

PROGRAM

March 6 (Thursday)

- 15:00–18:00 Registration at Okazaki Conference Center
18:00–20:00 Get-Together Party at Okazaki Conference Center

March 7 (Friday)

- 8:50 – 9:00 Welcome Address
Hideo Mohri (President, Okazaki National Research Institutes)
- 9:00 – 9:10 Opening Remarks
Teizo Kitagawa (Center for Integrative Bioscience)
Chair: Teizo Kitagawa (Center for Integrative Bioscience)
- 9:10 – 10:10 **Kenneth D. Karlin** (The Johns Hopkins University)
Bioinorganic “Oxygen Activation” Emphasizing Copper and Non-Heme Iron Enzymes & Model Chemistry
Chair: Masao Ikeda-Saito (Tohoku University)
- 10:10 – 11:10 **Yoshihito Watanabe** (Nagoya University)
Molecular Mechanisms on the Compound I Formation of Heme Enzymes
- 11:10 – 11:30 Coffee Break
Chair: Toru Shimizu (Tohoku University)
- 11:30 – 12:30 **Isao Morishima** (Kyoto University)
Molecular Mechanism of P450cam Catalyzed Oxygenation Reaction Regulated by the Association with Putidaredoxin
- 12:30 – 13:30 Lunch
- 13:30 – 15:00 **Poster Discussion** (Odd Numbers)
Chair: Osamu Yamauchi (Kansai University)
- 15:00 – 16:00 **Lucia Banci** (University of Florence)
NMR in Structural Genomics of Metalloproteins
Chair: Takamitsu Kohzuma (Ibaraki University)
- 16:00 – 17:00 **Gerard W. Canters** (Leiden University)
The Spectroscopy of Copper Proteins in Relation to Their Function
Chair: Isao Morishima (Kyoto University)
- 17:00 – 18:00 **Andrew J. Thomson** (University of East Anglia)
Magnetic and Optical Methods of Studying Metalloproteins

March 8 (Saturday)

Chair: Kiyoshi Fujisawa (Tsukuba University)

9:00 – 10:00 **Thomas V. O'Halloran** (Northwestern University)
Chemistry of the Cellular Cytoplasm: Receptors for Monitoring and
Controlling Metal Ion Activity

Chair: Hideo Akutsu (Osaka University)

10:00 – 11:00 **Eiichi Kimura** (Hiroshima University)
Macrocyclic Zinc(II)-Fluorophores for New Detectors of Apoptosis

11:00 – 11:20 Coffee Break

Chair: Norikazu Ueyama (Osaka University)

11:20 – 12:20 **Anthony G. Wedd** (The University of Melbourne)
Chemistry of the Transfer of Copper(I) between Copper-Binding Proteins

12:20 – 13:20 Lunch

13:20 – 15:00 **Poster Discussion** (Even Numbers)

Chair: Kenneth D. Karlin (The Johns Hopkins University)

15:00 – 15:30 **Shinobu Itoh** (Osaka City University)
Mechanism of Phenolase Reaction of Tyrosinase Enzymatic Reaction vs.
Model Reaction

15:30 – 16:00 **Wonwoo Nam** (Ewha Womans University)
Reactive Intermediates in Biomimetic Models of Heme and Nonheme
Iron Oxygenase Enzymes

16:00 – 16:30 **Prasat Kittakoop** (National Center for Genetic Engineering and
Biotechnology)
Biologically Active Compounds from Thai Plants and Microorganisms

16:30 – 16:50 Coffee Break

Chair: Anthony G. Wedd (The University of Melbourne)

16:50 – 17:20 **Takeshi Nishino** (Nippon Medical School)
Structure and Mechanism of Xanthine Oxidoreductase, a Molybdenum
Containing Iron-Sulfur Flavoprotein

17:20 – 17:50 **Periakaruppan T. Manoharan** (Indian Institute of Technology)
Subunit Heterogeneity in Reconstituted and Hybrid Hemoglobins

17:50 – 18:20 **Zijian Guo** (Nanjing University)
From Mechanistic Study to the Design of Metal-Based Anticancer
Complexes

18:30 – Steering Committee Meeting

March 9 (Sunday)

Chair: Thomas V. O'Halloran (Northwestern University)

- 9:00 – 9:30 **Shigetoshi Aono** (Center for Integrative Bioscience)
Structure and Function of the Heme-Based Sensor Proteins, CooA and HemAT-Bs
- 9:30 – 10:00 **Youn Soo Sohn** (Ewha Womans University)
Selective Tumor Targeting by EPR Effect. Synthesis, Biodistribution and Antitumor Activity of Polyphosphazene-Platinum(II) Conjugates
- 10:00 – 10:30 **Edward R. T. Tiekink** (National University of Singapore)
Triorganophosphinegold(I) Thiolates: Pharmacological Applications and Anti-Tumour Potential
- 10:30 – 11:00 Coffee Break

Chair: Lucia Banci (University of Florence)

- 11:00 – 11:30 **N. Jayaraman** (Indian Institute of Science)
Zinc(II)-Dithiolate Complex of Insulin B Chain
- 11:30 – 12:00 **Masatatsu Suzuki** (Kanazawa University)
Reversible O–O Bond Cleavage and Reformation of Peroxo Group of Peroxocarbonate Ligand of Iron(III) complex
- 12:00 – 12:30 **Wing-Tak Wong** (The University of Hong Kong)
Gadolinium Complexes Containing Polyamino Polycarboxylate Ligands for Magnetic Resonance Imaging (MRI) Contrast Agents
- 12:30 – 13:30 Lunch
- 13:30 – 15:00 **Poster Discussion**

Chair: Suresh V. S. Rana (Ch. Charan Singh University)

- 15:00 – 15:30 **Seog K. Kim** (Yeungnam University)
Simultaneous Binding of Ru(II)[(1,10-Phenanthroline)₂dipyridophenazine]²⁺ and Minor Groove Binder 4[6-Diamidino-2-Phenylindole to Poly[d(A-T)₂] and DNA Mediated Energy Transfer between the Drugs
- 15:30 – 16:00 **Bhaskar G. Maiya** (University of Hyderabad)
Photonuclease Activity of Co(III), Ni(II) and Ru(II) Complexes Containing Intercalatable, Photoactive Polypyridyl Ligands
- 16:00 – 16:20 Coffee Break

Chair: Gerard W. Canters (Leiden University)

- 16:20 – 16:50 **Pin Yang** (Shanxi University)
Double-Strand Hydrolysis of DNA by Some Artificial Nucleases
- 16:50 – 17:20 **Takamitsu Kohzuma** (Ibaraki University)
A Mechanistic Approach to the Crystal Growth of a Heme Protein,
Cytochrome *c*' in Space Experiment STS-107
- 17:20 – 17:50 **Nenad M. Kostic** (Iowa State University)
Selective Cleavage of Peptides and Proteins with Metal Complexes as
Artificial Enzymes
- 18:30 – 21:00 Banquet

March 10 (Monday)

Chair: Yoshihito Watanabe (Nagoya University)

- 9:00 – 9:30 **Shyamalava Mazumdar** (Tata Institute of Fundamental Research)
Effect of Variations in the Redox Potential of the Metal Center on the
Peroxidase Activity of a Hemeprotein
- 9:30 – 10:00 **Norikazu Ueyama** (Osaka University)
Regulation of Oxo-Transfer Reactivity by Intramolecular Hydrogen
Bond toward Ligating Atom in the Active Center of Mo-, W-Oxidases
and P450
- 10:00 – 10:30 **Hongzhe Sun** (University of Hong Kong)
Interactions of Antimony Antiparasitic and Bismuth Antiulcer Agents
with Peptides and Proteins: Insights into the Possible Mechanism of
Action
- 10:30 – 11:00 Coffee Break

Chair: Andrew J. Thomson (University of East Anglia)

- 11:00 – 11:30 **Takashi Ogura** (The University of Tokyo)
Resonance Raman Study on Cytochrome *c* Oxidase in Its Solubilized
State, in Intact Mitochondria and in Reconstituted Vesicles
- 11:30 – 12:00 **Yoshinori Naruta** (Kyushu University)
Preparation of Peroxo-Bridged Heme-Copper Complex and Its Crystal
Structure
- 12:00 – 12:30 **Sunney I. Chan** (Institute of Chemistry, Academia Sinica)
Stereospecific Hydroxylation of Small Alkanes by the Particulate
Methane Monooxygenase from *Methylococcus capsulatus* (Bath)
- 12:30 – 12:40 Concluding Remarks
Yoshihito Watanabe (Nagoya University)

Poster Presentation

P-1 Synthesis and Structure-Activity Relationships of Novel Platinum(II) Complexes of (N-Substituted) Dicarboxylic Amino Acids

Jin Kyu Kim¹, Yeong-Sang Kim^{1,2}, Rita Song^{1,3}, Moo Jin Jun², and Youn Soo Sohn^{1}*
(¹Ewha Womans University, Korea, ²Yonsei University, Korea, ³Korea Institute of Science and Technology, Korea)

P-2 Synthesis of Orally Active (Diamine)Platinum(IV) Complexes of Mixed Carboxylates

Joo Ik Kim^{1,2}, Sun Young Park¹, Yeong-Sang Kim^{1,2}, Rita Song³, and Youn Soo Sohn¹
(¹Ewha Womans University, Korea, ²Yonsei University, Korea, ³Korea Institute of Science and Technology, Korea)

P-3 The Detection of Polynuclear Pt(II) Species During the Reaction of Platinum Complexes and Biological Thiols

Qin Liu^{1,2}, Jun Lin¹, Longgen Zhu¹, and Zijian Guo^{1}* (¹Nanjing University, P. R. China, ²Nanjing College of Economics, P. R. China)

P-4 Synthesis and Antitumor Activity of DNA-Binding Cationic Porphyrin-Platinum(II) Complexes

Rita Song¹, Yeong-Sang Kim^{2,3}, Chong Ock Lee⁴, and Youn Soo Sohn² (¹Korea Institute of Science and Technology, Korea, ²Ewha Womans University, Korea, ³Yonsei University, Korea, ⁴Korea Research Institute of Chemical Technology, Korea)

P-5 Interaction of Certain Binuclear Cobalt(III)-Diimine Complexes with Calf Thymus DNA

*Pitchumony Tamil Selvi and Mallayan Palaniandavar** (Bharathidasan University, India)

P-6 Anion Recognition by Zn²⁺-(Guanidinylolethyl)cyclen in Aqueous Solution

Shin Aoki¹, Kenta Iwaida¹, Motoo Shiro², Kei Takeda¹, and Eiichi Kimura³
(¹Hiroshima University, Japan, ²Rigaku Corporation X-Ray Research Laboratory, Japan, ³Hiroshima University, Japan)

- P-7 Modification of DNA by the Platinum Complex of the Dimeric Zinc Complex Having a 2,2'-Bipyridyl Linker**
Mohd Zulkefeli¹, Rieko Okatani¹, Shin Aoki¹, Kei Takeda¹, and Eiichi Kimura²
(¹Hiroshima University, Japan, ²Hiroshima University, Japan)
- P-8 Reduction of Pentavalent Antimony(Sb^V) by Trypanothione and Formation of a Binary and Ternary Complex of Antimony(III) and Trypanothione**
Siucheong Yan, Fei Li and Hongzhe Sun (University of Hong Kong, China)*
- P-9 Biologically Active Copper(II) Complexes: Synthesis, Spectral and Electrochemical Characterization, DNA Intercalation and Biological Studies**
Gurusamy Rajagopal¹, Kasi Nehru², and Periakaruppan Athappan²* (¹Crescent Engineering College [Affiliated to Anna University], India, ²Madurai Kamaraj University, India)
- P-10 Binding Mode of the Cu(Brazilin) Complex to Native DNA and Its Active Species as Chemical DNA Nuclease**
*Hyun Mee Lee¹, Youn Hee Chae¹, Maeng-Joon Jung² and Seog K. Kim¹** (¹Yeungnam University, Republic of Korea, ²Sangju National University, Republic of Korea)
- P-11 Interaction of Metal Complexes Containing Tridentate Ligand with DNA**
V. G. Vaidyanathan and Balachandran Unni Nair (Central Leather Research Institute, India)
- P-12 Double Strand Cleavage by a Dinuclear Cu(II) Complex**
Junghee Kim and Soohyun Kim (Sun Moon University, Korea)*
- P-13 Hydrolytic Cleavage of DNA by Dinuclear Metal Complexes**
Fei Gao and Yin Caixia (Shanxi University, P. R. China)
- P-14 Selective Recognition of Nucleobases by Organometallic Ruthenium Complexes**
Rafael Fernández, Michael Melchart, Abraha Habtemariam, and Peter J. Sadler (University of Edinburgh, UK)

P-15 DNA Interactions of Ruthenium(II) Complexes Bearing a New Generation of Photoactive Ligands

Sastri, C. V. and Maiya, B. G (University of Hyderabad, India)*

P-16 Modulation of Heavy Metal Toxicity by Vitamins and Hormones

S. V. S. RANA (Ch. Charan Singh University, India)

P-17 Molecular Dynamic Correlation Analyses of the Metal-Protein Binding Motif, the Protein Profile and Biosorption-Toxicity Studies of Lead (Pb) and Cadmium (Cd) Resistant Marine Sediment Bacteria (*Bacillus spp.* 1 and 2 and *Chryseomonas sp.* 2) Isolated from Iligan Bay

Myrna S. Mahinay¹, Mannix P. Balanay², Franco G. Teves³, and Alexis C. Daquinag⁴ (¹MSU-Iligan Institute of Technology, Philippines, ²Siquijor State College, Philippines, ³MSU-Iligan Institute of Technology, Philippines, ⁴Baylor College of Medicine, USA)

P-18 Specification of Bio-Accumulated Toxic Metals-A Computer Modeling Study

T. Sive Rao and G. Nageswara Rao (Andhra University, India)

P-19 Studies on the Interaction between cis-[Ru(2,2,2-tet)Cl₂]ClO₄ with Human Serum Albumin and Human Serum Transferrin

Rong Chen, Ella Lai-Ming Wong, Hong-Zhe Sun, and Chi-Ming Che* (The University of Hong Kong, P. R. China)*

P-20 Hydrolysis of Phosphate Ester by Zinc(II) Complex of a Tetradentate Ligand Providing Sulfur and Nitrogen Donors

Fumio Akagi and Masami Ito (Oita University, Japan)

P-21 Hydrolysis by the Zinc Finger Peptides: Conversion of Structural Zinc Sites into Catalytic Zinc Sites

Akiko Nomura and Yukio Sugiura (Kyoto University, Japan)

P-22 Design of Dimetal-Binding α -Helical Coiled Coil Peptide

Toshihisa Mizuno¹, Mihoko Koike¹, Kiyoko Wada¹, Kunihiro Tajima², Jun-ichi Oku¹, and Toshiki Tanaka^{1} (¹Nagoya Institute of Technology, Japan, ²Kyoto Institute of*

Technology, Japan)

P-23 Towards the Design of Synthetic Enzymes

David Weber and Christin Choma (Rensselaer Polytechnic Institute, USA)

P-24 The Investigation of Bacterial Iron Transports Using Trihydroxamate Artificial Siderophores

Kenji Matsumoto, Masanori Hasebe, Tomohiro Ozawa, Koichiro Jitsukawa, and Hideki Masuda (Nagoya Institute of Technology, Japan)

P-25 Design, Expression, and Self-Assembling Properties of Hydrophobic Polypeptides Bearing Cysteine(s) as a Mimic of Bacterial Photosynthetic Antenna Complex

Takehisa Dewa^{1,2}, Taku Yamada¹, Taeko Mizuno¹, Makiko Ogawa¹, Kiyotaka Yoshida¹, Yoshiaki Nakao¹, Masaharu Kondo¹, Kouji Iida³, Keiji Yamashita¹, Toshiki Tanaka¹, and Mamoru Nango¹ (¹Nagoya Institute of Technology, Japan, ²PRESTO, JST, ³Nagoya Municipal Industrial Research Institute, Japan)

P-26 Structure and Biological Activity of Germatranes Containing Ge-C Bond

Edmunds Lukevics and Luba Ignatovich (Latvian Institute of Organic Synthesis, Latvia)

P-27 1,10-Phenanthroline Phosphorylates (Activates) MAP Kinase in *Xenopus* Oocytes

Ken-Ichi Watanabe, Toshinobu Tokumoto, and Katsutoshi Ishikawa (Shizuoka University, Japan)

P-28 Luminescent Terbium(III) Complex Showing Selectivity to Bicarbonate and Salicylate in Aqueous Solution: The Recognition Derived from Chelating Mode

Cong Li and Wing-Tak Wong (The University of Hong Kong, P. R. China)*

P-29 Structure and Spectrochemical Study Using Metal Substituted Blue Copper Model Complexes

Yuki Matsunaga, Naoko Ibi, Yoshitaro Miyashita, Kiyoshi Fujisawa, and Ken-ichi Okamoto (University of Tsukuba, Japan)

P-30 Magnetic, EPR and SOD Studies of Some Cu^{II}-Cu^{II}, Cu^{II}-Ni^{II} and Cu^{II}-Zn^{II}

Imidazolate Bridged Complexes

R. N. Patel (A. P. S. University, India)

P-31 A Sterically Hindered Salen Iron Complex as a Model for Mononuclear Non-Heme Iron Enzymes

Takuya Kurahashi¹, Hiroshi Fujii¹, Manabu Sugimoto², Takashi Ogura³, and Kenji Oda³ (¹Institute for Molecular Science, Japan, ²Kumamoto University, Japan, ³The University of Tokyo, Japan)

P-32 Efficient Olefin cis-Dihydroxylation and Epoxidation by Non-Heme Iron Catalysts with H₂O₂

Jinheung Kim, Ju Yeon Ryu, Wonwoo Nam, Lawrence Que, Jr. (Changwon National University, Korea, Ewha Womans University, Korea, University of Minnesota, USA)

P-33 Interaction of a Monodentate Ligand to Five-Coordinated Co(III) Complex with N₂S₃ Environment Directed to Nitrile Hydratase

Tomohiro Ozawa, Takayuki Goto, Yasuhiro Funahashi, Koichiro Jitsukawa, and Hideki Masuda (Nagoya Institute of Technology, Japan)

P-34 Cu(II) Regulation by Aromatic-Aromatic Ring Stacking Interaction

Akira Odani¹, Tetsuro Taniguchi², Maya Saita², Yoshihito Watanabe², and Osamu Yamauchi³ (¹Nagoya University, Japan, ²Nagoya University, Japan, ³Kansai University, Japan)

P-35 Synthesis and Reactivity of Dinuclear Transition Metal Complexes Supported by Binaphthyl-Containing Dinucleating Ligands with Axial Chirality

Takayuki Nagataki, Yoshimitsu Tachi, and Shinobu Itoh (Osaka City University, Japan)

P-36 Synthesis and Characterization of Tetranuclear Manganese Complexes of a Quinoline-Based Ligand

Yuji Mikata¹, Motoko Wakamatsu², Yuriko Abe², and Shigenobu Yano³ (¹Nara Women's University, Japan, ²Nara Women's University, Japan, ³Nara Women's University, Japan)

P-37 Synthesis and Characterization of the Dicopper(I) Complex Supported by Novel Unsymmetrical Penta-Pyridine Ligand

Kazuki Aita¹, Yoshimitsu Tachi¹, Shinichi Teramae², Shunichi Fukuzumi², and Shinobu Itoh¹ (¹Osaka City University, Japan, ²Osaka University, CREST, Japan)

P-38 Characterization of Isomerism between the μ - η^2 : η^2 -Peroxo and Bis(μ -oxo)dicopper Cores by Density Functional Theory

Ping-Yu Chen and Sunney I. Chan (Academia Sinica, Taiwan)

P-39 Dioxygen Reactivity of Mono- and Di-Copper(I) Complexes Supported by 1,3,5-Triethylbenzene Spacer Ligands Carrying Pyridylamine Didentate Metal Binding Sites

Hiroshi Ohi, Yoshimitsu Tachi, and Shinobu Itoh (Osaka City University, Japan)

P-40 Ternary Copper(II) Complexes with Axial Sulfur Ligation as Structural Models for the Cu_B Site of Dopamine β -Hydroxylase and Peptidylglycine β -Hydroxylating monooxygenase

Pattubala A. N. Reddy, Bidyut K. Santra, Munirathinam Nethaji, and Akhil R. Chakravarty (Indian Institute of Science, India)*

P-41 Bis(μ -Oxo)Dicopper Complex with Tetrahedral Distortion Introduced by Using (-)-Sparteine

Yasuhiro Funahashi¹, Yuko Wasada-Tsutsui¹, Shun Hirota², Mitsumi Kishida¹, Toshio Ouchi¹, Tomohide Nishikawa¹, Hidekazu Arai¹, Yasutaka Honda¹, Syuhei Yamaguchi¹, Tomohiro Ozawa¹, Koichiro Jitsukawa¹, and Hideki Masuda¹ (¹Nagoya Institute of Technology, Japan, ²Kyoto Pharmaceutical University, Japan)

P-42 Spectroscopic Characterization of the Reaction between Bis(μ -oxo)dicopper(III) Complex and Triphenylphosphine

Svitlana V. Pavlova¹, Huang-Chou Chen², and Sunney I. Chan^{1,2} (¹Academia Sinica, Taiwan, ²National Tsing-Hua University, Taiwan)

P-43 Low-Temperature Stopped-Flow Studies on the Reactions of Copper(II) Complexes and Hydrogenperoxide

Takao Osako, Yoshimitsu Tachi, and Shinobu Itoh (Osaka City University, Japan)

P-44 Characterization of the Copper C-Clusters of the Particulate Methane

Monooxygenase in *Methylococcus Capsulatus* (BATH)

Huang-Chou Chen^{1,2}, *Steve Sheng-Fa Yu*¹, *Sunney I. Chan*^{1,2} (¹*Academia Sinica, Taiwan*, ²*National Tsing-Hua University, Taiwan*)

P-45 The Hydroxylation Chemistry of Chiral Butanes Mediated by the Particulate Methane Monooxygenase from *Methylococcus Capsulatus* (BATH)

Steve Sheng-Fa Yu, *Lo-Ying Wu*, and *Sunney I. Chan* (*Academia Sinica, Taiwan*)

P-46 Recent Developments in the Synthesis of Mo/Fe/S Clusters. Pursuit for the Synthetic Nitrogenase Cofactor

Jaehong Han (*Virginia Polytechnic Institute and State University, USA*)

P-47 Preparation and Characterization of a (Cu, Zn)-pMMO From *Methylococcus Capsulatus* (BATH)

Chang-Li Chen^{1,2}, *Huang-Chou Chen*^{1,2}, *Shyue-Chu Ke*³, *Steve S.-F. Yu*², *Lo-Ying Wu*^{1,2}, and *Sunney I. Chan*^{1,2*} (¹*Academia Sinica, Taiwan*, ²*National Tsing-hua University, Taiwan*, ³*National Dong-hua University, Taiwan*)

P-48 Preparation, Purifications and Characterization of CODH/ACS from *Methanosarcina thermophila* and Its Interactions with CO and NO

*Tapan Kumar Kundu** and *Stephen W. Ragsdale* (*University of Nebraska Lincoln, U.S.A*)

P-49 Reaction Mechanism of Nitrile Hydratase; Analysis by Isovarelonitrile

Kayoko Taniguchi^{1,2}, *Masanari Tsujimura*¹, *Masafumi Odaka*¹, *Mikio Hoshino*³, *Hiroyuki Koshino*⁴, *Takuji Hirose*², *Isao Endo*⁵, and *Mizuo Maeda*¹ (¹*The Institute of Physical and Chemical Research (RIKEN), Japan*, ²*Saitama University, Japan*, ³*RIKEN, Japan*, ⁴*RIKEN, Japan*, ⁵*Utsunomiya University, Japan*)

P-50 Reaction Mechanism of Nitrile Hydratase; Analysis by Isobutyronitrile

*Masafumi Odaka*¹, *Masanari Tsujimura*¹, *Hiroshi Nakayama*², *Naoshi Dohmae*², *Hiroyuki Koshino*³, *Tadao Asami*⁴, *Mikio Hoshino*⁵, *Koji Takio*², *Mizuo Maeda*¹, and *Isao Endo*⁶ (¹*The Institute of Physical and Chemical Research (RIKEN), Japan*, ²*RIKEN, Japan*, ³*RIKEN, Japan*, ⁴*RIKEN, Japan*, ⁵*RIKEN, Japan*, ⁶*Utsunomiya University, Japan*)

**P-51 NMR Structure of the Transmembrane Domain⁴ of the Divalent Metal-Ion
Transporter DMT1**

Fei Li¹, Hongyan Li², Zhong-Ming Qian² and Hongzhe Sun^{1} (¹The University of
Hong Kong, P. R. China, ²The Hong Kong Polytechnic University, P. R. China)*

P-52 Structural Study of Iron Transporter Nramp1 by CD and Fluorescence

Miufan Kwan, Fei Li and Hongzhe Sun (The University of Hong Kong, P. R. China)*

P-53 ¹⁹F NMR Study on Heme Electronic Structure in Reconstituted Hemoproteins

*Yueki Hirai¹, Satoshi Nagao¹, Tatsunori Inose¹, Norifumi Terui¹, Yasuhiko Yamamoto¹,
and Akihiro Suzuki² (¹University of Tsukuba, Japan, ²Nagaoka National College of
Technology, Japan)*

**P-54 Characterization of the F20A Mutant of Cytochrome *c*₃ from *D. vulgaris* Miyazaki
F**

*Yuki Takayama¹, Rie Kobayashi², Erisa Harada^{1,3}, Kiyoshi Ozawa² and Hideo
Akutsu^{1,4} (¹Osaka University, Japan, ²Yokohama National University, Japan, ³Japan
Biological Informatics Consortium, Japan, ⁴Institute for Molecular Science, Japan)*

**P-55 The Effects of Surface Charges in Cytochrome *c*₃ from *D. Vulgaris* Miyazaki F on
Its Reduction by Hydrogenase**

*Naoki Yahata¹, Kiyoshi Ozawa², and Hideo Akutsu^{1,3} (¹Osaka University, Japan,
²Yokohama National University, Japan, ³Institute for Molecular Science, Japan)*

**P-56 The Role of Substrate Binding on the Stability of the Heme Cavity and the Overall
Structure of Cytochrome P450cam**

R. Murugan and S. Mazumdar (Tata Institute of Fundamental Research, India)

**P-57 Molecular Mechanism of the Structural Changes in Cytochrome P450cam upon
the Binding of Putidaredoxin**

*Takehiko Toshi¹, Haruyuki Harada¹, Shiro Yoshioka¹, Satoshi Takahashi¹, Koichiro
Ishimori¹, Isao Morishima¹, Shingo Nagano², Jason K. Yano², and Thomas L.
Poulos² (¹Kyoto University, Japan, ²University of California, Irvine, USA)*

P-58 Crystallographic and Spectroscopic Characterization of Nonheme Fe(IV)=O

Complexes

Jun-Hee In¹, Jan-Uwe Rohde², Mi Hee Lim¹, Audria Stubna³, Yon-Ok Ryu¹, Eckard Münck³, Lawrence Que, Jr.², and Wonwoo Nam¹ (¹Ewha Womans University, Korea, ²University of Minnesota, USA, ³Carnegie Mellon University, USA)

P-59 Evolution of Copper-Binding Sites in Cu-Oxidases Estimated from Structural and Functional Similarities

Kensuke Nakamura¹, Takeshi Kawabata¹, Kei Yura², and Nobuhiro Go² (¹Nara Institute of Science and Technology, Japan, ²Japan Atomic Energy Research Institute, Japan)

P-60 Resonance Raman Spectra of Cytochrome *c* Oxidase of Intact Mitochondria

Toshinari Takahashi¹, Shinya Yoshikawa², and Takashi Ogura¹ (¹The University of Tokyo, Japan, ²Himeji Institute of Technology, Japan)

P-61 Activation Mechanism of Soluble Guanylate Cyclase in the Presence of CO and YC-1

Biswajit Pal¹, Zhengqiang Li¹, Shigeo Takenaka², Takeshi Tomita¹, Shingo Tsuyama², and Teizo Kitagawa¹ (¹Center for Integrative Bioscience, Japan, ²Osaka Prefecture University, Japan)

P-62 Molecular Mechanism of the Catalase Reaction Studied by Myoglobin Mutants

Shigeru Kato¹, Takafumi Ueno², Shunichi Fukuzumi³, and Yoshihito Watanabe² (¹The Graduate University for Advanced Studies, Japan, ²Nagoya University, Japan, ³Osaka University, Japan)

P-63 Mechanistic Studies of Olefin Epoxidations by Manganese Complexes of Salen and Porphyrin Ligands

Na Young Oh¹, Se-Eun Park¹, In Kyung Lim¹, Chang Young Cho¹, Jinheung Kim², and Wonwoo Nam¹ (¹Ewha Womans University, Korea, ²Changwon National University, Korea)

P-64 Formation of Iodosylbenzene-Iron Porphyrins on the Reaction of Oxoiron(IV) Porphyrin Cation Radicals and Iodobenzene

Ying Ji Sun¹, Sun Kyung Choi¹, Mi Hee Lim¹, Sun Ok Kim¹, Jan-Uwe Rohde², Lawrence Que, Jr.², and Wonwoo Nam¹ (¹Ewha Womans University, Korea, ²University of Minnesota, USA)

P-65 Functionalization of Myoglobin by Reconstitution with an Artificial Heme Having a Substrate Binding Region

Hideaki Sato, Takaaki Matsuda, Takashi Hayashi, Tsutomu Ando and Yoshio Hisaeda (PRESTO, Japan Science and Technology Corporation, Kyushu University, Japan)

P-66 Semisynthesis of Metalloproteins, Fe(Schiff Base)•Apo-Mb: Control of Cyanide Binding by Ala71->Gly Mutation

Takafumi Ueno¹, Masataka Ohashi², Masaharu Kono³, Atsuo Suzuki³, Takashi Yamane³, and Yoshihito Watanabe⁴ (¹Nagoya University, Japan, ²The Graduate University for Advanced Studies, Japan, ³Nagoya University, Japan, ⁴Nagoya University, Japan)

P-67 Rational Design of Cr (Schiff base)•apo-Mb for Enantioselective Sulfoxidation

Tomomi Koshiyama¹, Takafumi Ueno², Masataka Ohashi⁴, Masaharu Kono³, Atsuo Suzuki³, Takashi Yamane³, and Yoshihito Watanabe¹ (¹Nagoya University, Japan, ²Nagoya University, Japan, ³Nagoya University, Japan, ⁴The Graduate University for Advanced Studies, Japan)

P-68 Regulation of Cyanide Binding to Fe^{III}(Schiff base)•apo-myoglobin by the Schiff Base Ligand Structure

Masataka Ohashi¹, Takafumi Ueno², and Yoshihito Watanabe² (¹The Graduate University for Advanced Studies, Japan, ²Nagoya University, Japan)

P-69 Model Study on Electron Transfer Reaction within Protein-Protein Complexes Using a Reconstituted Myoglobin

Tsutomu Ando¹, Takashi Hayashi^{1,2}, Hideaki Sato², and Yoshio Hisaeda¹ (¹Kyushu University, Japan, ²PRESTO, Japan Science and Technology Corporation)

P-70 Use of Lanthanide Ions as NMR Structure Probes: Bioinorganic Conformational Analysis

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P-71 Gd³⁺ Polyaminocarboxylate Complexes Containing Macrocycles as Magnetic Resonance Imaging (MRI) Contrast Agents (CAs)

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P-72 Determining the Potentials of Rieske Clusters: How Is Cluster Redox State Coupled to Histidine Protonation State ?

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P-73 Self-Assembly of Polyethylenimine (PEI)-Linked Metalloporphyrin on an Electrode And It's Electron Transferability

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P-74 Metal-Nucleobase Interaction: Supramolecular Self-Assembly via Hydrogen Bonding and Coordination in Polymeric Cadmium Complex of N⁶-Benzyladenine

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P-75 Identification of Functional Peptides for Gb3 Isolated from a Random Peptide Library

Yoshiko Miura, Yuki Sasao, Akio Sakaki, and Kazukiyo Kobayashi (Nagoya University, Japan)

P-76 3D and Electronic Structural Analysis of Metalloproteins by the DV-Xa Analysis

Akihiro Kikuchi (RIKEN Harima Institute/SPring-8, Japan)

P-77 A Useful Sieve-Supported Cobalt(II)/Acetate Mimic System for Catalytic Alkane Oxidation with Tert-Butyl Hydroperoxide

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