursion at Konza Prairie, Manhattan, Kansas. More photos can be found from our website: <https://www.k-state.edu/chem/conferences/dmwc2019/photo.html>

Workshop/Seminar Agenda:

Department of Chemistry

Kansas State University

213 CBC Building

1212 Mid-Campus Dr North

Manhattan, KS 66506-0401 chemdept@k-state.edu

Schedule

Thursday, August 15, 2019

5:30pm - 7:30pm

Reception - International Grains Program Conference Center
1980 Kimball Avenue, Manhattan, KS 66502

Friday, August 16, 2019

8:10am - 8:20am

Welcome and Opening Remarks
Prof and Head Daniel Higgins & Conference Organizer and Prof Duy Hua

8:20am - 8:50am

JSPS International Program Information
Director Kohji Hirata and Mr. Hideki (<http://jpspsusa.org/wp/>)

8:50am - 9:50am

Novel Methods in Chemical Synthesis
Prof. Kiyosei Takes, Pharmaceutical Sciences, Kyoto University, Japan

9:50am - 10:00am

Break

10:00am - 12:00pm

Biopolymers and Macromolecules
Prof's Nicolas A. Wallace (Biology, KSU), Si Wu (University of Oklahoma),
Yonghui Li (Grain Sciences and Industry, KSU)

12:00pm - 1:00pm

Lunch Break and Posters (Chemistry, CBC Foyer)

1:00pm - 3:00pm

Drug Discovery and Chemical Synthesis
Prof's Keiji Maruoka (Kyoto University, Japan), Ho Leung Ng (Biochemistry,
KSU), James Takacs (Chemistry, University of Nebraska)

3:00pm - 3:10pm

Break

3:10pm - 5:10pm

Nanostructured Materials and Applications
Prof's Shin Moteki (Chemistry, University of Missouri), Nathan Oyler (Chemistry,
University of Missouri), Jun Li (Chemistry, KSU)

5:10pm - 6:00pm

Posters (Chemistry, CBC Foyer)

Saturday, August 17, 2019

10:00am - 1:00pm

Excursion, Konza Prairie (Interested Participants)
