



JSPS



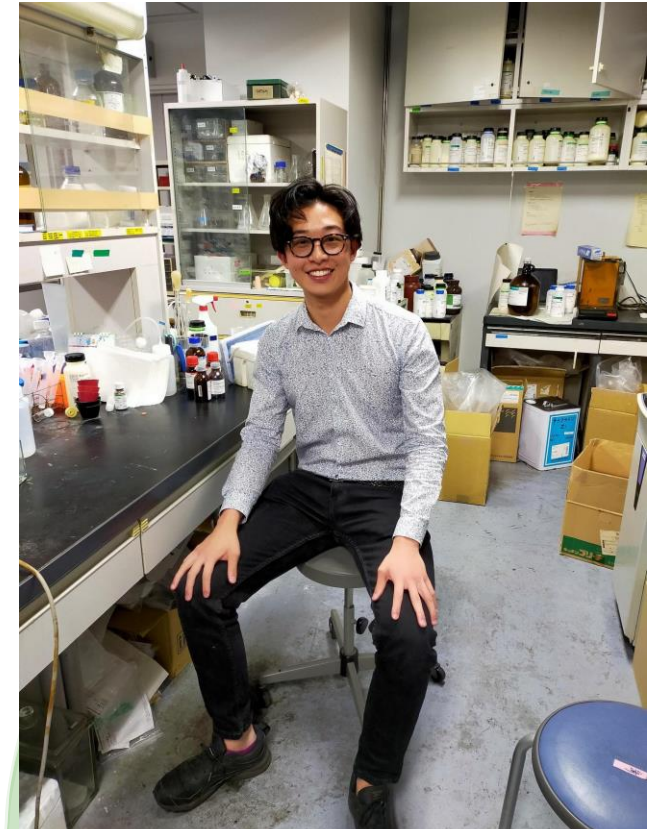
JSPS Summer Program (LONDON)

Henrik PH WONG

Postgraduate Researcher and Teaching Associate at The University of Manchester / Student Researcher at RIKEN

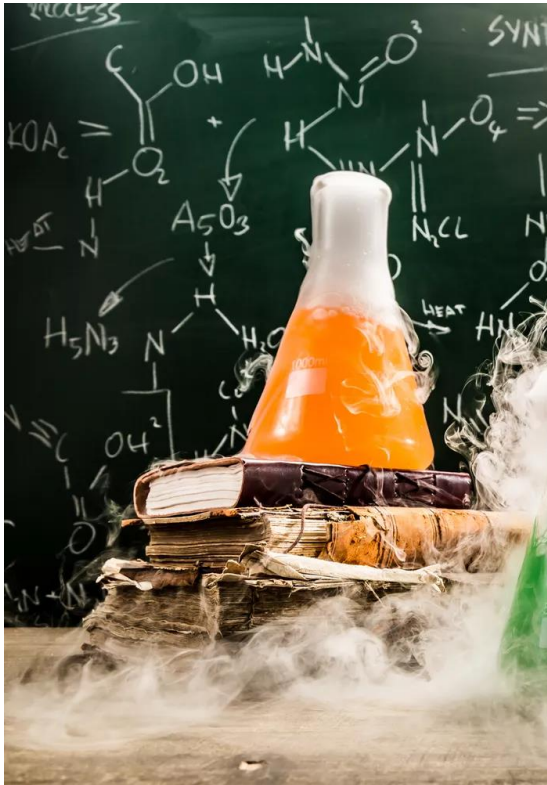
JSPS Fellow 2023

Friday 26th April 2024



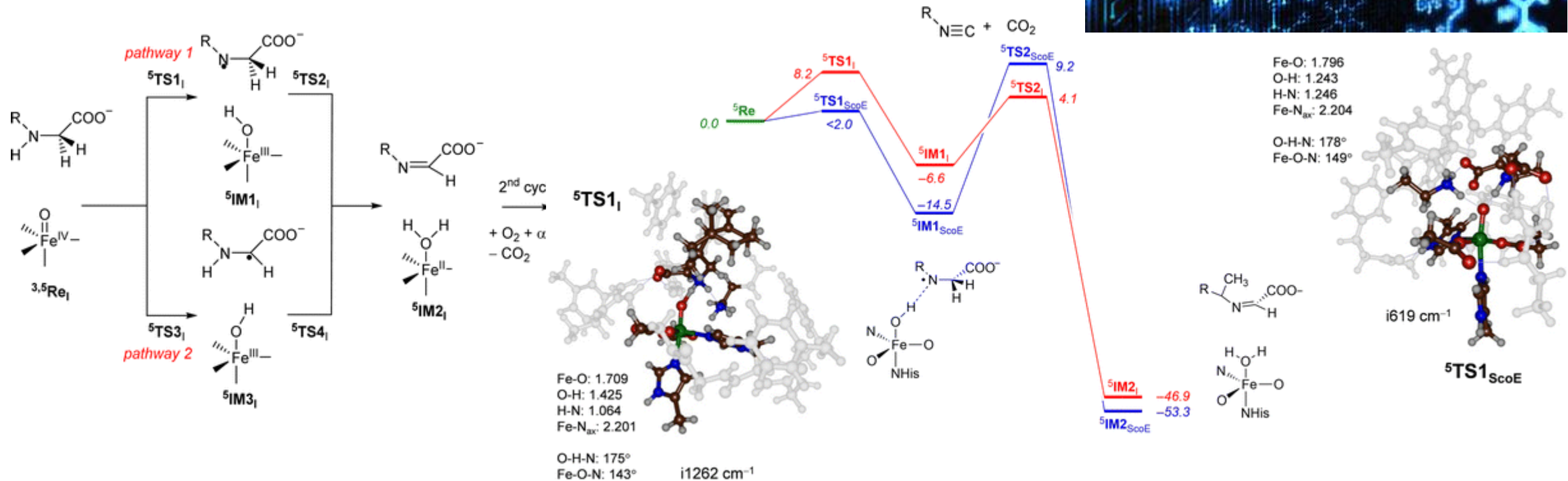
Background

Is there more?



Background

A → B



Introduction

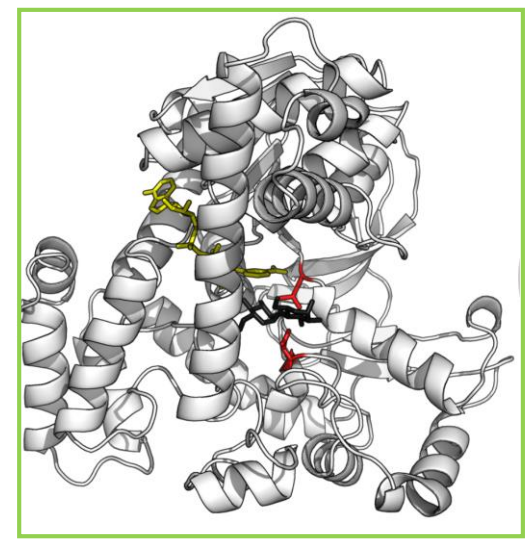
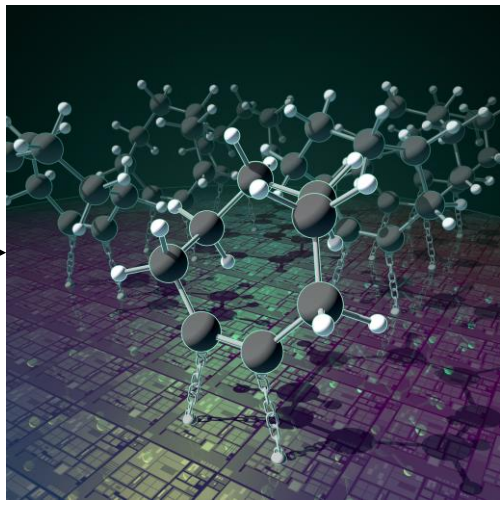
2nd Year PhD Chemical Engineering student at the University of Manchester

- MEng Chemical Engineering (2018-2022)
- PhD Chemical Engineering (2022 – Present)

❖ Molecular Engineering and Simulation



Supercomputer
MD / QM



Material Design
Catalysts
(Biocatalysts)
Enzymes

Introduction (Host)

The University of Tokyo (東京大學)

- Graduate school of Pharmaceutical Science, Natural Product Lab
Lab found in **(1893)** by Professor Jun'Ichiro SHIMOYAMA

Lab Specification

- 20+ People ranging from (B.S ~ Post-Doctoral)
- 70:30 (Japanese : International)

Lab Specialities:

- The biosynthesis of natural products (genome mining, **engineered biosynthesis**)
- The enzyme biocatalysts (**structure-based engineering, mechanistic studies**)
- The search for bioactive substances (isolation, structure elucidation, synthesis)



Professor Jun'Ichiro
SHIMOYAMA



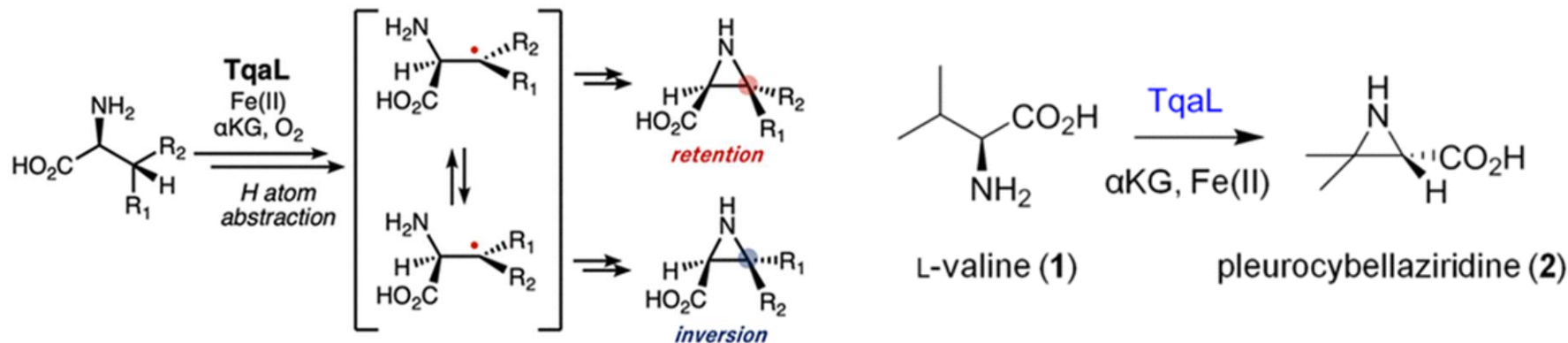
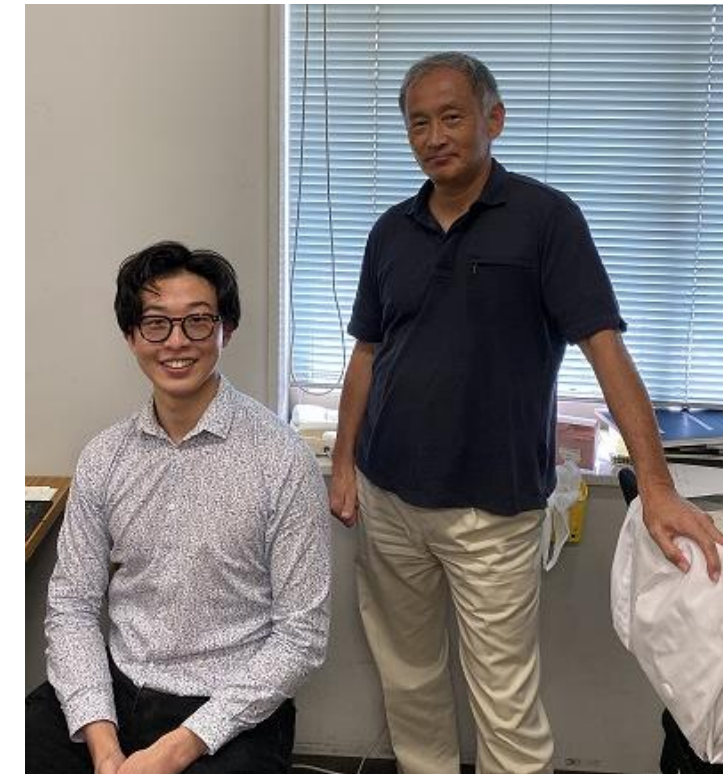
Professor Ikuro ABE
B.S, M.S, Ph.D Tokyo University

Develops strategies for discovering and exploiting small molecules, essential for **future drug discovery** efforts.

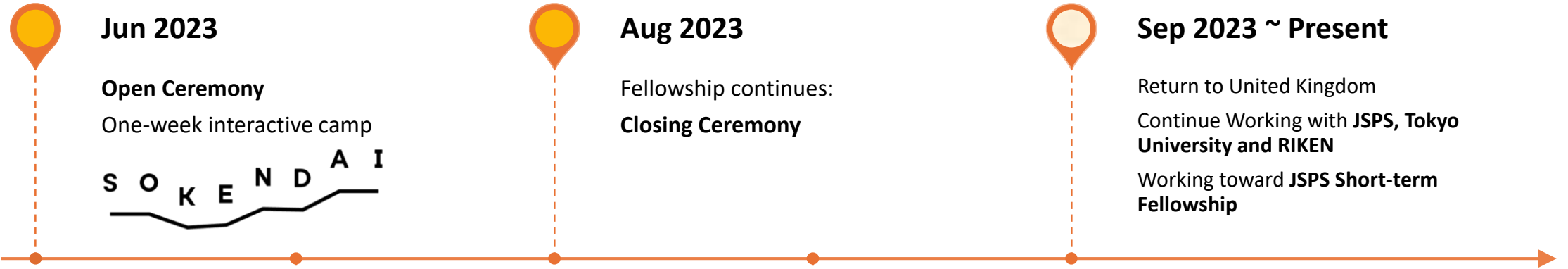
JSPS Summer Research

Origin of the selectivity Specificity of the Fe(II)/ α -Ketoglutarate Dependent Oxygenase TqaL

- Explore TqaL unusual aziridine formation
- Development of Mechanistic Pathways from A to B
- Prediction and testing of the proposed pathway



JSPS Summer Overview



Fellowship Begins
Tokyo University
Homestay program
July 2023



東京大学
THE UNIVERSITY OF TOKYO

JSPS Contract Extended
RIKEN extension
Sep 2023



理化学研究所



SOKENDAI



- One week before the JSPS Fellowship begins.
- Meet fellows from **around the world!**
- Poster presentation session
- Remember to bring your poster!



Origin of the selectivity Specificity of the Fe(II)/ α -Ketoglutarate Dependent Oxygenase Tqal

Henrik P.H Wong,^[1] Sam. P de Visser,^[1] and Ikuro Abe^[2]
^[1]Manchester Institute of Biotechnology and Department of Chemical Engineering, The University of Manchester, 131 Princess Street, Manchester M1 7DN, United Kingdom
^[2]Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo 113-0033, Japan

ABSTRACT

Non-heme iron enzymes are versatile catalysts in the biosynthesis of medicinal natural products and have attracted increasing attention as practical catalytic tools in chemical synthesis due to their ability to perform chemically challenging transformations. The nonheme iron enzyme Tqal is a recently discovered enzyme that catalyzes the unique reaction whereby the azidation of a valine amino acid is catalyzed. This is an important reaction in, for example, drug synthesis reactions and few biotechnological examples are known of selective azidation reactions at ambient temperatures. Currently, the mechanistic details as well as the synthetic potential of the Tqal-catalyzed ring closure reaction remain unclear. The work using Tqal, catalyzed L-valine by molecular modeling through the use of Molecular Dynamics (MD) simulations, Quantum Chemical (QM) packages such as density functional theory (DFT) and electric field effect to improve and establish the potential reaction mechanisms. We aim to investigate if Tqal can be an excellent candidate for use as a pharmacophore in a variety of drug development and discovery applications.

Introduction

Enzymes are flexible catalysts that are essential components of all forms of life and typically contain transition metal cofactors in nature. Mononuclear nonheme iron dioxygenases are found in all forms of life, including plants, people, and microbes, and catalyze oxygen atom transfer reactions to substrates. Non-heme iron oxygenases are involved in a variety of biological processes in plants, including growth signalling, stress responses, and secondary metabolism.^[1-7] Tqal catalyses unusual azidation formation from L-val via cleavage of the unactivated C-H bond. Which is crucial to several drugs such as aziridine rings, including mitomycin C, perfenoxin, and zimonicin B (carzinophilin). This adds to the possibilities of the employment of enzymes as a variety of ways.

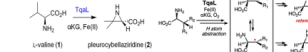


Figure 1: Suggested reaction with starting substrate from chosen substrate (L-valine) glycine to phenacyl glycidyl azidate (LGA) with proposed reaction mechanism of azidation formation using a non-heme iron (II)-dependent oxidase (Tqal) undergoing hydrogen atom abstraction (Right)

Aims and Objectives

The objectives of this study are to explore the potential of Tqal-catalyzed ring closure reactions and to investigate the mechanism and synthetic potential of this reaction using electric field effects.

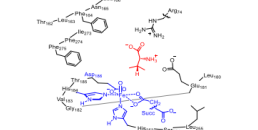


Figure 2: Preliminary model of Tqal from MD Simulation at Snapshot 2453.

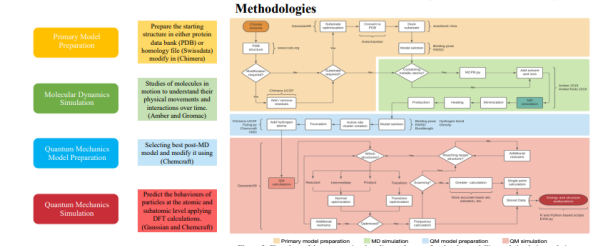


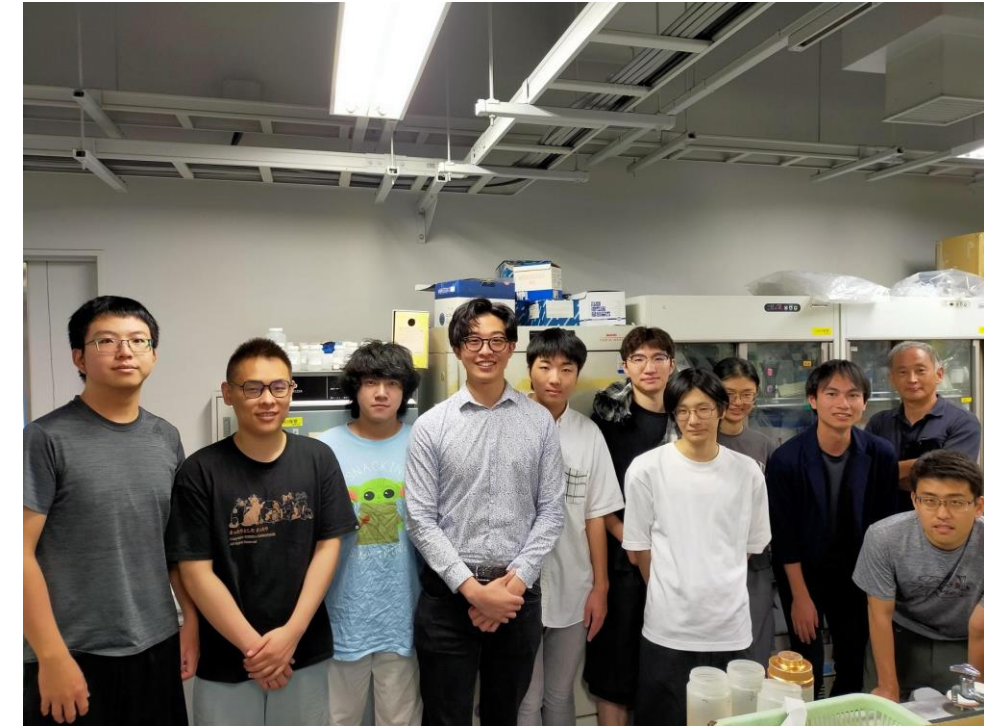
Figure 3: Flowchart of the computational workflow for molecular modeling and simulation techniques

Acknowledgement
 This work is supported by the Japan Society for the Promotion of Science (JSPS) summer fellowship in grants and Grant-in-Aid for Scientific Research and supercomputer facilities from The University of Tokyo and RIKEN in collaboration with Prof. Uchiyama's group. The University of Manchester computer shared facility (CSF) and Postgraduate Research Teaching Associate (PGRTA) Scholarships Ioh Cha, Jun C. Poon, Brady Zarella, Masha Shteyn, Angeli Yao, Yung Gao, and Wei-chen Cheng also provided support.



Tokyo University (東京大學)

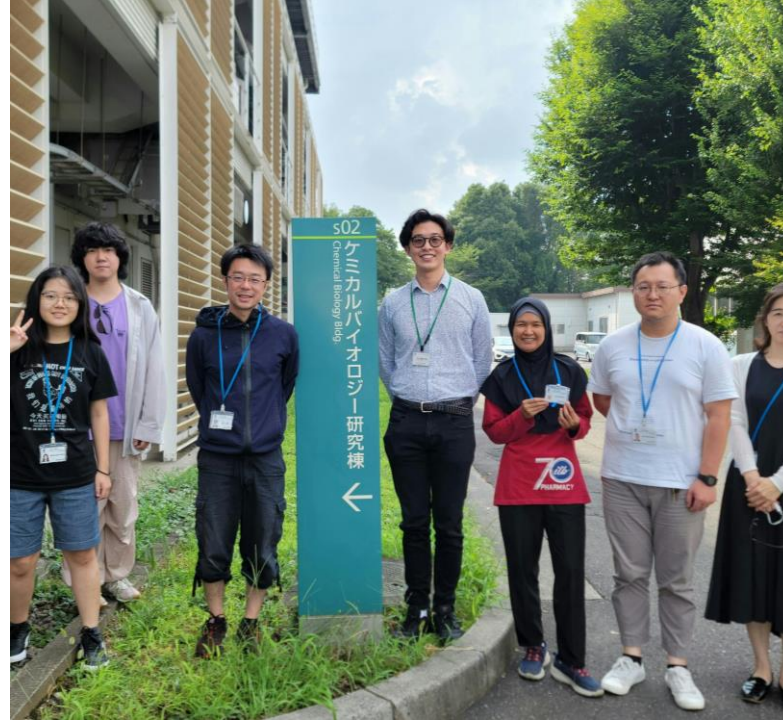
- Collaborate with undergraduate and postdoctoral students
- Participate in weekly meetings
- Conduct ongoing computational studies on enzymes
- Engage in learning, cultural exchanges, and meals with **new friends!**



RIKEN (理化学研究所)

Founded in 1917, it is the largest research institute in Japan!

- Birthplace of Nihonium 113!
- Home to the Fugaku supercomputer. (World No.1 <2022)
- Special collaboration with **RIKEN** and **Tokyo University**





Homestay

Late July *

- 3 days 2 nights
- Wishes, wishes and wishes!!

(Sushi, Firework, Temple and Many MORE!!)



Preparation: Pre-departure

Documentation

VISA!!

Certificate of Eligibility



Don't bring too many clothes!

Gifts for Host & Homestay
(Gifts + Letter)

Travel



Google Maps

Finance

1% Cash Back!



Cash



Accommodation



Communication

E-Sim or Sim

LINE (Homestay)

Whatsapp Group chat (Fellow)



Optional:

Business Card*

Diary**

External Harddrive**

Split Luggage!

Chopstick

*(Check with University)

** (Buy in Japan)

Research Culture
Can be very different

During Fellowship

Tips & Tricks
Bring your own bin
Talk quietly
Avoid handshakes & hugs

Travel



Shop



Etiquette



家でやろう。
Please do it at home.



座席の譲り占めはご遠慮ください。
Please share the seat with others.

飲屋でやろう
Please do it at the pub.



飲み過ぎのご来庫はご遠慮ください。
After a night drinking with buddies, please refrain from propping snoring on the train.

Post-Fellowship

- Maintains and creates academic links with Japan
- Provides guidance and support to new Fellows and Japanese researchers in the UK
- Conducts joint activities with academic institutions and counterpart agencies
- Facilitates the exchange of information among Alumni members
- Networking opportunities at Alumni Evenings



Career Aspects

The Fellowship Extend Beyond JAPAN

- **Student Researcher at RIKEN**
- **Gain connections** with prestigious Japanese universities and research institutes.
- **JSPS Alumni Association!**



Working Toward - JSPS Short-Term Fellowship!!

Contact Me!

For more tips and guidance.

Please contact me using below methods:

LinkedIn: Henrik Pak Hong WONG

Email: Henrik.wong@manchester.ac.uk

X: @HenrikPHWong



SCAN ME!



Henrik Pak Hong WONG

PhD & PGRTA Scholar @UOM | Student Researcher @RIKEN
| Former Research Fellow @JSPS | AFHEA
Manchester Area, United Kingdom
926 followers · 500+ connections

 RIKEN

 The University of Manchester

 Company Website [↗](#)

Happy to chat at any time! =)

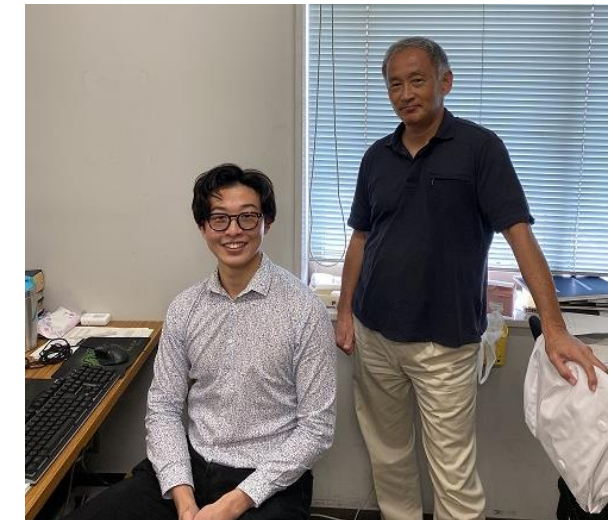
Thank you very much for your time!

Acknowledgements

- JSPS & JSPS London
- SOKENDAI
- Prof ABE's Lab @Tokyo University
- Prof AWAKAWA's Lab @RIKEN

Special Offers!

Nobuko San @Ramen Isshin,
Hongo (らーめん 一信)



FAQ

- An introduction to my research work and host institution in Japan
- What the summer programme fellows can expect from their orientation week at Sokendai, the home stay and research at the host institution
- Preparations fellows should make with visas, currency, splitting up luggage, taking business cards, research requirements
- Life in Japan including accommodation, mobile phones, Wi Fi access and travel
- Working in Japan including the research culture, etiquette, what to expect
- Challenges including the language and general culture
- Future collaborations with researchers in Japan and importance of joining the JSPS Alumni Association to maintain those links and the schemes we offer
- Any other advise you wish you had known before you went to Japan as a JSPS Fellow

FAQ

- How to find accommodation
(Sakura House, Oakhouse, Google for short-term lets) *Francis
- Working and living in Japan with limited Japanese language skill
(Learn Basic Japanese!)
- Social life in Japan- how to meet Japanese and international people
(Be yourself and take it slow)
- Accessing Japanese lessons through JSPS, the host institution and elsewhere
(Duolingo, JSPS provided material is sufficient)
- Using public transport
(Metro, Bus and E-Scotter)

