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PART I ANNUAL REPORTS

1. Abstracts of Papers Published in Journals

MATHEMATICS

A characterization of Conway-Coxeter friezes of zigzag type by rational links

Takeyoshi Kogiso, Michihisa Wakui[*1] (*1 Department of Mathematics, KansaiUniversity)
Osaka J. Math. **59** (2022), no. 2, 341-362.

The present paper show that Conway-Coxeter friezes of zigzag type are characterized by (unoriented) rational links. As an application of this characterization Jones polynomial can be defined for Conway-Coxeter friezes of zigzag type. This gives a new method for computing the Jones polynomial for oriented rational links.

Homogeneous Sasaki and Vaisman manifolds of unimodular Lie groups

D. Alekseevsky, K. Hasegawa, Y. Kamishima
Nagoya Math. J. 83-96 (2021).

We show the basic structure theorem of simply connected homogeneous Sasaki and Vaisman manifolds of unimodular Lie groups, up to holomorphic isometry. A compact locally homogeneous Vaisman manifold is described as a complex manifold which is an S^1-bundle over a Sasaki manifold or a holomorphic nontrivial complex torus bundle over a Kähler manifold.

Construction of contractible complete quaternionic almost Hermitian manifolds with compact isometry group

Y. Kamishima
Josai Mathematical Monograph, **13**, 52-66 (2021).

The 4n+3-dimensional quaternionic Heisenberg nilpotent Lie group M admits a quaternionic contact structure. There exists a three dimensional simply connected non-abelian solvable Lie group R acting properly on M. We show that the quotient of M by R admits a quaternionic almost Hermitian metric g. Moreover, one almost complex structure, say J from the quaternionic structure is shown to be integrable for which $(M/R, J)$ is a Bochner flat Kähler manifold.

Quaternionic contact $4n+3$-manifolds and their $4n$-quotients

Y. Kamishima
Annals of Global Analysis and Geometry, **59**(4) 435-455 (2021).

This is a sequel to (2). We study some quaternionic contact-Einstein manifolds (qc for short) with zero qc-scalar curvature. We constructed a family of quaternionic Hermitian metrics $(g_a, \{J_\alpha\}_{\alpha=1}^3)$ on the domain Y of the standard quaternion space $\mathbb{H}^n$ one of which, say (g_a, J_1) is a Bochner flat Kähler metric. We verify that the compact quaternionic Heisenberg infranilmanifold is such an example.

Algebraic analysis of Siersma's non-isolated hypersurface singularities

Shinichi Tajima, Yoko Umeta
Hokkaido Math. J. **51**(1), 2022, 117-151.

In the context of algebraic analysis, we examine non-isolated line singularities studied by D.Siersma. We compute a Grörbner basis of the annihilator in a non-commutative ring associated with these singularities by using Poincaré-Birkhoff-Witt algebra. We compute local cohomology solutions of the associated holonomic D-modules by utilizing the Gröbner basis of the annihilator, and then determine the monodromy structure of the local cohomology solutions along a singular stratum of hypersurfaces. We obtain micro-local b-functions of the singularities in an explicit manner.

Holonomic D-modules associated with a simple line singularity and vertical monodromy

Shinichi Tajima, Yoko Umeta
Funkcialaj Ekvacioj, **64**(1), 2021, 17-48.

We study holonomic D-modules associated with certain kind of non-isolated hypersurface singularities introduced by T. de Jong. Structures of these holonomic D-modules such as characteristic variety, monodromy are explicitly determined. An application to Betti numbers of local Milnor fibers is also discussed.

Some kinds of of uncertainty relations represented by tracial or non-tracial positive linear maps

Kenjiro Yanagi
Proceedings of the International Conference on Nonlinear Analysis and Convex Analysis & International Conference on Optimization:Techniques and Applications II, 2021, pp. 311-321.

Uncertainty relations are inequalities representing the impossibility of simultaneous measurement in quantum mechanics. The most well-known uncertainty relations were presented by Heisenberg and Schrodinger. We aim to replace the usual trace Tr by positive linear map from $M_n(\mathbb{C})$ to $M_m(\mathbb{C})$ and to replace x^α and $x^{1-\alpha}$ by functions f and g under certain conditions. We obtain some extensions of uncertainty relations represented by tracial or non-tracial positive linear map.

Refined Hermite-Hadamard inequality and its application

Kenjiro Yanagi
Linear and Nonlinear Analysis, vol. **7**, no. 2, 2021, pp. 173–183.

There are many generalizations of Hermite-Hadamard inequality for convex function f defined on $[a, b]$. Recently we gave several types of refined Hermite-Hadamard inequality and obtained inequalities satisfied by weighted logarithmic mean. In this article we give several relations of upper bounds or lower bounds of refined Hermite-Hadamard inequality. Futhermore, we apply to different type of inequalities under some conditions.

Refinements of bounds for entropy and relative entropy

Kenjiro Yanagi
Linear and Nonlinear Analysis, vol. **8**, no. 2, 2022, pp. 197–215.

There are many generalizations of Hermite-Hadamard inequality for convex function f defined on $[a, b]$. Recently we gave several relations of upper bounds or lower bounds of refined Hermite-Hadamard inequality and apply to different types of inequalities under some conditions. In this article we give detailed lower and upper bounds for Tsallis entropy and Tsallis relative entropy. As applications we give bounds for Tsallis relative operator entropy in the case of operators satisfying the condition $1A \leq B \leq LA$, with $1<L$.

Refined Hermite-Hadamard inequalities and some norm inequalities

Kenjiro Yanagi
Symmetry, vol. **14**, no. 12, 2022, pp. 2522–1–9.

It is well known that the Hermite-Hadamard inequality (called the HH inequality) refines the definition of convexity of function $f(x)$ defined on $[a, b]$ by using the integral of $f(x)$ from a to b. There are many generalizations or refinements of HH inequality. Furthermore HH inequality has many applications to several fields of mathematics, including numerical analysis, functional analysis, and operator inequality. Recently we gave several types of refined HH inequalities and an N-variable HH inequality and apply to some norm inequalities under certain conditions. As applications, we obtain several inequalities which are satisfied by means defined by symmetry. Finally, we obtain detailed integral values.

***N* variable logarithmic mean**

Kenjiro Yanagi
Linear and Nonlinear Analysis, vol. **8**, no., 2022, pp. 249–253.

It is well known that the Hermite-Hadamard inequality refines the definition of convexity of function $f(x)$ defined on $[a, b]$ by using the integral of $f(x)$ from a and b. There are many generalizations or refinements of the Hermite-Hadamard inequality. In this article, we give an N variable Hermite-Hadamard inequality and apply to give the definition of N variable logarithmic mean.

微小拡散 SEIR モデルのパラメータ推定

清水優祐
日本応用数理学会論文誌, **31**(4), 278-287, 2021.

感染症の数理モデルである SIR モデルや，潜伏期間を考慮した SEIR モデルは，感染症の短期的な流行を決定論的に記述した微分方程式型であるが，現実の感染拡大の様相は偶発的であり，人口のダイナミクスをモデルで表現するためには，ランダムな微小変動を取り込む必要があると考え，SEIR モデルに拡散項を加えた，微小拡散 SEIR モデルを考案し，パラメータの推定量の漸近分布を導出した。また，統計解析ソフトウェア R を用いて人口動態の数値実験を行った。

CHEMISTRY

分子軌道エネルギーと機械学習による分子物性の予測

寺前裕之，松尾哲秀，庭月野一眞，井上竜太，野口晋治，玄　美燕[*1]，山下　司[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
J. Comput. Chem. Jpn., **19**, 43-45 (2020); https://doi.org/10.2477/jccj.2020-0005.

The values of the internuclear distances and the dipole moments of 14 small molecules have been estimated by machine learning with only molecular orbital energies as the explanatory variables. We use four regression methods, partial least square (PLS), random forest (RF), Radial Basis Function Kernel Regularized Least Squares (krlsRadial), and Baysian Regularized Neural Networks (BRNN) and we report only BRNN results for the internuclear distances,and PLS results for the dipole moments. The coefficients of determination for the internulear distances and the dipole moments are 0.9318 and 0.7265, respectively. It has been proved that the internuclear distances and the dipole moments can be predicted by the molecular orbital energies only.

Prediction of molecular properties with machine learning and molecular orbital energies

Hiroyuki Teramae, Meiyan Xuan[*1], Jun Takayama[*1], Mari Okazaki[*1] and Takeshi Sakamoto[*1]（*1 Faculty of Pharmaceutical Sciences, Josai University）
AIP Conference Proceedings **2611**, 020007 (2022); https://doi.org/10.1063/5.0119589.

The prediction by the machine learning using molecular orbital energies as an explan-

atory variable is attempted to predict the strength of anxiolytics, anti-anxiety, and muscle relaxant of benzodiazepine anxiolytics. We also attempt to predict half-life of concentration in the body $T_{1/2}$, and time to reach maximum body concentration T_{max} of benzodiazepine anxiolytics with the same procedure. The molecular orbital calculations are performed at 6-31G (d, p) level and random forest is used as regression method. The number of molecular orbitals is varied from 2 to 20 and it is found that 4 or 6 is almost sufficient for the prediction of these 5 objective variables. Finally, the predictions of five properties in the present study are fairly well agreed with the experiments by machine learning employing the molecular orbital energies as the only explanatory variables.

Overexpression and purification of a toxic peptide LaIT2 from Japanese scorpion, *Liocheles australasiae*

Maiki Tamura, Chiharu Tatsushiro, Eugene Hayato Morita, Shinya Ohki
Protein Expr. Purif. **182** (2021) 105835.

In Japan, there are two species of scorpions, Madara scorpion (*Isometrus maculatus*) and Yaeyama scorpion (*Liocheles australasiae*), and both of them are living in Yaeyama island. It has been shown that *Liocheles australasiae* has venom including β-toxin acting on K+-channels (β-KTx) (Juichi et al., 2018) [1]. Interestingly, LaIT2, one of the toxins found in the venom of *Liocheles australasiae*, displays the virulence for insects but almost not for mammals. Until now, molecular mechanism of the functional specificity of LaIT2 is unknown. To clear this issue, we tried to establish the overexpression system of LaIT2 in Rosetta-gami B (DE3) pLysS, which have trxB/gor mutations to induce the disulfide bond formation. In this study, we have succeeded to overexpress the recombinant LaIT2 (rLaIT2) as a thioredoxin (Trx)-tagged protein, and established the purification protocol with Ni^{2+}-NTA column chromatography, enterokinase digestion, and HPLC. We succeeded to obtain approximately 0.5 mg of rLaIT2 from the *E. coli* cells cultured in 1 L of M9 culture medium. Intramolecular disulfide bonding pattern of rLaIT2 was identified by endopeptidase fragmentation and mass spectrometry. rLaIT2 showed insecticidal activity and antimicrobial activity, and these are almost identical to those of natural LaIT2. ^{1}H-^{15}N HSQC spectrum of ^{15}N-labelled rLaIT2 indicated that the rLaIT2 has a stable conformation.

Structural and functional studies of LaIT2, an antimicrobial and insecticidal peptide from *Liocheles australasiae*

Maiki Tamura, Chiharu Tatsushiro, Eugene Hayato Morita, Shinya Ohki
Toxicon **214**, (2022) 8-17.

LaIT2, composed of 59 amino acid residues, is a peptide toxin isolated from the venom of the Yaeyama scorpion, *Liocheles australasiae*. LaIT2 is toxic to insects but not most mammals. The N- and C-domains of LaIT2 are known to possess antimicrobial and insecticidal activities,

respectively. However, the molecular mechanisms are largely unknown because of the lack of a three-dimensional structure of LaIT2. Thus, we elucidated the solution NMR structure of LaIT2. LaIT2 adopts a β-KTx-like two-domain structure, in which the N- and C-terminal domains form a random coil and an α-β-β motif, respectively. Trifluoro ethanol and liposomes titration experiments showed that the unstructured N-domain of LaIT2 has the ability to form an α-helix. The N-terminal helix is amphiphilic, and one side of the helix is positively charged. Measurements of the antimicrobial and insecticidal activities of LaIT2 mutants suggested K15 in the N-domain was found to be responsible for the antimicrobial activities, whereas L53 and L54 in the C-domain were key residues involved in the insecticidal activity. Moreover, K21 in the N-domain is important for both activities. Therefore, two domains are suggested that they work together to show antimicrobial and insecticidal activity.

3′-Aminofluorene-9-spiro-5′-imidazolidine-2′,4′-dithione as a sensing material for planar aromatic solvents

T. Sakata, M. Suzuki
Indian. J. Adv. Chem. Sci., **10**(1), (2022) 22.

Herein, we investigate the non-covalent interactions between aromatic compounds and a spirocycle-bearing imidazolidinedithione molecule 3′-aminofluorene-9-spiro-5′-imidazolidine-2′,4′-dithione (**HM**). **HM** and planar aromatic solvent molecules, such as benzene, pyrrole, and thiophene, form molecular compounds with a composition ratio of 2:1 via NH$\cdots\pi$ interactions. These compounds exhibit weak emission in the λ_{max} range of 515–544 nm, which were estimated from the sum of the squares of the differences between the electronegativities of the bonded atoms comprising the guest molecule structures without employing quantum calculations. Moreover, a linear correlation between the desorption temperature and NH$\cdots\pi$ interactions is determined from the heats of formation of **HM**, guest molecules, and corresponding molecular compounds.

Ligand Rotation Induced Oxidation State Change and Spin Appearance of the Bis (phthalocyaninato) cerium ($CePc_2$) Molecule on the Au (111) Surface

Islam Saiful[*1], Mohammad Ikram Hossain[*1], Keiichi Katoh, Masahiro Yamashita[*1,2], Ryuichi Arafune[*3], Syed Mohammad Fakruddin Shahed[*1], and Tadahiro Komeda[*1] (*1 Tohoku University, *2 Nankai University, *3 National Institute for Materials Sciences)
J. Phys. Chem. C, **126**(40), (2022) 17152–17163.

We show that the valence state of the Ce atom in bis (phthalocyaninato) cerium ($CePc_2$) adsorbed on Au (111) is reduced from 4+ to 3+ by using the scanning tunneling microscope (STM). It is indicating that the magnetic moment of the $CePc_2$ molecule is turned on by geometric constraints on Au (111) surface.

Comparison between $DySc_2N@C_{80}$ and $Dy_2ScN@C_{80}$ single-molecule magnetic metallofullerenes encapsulated in single-wall carbon nanotubes

Satoshi Ito[*1], Ryo Nakanishi[*1], Keiichi Katoh[*1], Brian K. Breedlove[*1], Tetsu Sato[*1], Zhao-Yang Li[*2], Yoji Horii[*3], Masanori Wakizaka[*1] and Masahiro Yamashita[*1,2] (*1 Tohoku University, *2 Nankai University, *3 Nara Women's University)
Dalton Trans., **51**, (2022) 6339–6344.

The effect encapsulation of $DySc_2N@C_{80}$ and $Dy_2ScN@C_{80}$ single-molecule magnet in single-walled carbon nanotubes (SWCNTs) has been explained in terms of intermolecular magnetic interactions and charge transfer between metallofullerenes and SWCNTs.

^{161}Dy synchrotron-radiation-based Mössbauer absorption spectroscopy

Ryo Masuda[*1,2], Shinji Kitao[*3], Hiroyuki Tajima[*3], Hiroki Taniguchi[*3], Takaya Mitsui[*4], Kosuke Fujiwara[*4], Yoshitaka Yoda[*2], Nobumoto Nagasawa[*2], Daisuke Ishikawa[*2,5], Alfred. Q. R. Baron[*2,5], Takefumi Yoshida[*6], Tetsu Sato[*7], Keiichi Katoh, Hisao Kobayashi, Makoto Seto[*3,4] (*1 Hirosaki University, *2 Japan Synchrotron Radiation Research Institute, *3 Kyoto University, *4 National Institute for Quantum Science and Technology, *5 RIKEN, *6 The University of Electro-Communications, *7 Tohoku University, *8 University of Hyogo)
Hyperfine Interactions, **243**(1), (2022) 17-1-8.

We used the measurement system for synchrotron-radiation-based Mössbauer absorption spectra with ^{161}Dy using the 25.7 keV nuclear first excited state to measure the Mössbauer spectra of DyF_3, Dy metal and $DyPc_2$ (Pc = phthalocyaninato). The ground state of Dy in each compound could be estimated from the observed magnetic hyperfine field of Dy.

Electro-Conductive Single-Molecule Magnet Composed of a Dysprosium(III)-Phthalocyaninato Double-Decker Complex with Magnetoresistance

Tetsu Sato[*1], Brian K. Breedlove[*1], Masahiro Yamashita[*1,2], Keiichi Katoh (*1 Tohoku University, *2 Nankai University)
Angewandte Chemie International Edition, **60**(39), (2021) 21179-21183.
Hot paper, Front cover

A one-dimensional (1D) arrangement of partially oxidized dysprosium(III)-phthalocyaninato double-decker complex, $[DyPc_2]I_x$ (I = iodide; $1.93<x<2.26$), was obtained by using electro-oxidation and chemical oxidation. The conductivity of $[DyPc_2]I_x$ was observed at temperatures lower than the blocking temperature (T_B), magnetoresistance (MR) effects corresponding to a magnetic hysteresis of single-molecule magnet (SMM) were observed at 2.2 K.

Terbium(III) bis-phthalocyaninato single-molecule magnet encapsulated in a single-walled carbon nanotube

Keiichi Katoh, Junya Sato[*1], Ryo Nakanishi[*1], Ferdous Ara[*2], Tadahiro Komeda[*2], Yuki Kuwahara[*3], Takeshi Saito[*3], Brian K. Breedlove[*1], Masahiro Yamashita[*1,4] (*1 Tohoku University, *2 Institute of Multidisciplinary Research of Advanced Materials, Tohoku University, *3 National Institute of Advanced Industrial Science and Technology (AIST), *4 Nankai University)

Journal of Materials Chemistry C, **9**(33), (2021) 10697-10704.
Front cover

A terbium(III)-phthalocyaninato double-decker single-molecule magnets ($TbPc_2$) were encapsulated in the single-walled carbon nanotubes (SWCNTs) for the first time. The magnetic and electronic properties of the $TbPc_2$@SWCNT hybrids were investigated. It appears that the electron correlation between $TbPc_2$ and SWCNT can affect the electrotransport and electromagnetic properties. This strategy may pave the way for the construction of SMM@SWCNT hybrid materials.

Single molecular adsorption of terbium (III) bis-phthalocyaninato ($TbPc_2$) governed by two surface reconstructions of perovskite type $SrVO_3$ epitaxial ultrathin film

Hirofumi Oka[*1,2], Keiichi Katoh, Yoshinori Okada[*1,3], Daichi Oka[*4], Taro Hitosugi[*1,5], Masahiro Yamashita[*1,2,3,6], Tomoteru Fukumura[*1,2,3] (*1 Advanced Institute for Materials Research, Tohoku University, *2 Core Research Cluster for Materials Science, Tohoku University, *3 Okinawa Institute of Science and Technology Graduate University, *4 Tohoku University, *5 Tokyo Institute of Technology, *6 Nankai University)

Chemistry Letter, **50**(8), (2021) 1489-1492.

We observed a single molecule magnet, terbium(III)-phthalocyaninato double decker molecule ($TbPc_2$), adsorbed on a perovskite type transition metal oxide ($SrVO_3$) ultrathin film by using low temperature scanning tunneling microscopy (STM). The high-resolution STM images reveal that the adatom structure of each surface reconstruction dominates the adsorption arrangement according to the proposed adsorption configurations.

Structural, magnetic and theoretical analyses of anionic and cationic phthalocyaninato-terbium(III) double-decker complexes: Magnetic relaxation via higher ligand-field sublevels enhanced by oxidation

Yoji Horii[*1], Marko Damjanović[*2], Keiichi Katoh, Masahiro Yamashita[*3,4]
(*1 Nara Women's University, *2 Heidelberg University, *3 Tohoku University, *4 Nankai University)

Dalton Transactions, **50** (28), (2021) 9719-9724.

Crystallographic and magnetic analyses have been performed on the anionic and cationic forms of terbium(III)-phthalocyaninato double-decker single molecule magnets (SMMs). The cationic form exhibits a longer magnetic relaxation time (τ) and higher activation energy of spin-flip (ΔE) than anionic one.

Visible-Light-Induced Synthesis of 1,2,3,4-Tetrahydroquinolines through Formal [4+2] Cycloaddition of Acyclic α,β-Unsaturated Amides and Imides with N,N-Dialkylanilines

K. Itoh[*1], S. Nagao[*1], K. Tokunaga[*2], S. Hirayama[*1], F. Karaki[*1], T. Mizuguchi[*1], K. Nagai[*1], N. Sato[*1], M. Suzuki, M. Hashimoto, H. Fujii[*1] (*1 Kitasato University, *2 Kogakuin University)
Chem. Eur. J. **27**, (2021) 5171–5179, *Chem. Eur. J.* **27**, (2021) 5053–5053 (Cover Picture).

The cooperative action of an Ir^{III} complex photosensitizer, a thiourea, and an azo compound enables the visible-light-induced formal [4+2] cycloaddition of acyclic α,β-unsaturated amides and imides with *N,N*-dialkylanilines to synthesize structurally diverse 1,2,3,4-tetrahydroquinolines possessing contiguous stereogenic centers in a highly diastereoselective manner. The chemoselective removal of the auxiliary can be achieved.

Synthesis and Antifungal Activity of Polycyclic Pyridone Derivatives with Anti-Hyphal and Biofilm Formation Activity against Candida Albicans

H. Kamauchi*, Y. Kimura*, M. Ushiwatari*, M. Suzuki, T. Seki*, K. Takao*, Y. Sugita* (* Faculty of Pharmacy and Pharmaceutical Science, Josai University)
Bioorg. Med. Chem. Lett. **37**, (2021) 127845.

Thirty-five pyridone derivatives were synthesized, with derivatization conducted on polycyclic pyridone scaffolds, including *cis*- or *trans*-oxydecalin and other cyclic structures, by domino-Knoevenagel-electrocyclic reactions. The anti-fungal activities of the synthesized compounds were tested against *Candida albicans*. Ten compounds inhibited hyphal formation without inhibiting growth. Pyridones with anti-hyphal formation activity (**4c**, **6d**, **12a** and **12c**) were tested for their ability to inhibit biofilm formation. Compound **6d** showed both anti-hyphal and biofilm inhibition activity.

Effect of Lactic Acid Content into on during Miconazole Eye Drops to be Used for Infection Preventive

K. Yoshimura*, Y. Inoue*, A. Koizumi*, M. Suzuki, S. Itakura*, H. Todo*, I. Murata*, I. Kanamoto* (* Faculty of Pharmacy and Pharmaceutical Science, Josai University)
J. Drug Res. Dev. **7**, (2021) dx.doi.org/10.16966/2470-1009.160.

The aims of this study were to prepare a 0.1% Miconazole (MCZ) eye-drop solution and to evaluate the stability and physical properties of the preparation. MCZ eye-drops diluted

with physiological saline showed a reduction in MCZ content to approximately 90% after 2 weeks of storage at 4°C, and precipitates were confirmed in the eye-drop solution. The pH was maintained at 4.8 and the osmolality at 280mOsmol/kg. When lactic acid was added at concentrations of 1% and 0.5%, MCZ precipitation was confirmed after storage for 4 weeks, and the MCZ content decreased to ≤ 90%, with a pH of approximately 3.0–3.5. However, when 0.3% lactic acid was added, the MCZ content was maintained after 4 weeks, but the pH dropped to about 3.9. These results suggest that storing MCZ eye-drops at 4°C for 7 days is reasonable. In addition, the storage period could be extended up to 4 weeks under conditions of 25°C, RH84% or 40°C, RH82%. MCZ eye-drop solution containing 0.3% lactic acid can remain stable for 2 weeks when stored at 4°C.

Inclusion Complexes of Daidzein with Cyclodextrin-Based Metal-Organic Framework-1 Enhance Its Solubility and Antioxidant Capacity

Y. Inoue*, M. Yoshida*1, T. Ezawa*1, T. Tanikawa*1, F. Arce*2, G. L. See*2, J. Tomita*3, M. Suzuki, T. Oguchi*4 (*1 Faculty of Pharmacy and Pharmaceutical Science, Josai University, *2 University of San Carlos, Cebu, *3 Instrument Analysis Center, Josai University, *4 University of Yamanashi)
AAPS PharmSciTech. **23**, (2022) 2.

Daidzein, an aglycone-type isoflavone, is useful in the prevention of atherosclerotic cardiovascular diseases. However, the solubility of daidzein remains relatively low even with pharmaceutical interventions (e.g., γ-cyclodextrin inclusion complex). In the present study, daidzein-cyclodextrin-metal organic framework solid dispersion complexes were prepared by the solvent evaporation method. The physicochemical properties of the complex and its effect on the solubility of daidzein were evaluated. The enhancement effect of a cyclodextrin-metal organic framework on the antioxidant properties of daidzein was verified using a diphenyl-picrylhydrazyl radical scavenging test. Powder X-ray diffraction results showed that the characteristic diffraction peaks of daidzein and cyclodextrin-metal organic framework disappeared and new peaks ($2\theta = 7.1°$, 16.5°) were observed. FT-IR measurements showed that the peak derived from the carbonyl group of daidzein shifted to the lower wavenumber. NOESY 1H-1H NMR showed cross peaks at the proton on the resorcinol side of daidzein and the proton (H-5, H-6) in a cyclodextrin-metal organic framework. Dissolution rate of daidzein at 5 min in distilled water was 0.06% for daidzein alone while the daidzein inclusion complex was about 100%. When fasted state simulated intestinal fluid was used, the dissolution rate of the daidzein complex was about 71% compared with that of daidzein alone (～3.0%) at 5 min. The daidzein inclusion complex improved the antioxidant capacity to～1.3 times (17.8 μg/mL) compared to the IC_{50} of daidzein alone (22.9 μg/mL). Preparations of cyclodextrin-metal organic framework inclusion complexes will be a platform in developing pharmaceutical formulations to enhance the bioavailability and activity of drugs.

A benzaldehyde derivative obtained from Hypoxylon truncatum NBRC 32353 treated with hygromycin B

H. Kamauchi*, M. Suzuki, K. Takao*, Y. Sugita* (* Faculty of Pharmacy and Pharmaceutical Science, Josai University)
J. Antibiot. **75**, (2022) 1–8.

The ribosome-targeted antifungal agent hygromycin B (HygB) alters the secondary metabolite profiles of fungi. *Hypoxylon truncatum* NBRC 32353 fermented in the presence of hygromycin B in barley medium activated secondary metabolite synthesis. A new benzaldehyde derivative truncaaldehyde (**1**) was obtained, along with thirteen known compounds (**2**–**14**). The structures of the new compounds were revealed using NMR and single-crystal X-ray crystallography. The total synthesis of (±)-**1** was achieved using a four-step sequence, and chiral separation was accomplished. The isolated compounds were tested for their monoamine oxidase (MAO) -A and -B inhibitory activities, with six compounds ((±)-**1**, **4**, **5**, **7**, **8**, and **10**) showing inhibitory activity.

Preparation, Characterization, Solubility, and Antioxidant Capacity of Ellagic Acid-Urea Complex

H. Sakurai*1, M. Suzuki, S. Itakura*1, H. Todo*1, F. Arce*2, G. L. See*2, T. Tanikawa*1, Y. Inoue*1 (*1 Faculty of Pharmacy and Pharmaceutical Science, Josai University, *2 University of San Carlos, Cebu)
Materials **15**, (2022) 2836.

Ellagic acid (EA), a natural polyphenol found in berries, has high antioxidant capacity. This study aimed to improve EA solubility by complex formation with urea (UR) using solvent evaporation method and evaluate its solubility, antioxidant capacity, and physical properties. The solubility test (25 °C, 72 h) showed that the solubility of EVP (EA/UR = 1/1) was approximately two-fold higher than that of EA (7.13 μg/mL versus 3.99 μg/mL). Moreover, the IC_{50} values of EA and EVP (EA/UR = 1/1) (1.50 μg/mL and 1.30 μg/mL, respectively) showed higher antioxidant capacity of EVP than that of EA. DSC analysis revealed that the UR peak at 134 °C disappeared, and a new endothermic peak was observed at approximately 250 °C for EVP (EA/UR = 1/1). PXRD measurements showed that the characteristic peaks of EA at $2q$ = 12.0° and 28.0° and of UR at $2q$ = 22.0°, 24.3°, and 29.1° disappeared and that new peaks were identified at $2q$ = 10.6°, 18.7°, and 26.8° for EVP (EA/UR = 1/1). According to 2D NOESY NMR spectroscopy, cross-peaks were observed between the -NH and -OH groups, suggesting intermolecular interactions between EA and UR. Therefore, complexation was confirmed in EA/UR = 1/1 prepared by solvent evaporation, suggesting that it contributed to the improvement in solubility and antioxidant capacity of EA.

Understanding the Nature and Strength of Noncovalent Face-to-Face Arene-Fullerene Interactions

M. Yamada*, Y. Kurihara*, M. Koizumi*, K. Tsuji*, Y. Maeda*, M. Suzuki (* Tokyo Gakugei University)
Angew. Chem. Int. Ed. **61**, (2022) e202212279.

Face-to-face noncovalent arene−fullerene interactions are important in several research fields such as synthetic chemistry, materials chemistry, and medicinal chemistry; however, their nature and strength are still poorly understood. In this study, we prepare a fullerene-based torsion balance containing thioanisole, phenol, naphthalene, azulene, and pyrene moieties as a unimolecular model system. Moreover, we compare the folding free energies between the folded and the unfolded conformers of a series of the molecular torsion balances to quantify noncovalent interactions between arenes and the fullerene surface. This work demonstrates that the contributions of polarizabilities, anionic charges, electronic dipole moments, and the number of arene rings to the interactions can be experimentally measured by analyzing the folding equilibrium of the molecular torsion balances.

川越市小・中・大学連携理科ふれあい事業への取り組み～2018，2019 年度

石黒直哉，宇和田貴之，北川浩子†
城西大学教職課程センター紀要，**5**, 61-64 (3 月 2021).

川越市が市内の小・中学生の理科に対する興味・関心や知的好奇心，探究心を醸成するため毎年度開催している川越市「小・中・大学連携理科ふれあい事業」では，川越市近隣大学（埼玉大学，東洋大学および本学）の教員および学生を小・中学校に招き，理科に関する実験・実習を行っている。本学理学部化学科の教員は本事業に継続的に参加し貢献している。本稿では 2018 ～ 2019 年度の我々の本事業への取り組み内容を報告し，アンケート結果から今後の展開を考察する。

Establishment of a detection system for the invasive species *Chelydra serpentina* using environmental DNA

Ishiguro N, Jinno K, Saito T, Kato H
DNA 鑑定，**12**, 17-26 (2021).

The common snapping turtle (*Chelydra serpentina*), designated as an invasive alien species by law in Japan, is a large freshwater turtle native to North America. Because this species is larger in body- and clutch-size than the Japanese native turtles, the impacts of predation and interspecific competition on the ecosystem are expected to be considerably large. In recent years, environmental DNA (eDNA) analytical methods that complement traditional surveys have been developed. In this study, we developed an eDNA-based detection method

for *C. serpentina* and applied it to natural habitats. First, we tested our method in 1 L of water from the tank, for which a male *C. serpentina* was bred. Next, we applied this method at four sites in surveying rivers with the target species and detected the eDNA of *C. serpentina* at all the sites. These results suggest that eDNA analysis is useful for the monitoring of this species.

環境 DNA 分析にも有効なスナヤツメ隠蔽種判別法の確立

石黒直哉，高山晃徳，齊藤達也，金澤　光
DNA 鑑定，**12**, 41–49 (2021).

Two cryptic lamprey species, *Lethenteron* sp. N (northern species) and *L.* sp. S (southern species), which have high genetic differentiation, exist in Japan. A rapid and reliable method of identifying mitochondrial DNA (mtDNA) from these lamprey species was designed for PCR-based genotyping of the mtDNA cytochrome *b* (CYB) region, which is also effective in environmental DNA (eDNA) analysis. Two allele-specific primers were developed for the mtDNA CYB region of each species: Let1-L and Let1-H for *L.* sp. N and Let2-L and Let2-H for *L.* sp. S. Agarose gel electrophoresis suggested that all 14 individuals collected in Saitama Prefecture were *L.* sp. N. In addition, surface water was collected from two sites of Kanabori Brook where 10 individuals of *L.* sp. N were found via survey. Using PCR-based eDNA analyses, *L.* sp. N eDNA was detected in samples from the sites, but *L.* sp. S eDNA was not.

Expression and antimicrobial activity of liver-expressed antimicrobial peptides in the ovaries of the viviparous teleost *Xenotoca eiseni*

Atsuo Iida, Risako Nakai, Junki Yoshida, Kaori Sano, Eiichi Hondo.
Fish Shellfish Immunol, **118**, 405–410 (2021).

The mechanism via which the mothers of viviparous animals regulate the internal environment of pregnancy-associated organs for maintaining offspring growth is poorly understood. Environmental niches in organs contain fluid components for supporting embryonic growth; however, they may serve as nutrients for microbes. In this study, we investigated the antimicrobial factors in a viviparous teleost, *Xenotoca eiseni*. According to the RNA-Seq analysis, high expression of leap1a was detected in the ovaries of both pregnant and non-pregnant fish. Moreover, the ovary extracts from X. eiseni and transformed leap genes exhibited antimicrobial activity against Escherichia coli. Our results suggest that viviparous teleosts utilize antimicrobial peptides to reduce the risk of infection in the ovarian lumen.

Cubam receptor-mediated endocytosis in hindgut-derived pseudoplacenta of a viviparous teleost (*Xenotoca eiseni*)

Atsuo Iida, Kaori Sano, Mayu Inokuchi, Jumpei Nomura, Takayuki Suzuki, Mao Kuriki, Maina Sogabe, Daichi Susaki, Kaoru Tonosaki, Tetsu Kinoshita, Eiichi Hondo.

J Exp Biol, **224**, jeb242613. (2021).

In the viviparous teleost Xenotoca eiseni (family Goodeidae), the intraovarian embryo intakes the maternal component secreted into the ovarian fluid via the trophotaenia. However, the molecules responsible for the absorption were still elusive. We focused on Cubam (Cubilin-Amnionless) as a receptor involved in the absorption, and cathepsin L as a functional protease in the vesicles. Our results indicated that the Cubam receptor is distributed in the apical surface of the trophotaenia epithelium and then is taken into the intracellular vesicles. Our findings suggest that the viviparous teleost acquired trophotaenia-based viviparity from a modification of the intestinal absorption system common in vertebrates.

Lineage-specific evolution of zona pellucida genes in fish

Kaori Sano, Sho Shimada, Hideki Mibu, Mizuki Taguchi, Takasumi Ohsawa, Mari Kawaguchi, Shigeki Yasumasu.
J Exp Zool B Mol Dev Evol, **338,** 191–191. (2022).

The zona pellucida (ZP) protein constitutes the egg envelope, which surrounds the vertebrate embryo. We performed a comprehensive study on the molecular evolution of ZP genes in Teleostei by cloning and analyzing the expression of ZP genes in fish of Anguilliformes in Elopomorpha, Osteoglossiformes in Osteoglossomorpha, and Clupeiformes in Otocephala to cover unsurveyed fish groups in Teleostei. The present results confirmed findings from our previous reports that the principal organ of ZP gene expression changed from ovary to liver in the common ancestors of Clupeocephala. These results suggest that teleost ZP genes have independently evolved to maintain fish-specific functions, such as egg envelope hardening and egg envelope digestion, at hatching.

Vanillin reduction in the biosynthetic pathway of capsiate, a non-pungent component of *Capsicum* fruits, is catalyzed by cinnamyl alcohol dehydrogenase

Kaori Sano, Yuya Uzawa, Itsuki Kaneshima, Saika Nakasato, Masashi Hashimoto, Yoshiyuki Tanaka, Sachie Nakatani, Kenji Kobata.
Sci Rep, **12**(1): 12384 (2022).

Capsicum fruits synthesize capsaicin from vanillylamine, which is produced from vanillin in a reaction catalyzed by a putative aminotransferase (pAMT). Capsiate, a non-pungent compound that is structurally similar to capsaicin, is synthesized from vanillyl alcohol rather than vanillylamine. In the present study, we revealed that the vanillin reductase in the capsiate biosynthetic pathway is cinnamyl alcohol dehydrogenase (CAD), which is an enzyme involved in lignin synthesis. Our results raises the possibility that in the genus Capsicum, the capsiate biosynthetic pathway emerged before the pAMT-encoding gene was acquired as the final trigger for capsaicin biosynthesis.

Second-order phase transition behavior behind polymer glass transition

Mitsuru Ishikawa, Taihei Takahashi, Yu-ichiro Hayashi, Maya Akashi, Takayuki Uwada
DOI 10.26434/chemrxiv-2021-66w4j-v6（Oct 19, 2021）.

Glass transition has similarity to the second-order phase transition in temperature dependent changes in entropy, non-Arrhenius viscosity, and heat capacity of glass forming materials. However, it has primarily been considered to be not phase transition. Recent single-molecule spectroscopy developments prompted re-investigating glass transition at the nanometer scale probing resolution, showing that glass transition includes phenomena similar to the second-order phase transition. They are characterized by microscopic collective polymer motion and discontinuous changes in temperature dependent relaxation times, the latter of which resembles the critical slowing down of second-order phase transitions, within a temperature window above the polymer calorimetric glass transition temperature. Simultaneous collective motion and critical slowing down occurrences disclose that the second-order phase transition hides behind polymer glass transition.

Polymer relaxation time enhancement at temperatures above glass transition temperatures predicted by idealized mode-coupling theory

Mitsuru Ishikawa, Keita Matsumoto, Tomoya Yamazaki, Risa Fukase, Yutaka Ichikawa, Takayuki Uwada
DOI 10.26434/chemrxiv-2022-fr63d-v2（Oct 11, 2022）.

The mode-coupling theory of glass transition predicts the relaxation time divergence of glass-forming materials at the crossover temperature, which is approximately 1.2 times the calorimetric glass transition temperature. However, this divergence has not been experimentally observed. This is known as the most serious drawback of the mode-coupling theory. The use of viscosity-sensitive single molecule fluorescence probes enables the detection of the poly（vinyl acetate）and poly（ethyl methacrylate）relaxation time enhancement around the crossover temperature, thereby supporting the prediction by the mode-coupling theory.

化学実験実習におけるオンラン教材を活用した反転授業の実践

宇和田貴之
城西大学教職課程センター紀要, **6**, 13-22（2022）.

2021 年度に城西大学理学部化学科 2 年生必修科目の基礎化学実験において反転授業を導入した経緯と実践方法を紹介した。2020 年度のコロナ禍を通して教員および学生のオンライン授業へのリテラシーが大きく向上したことと，その際の授業動画および資料の蓄積があって初めて可能となった反転授業であったが，受講生の十分な予習をもとにした理解向上や滞りや危険のない実験，提出物の質向上など大きな利点があることがわかった。また，反転授業を行う場合の学生

のコンピュータリテラシーの重要性について考察した。

Tumor-Specificity, Neurotoxicity, and Possible Involvement of the Nuclear Receptor Response Pathway of 4,6,8-Trimethyl Azulene Amide Derivatives

Kotone Naitoh, Yuta Orihara, Hiroshi Sakagami[*1], Takumi Miura, Keitaro Satoh[*2], Shigeru Amano[*1], Kenjiro Bandow[*3], Yosuke Iijima[*4], Kota Kurosaki[*5],Yoshihiro Uesawa[*5], Masashi Hashimoto and Hidetsugu Wakabayashi （*1 Research Institute of Odontology, Meikai University, *2 Research Institute of Odontology, Meikai University, *3 Division of Pharmacology, Department of Diagnostics and Therapeutics Sciences, Meikai University School of Dentistry, *4 Department of Oral and Maxillofacial Surgery, Saitama Medical Center, Saitama Medical University, *5 Department of Medical Molecular Informatics, Meiji Pharmaceutical University）

Int. J. Mol. Sci. **23** (5), 2601-2614 (2022).

Very few papers covering the anticancer activity of azulenes have been reported, as compared with those of antibacterial and anti-inflammatory activity. This led us to investigate the antitumor potential of fifteen 4,6,8-trimethyl azulene amide derivatives against oral malignant cells. 4,6,8-Trimethyl azulene amide derivatives were newly synthesized.

Anticancer activity was evaluated by tumor-specificity against four human oral squamous cell carcinoma (OSCC) cell lines over three normal oral cells. Neurotoxicity was evaluated by cytotoxicity against three neuronal cell lines over normal oral cells. Apoptosis induction was evaluated by Western blot and cell cycle analyses.

Among fifteen derivatives, compounds 7, 9, and 15 showed the highest anticancer activity, and relatively lower neurotoxicity than doxorubicin, 5-fluorouracil (5-FU),and melphalan. They induced the accumulation of a comparable amount of a subG1 population, but slightly lower extent of caspase activation, as compared with actinomycin D, used as an apoptosis inducer. The quantitative structure-activity relationship analysis suggests the significant correlation of tumor-specificity with a 3D shape of molecules, and possible involvement of inflammation and hormone receptor response pathways. Conclusions: Compounds 7 and 15 can be potential candidates of a lead compound for developing novel anticancer drugs.

Visible-Light-Induced Synthesis of 1,2,3,4-Tetrahydroquinolines through Formal [4+2] Cycloaddition of Acyclic α,β-Unsaturated Amides and Imides with N,N-Dialkylanilines

K. Itoh[*1], S. Nagao[*1], K. Tokunaga[*2], S. Hirayama[*1], F. Karaki[*1], T. Mizuguchi[*1], K. Nagai[*1], N. Sato[*1], M. Suzuki, M. Hashimoto, H. Fujii[*1] (*1 Kitasato University, *2 Kogakuin University)

Chem. Eur. J. **27**, (2021) 5171-5179, *Chem. Eur. J.* **27**, (2021) 5053-5053 (Cover Picture).

The cooperative action of an Ir^{III} complex photosensitizer, a thiourea, and an azo compound enables the visible-light-induced formal [4+2] cycloaddition of acyclic α,β-unsaturated amides and imides with *N,N*-dialkylanilines to synthesize structurally diverse 1,2,3,4-tetrahy-

droquinolines possessing contiguous stereogenic centers in a highly diastereoselective manner. The chemoselective removal of the auxiliary can be achieved.

Visible-light-induced formal [3 + 2] cycloaddition of α,β-unsaturated imides or amide with N,N,N′,N′-tetramethyldiaminomethane for the synthesis of 4-alkyl- and 4-aryl-1-methyl-2-pyrrolidinones

K. Itoh[*1], S. Nagao[*1], K. Tokunaga[*2], T. Mizuguchi[*1], F. Karaki[*1], S. Hirayama[*1], Y. Shibagaki[*1], M. Hashimoto, H. Fujii[*1] (*1 Kitasato University, *2 Kogakuin University)
Heterocycles. **104**, (2022) 2169-2178,

Photochemical reaction to synthesize 4-alkyl- and 4-aryl-1-methyl-2-pyrrolidinones through the formal [3 + 2] photocycloaddition of α,β-unsaturated imides or amide with N,N,N′,N′-tetramethyldiaminomethane, where an iridium(III) complex acts as a photosensitizer. The reaction is driven by visible-light-induced single-electron transfer between a photoexcited iridium(III) complex and N,N,N′,N′-tetramethyldiaminomethane to generate an α-aminoalkyl radical.

Multi-faceted elastic flexibility of 1-naphthyl and 9-anthryl 2,2′:6′,2″-terpyridine crystals

S. Kusumoto[*1], K. Oishi[*1], M. Nakaya, R. Suzuki[*2], M. Tachibana[*2], Y. Kim[*3], Y. Koide[*1] and S. Hayami[*3] (*1 Kanagawa Univ., *2 Yokohama City University, *3 Kumamoto Univ.)
Cryst. Eng. Commun. **24,** 8303-8308 (2022).

Functional molecular crystals capable of multidirectional deformation by external stimuli have the potential to be used in various applications such as mechanosensors and flexible devices. We report two organic crystals of 2,2′:6′,2″-terpyridine derivatives each substituted with luminescent naphthyl (**1**) and anthryl (**2**) moieties, displaying multi-faceted flexible bending with elasticity in response to mechanical stress, whose properties are evaluated in detail using their nanoindentations, single crystal X-ray structure analyses, and energy frame calculations.

Zero area thermal expansion of honeycomb layers via double distortion relaxation in $(PPh_4)[Cu_2(CN)_3]$

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Cryst. Eng. Commun. **24,** 5880-5884 (2022).

The zero area thermal expansion (TE) of a cyanide-bridged honeycomb layer was demonstrated by $(PPh_4)[Cu_2(CN)_3]$ (PPh_4^+ = tetraphenyl phosphonium) via double distortion relaxation. This characteristic TE behaviour involves in-plane anisotropy of the distorted layer with positive and negative TE. The conformation change in distorted PPh4+ tetrahedrons

also occurred between the layers. This was coupled with the anisotropic TE of the layers in accordance with complementary structural changes in the cation and anion counterparts.

Modulation of the elasticity of single crystal, 1-D metal dimethylglyoximato complexes via solid solution effect

A. Sugimoto[*1], S. Kusumoto[*2], M. Nakaya, Y. Sekine[*1], L. F. Lindoy[*3] and S. Hayami[*1] (*1 Kumamoto Univ., *2 Kanagawa University, *3 The University of Sydney)
Cryst. Eng. Commun. **24**, 4656-4660 (2022).

The fabrication of single crystal material with a desired degree of flexibility is a challenging topic in material science and crystal engineering. In this communication, we demonstrate the modulation of elasticity via a solid solution effect occurring in single crystals of one-dimensional, heterometal chain complexes.

A Ferroelectric Metallomesogen Exhibiting Field-Induced Slow Magnetic Relaxation

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Chem. Eur. J. **28**, e2021033 (2022).

Magnetoelectric (ME) materials exhibiting coupled electric and magnetic properties are of significant interest because of their potential use in memory storage devices, new sensors, or low-consumption devices. Herein, we report a new category of ME material that shows liquid crystal (LC), ferroelectric (FE), and field-induced single molecule magnet (SMM) behaviors. Co(II) complex incorporating alkyl chains of type $[Co(3C16\text{-}bzimpy)_2](BF_4)_2$ (**1**; $3C_{16}$-bzimpy=2,2′-(4-hexade-cyloxy-2,6-diyl)bis(1-hexadecyl-1H-benzo[d]imidazole)) displayed a chiral smectic C mesophase in the temperature range 321 K – 458 K, in which distinct FE behavior was observed, with a remnant polarization (88.3 $nCcm^{-2}$). Complex **1** also exhibited field-induced slow magnetic relaxation behavior that reflects the large magnetic anisotropy of the Co (II) center. Furthermore, the dielectric property of **1** was able to be tuned by an external magnetic field occurring from both spin-lattice coupling and molecular orientational variation. Clearly, this multifunctional compound, combining LC, FE, and SMM properties, represents an entry to the development of a range of next-generation ME materials.

Engineering ferromagnetism in $Ni(OH)_2$ nanosheets using tunable uniaxial pressure in graphene oxide/reduced graphene oxide

Y. Shudo[*1], Md. S. Islam[*1], H. Zenno[*1], M. Fukuda[*1], M. Nakaya, N. N. Rabin[*1], Y. Sekine[*1], L. F. Lindoy[*2] and S. Hayami[*1] (*1 Kumamoto University, *2 The University of Sydney)
Phys. Chem. Chem. Phys., **23**, 24233-24238 (2021).

The interlayer spaces in two dimensional (2D) layered materials such as graphene, metal oxides and metal chalcogenides can be used in a number of roles that include the trapping of gases, for ion transfer and for water purification applications. In such spaces, "inner" pressure occurs on guest species enclosed between the layers and its variation can, in principal, be used for precisely controlling particular guest properties. In this study, a mixture of two 2D materials including graphene oxide (GO) and nickel hydroxide ($Ni(OH)_2$), was employed to yield an anisotropic GO-$Ni(OH)_2$ hybrid 2D sheet. The inner pressure associated with this material was able to be tuned by reduction of the GO (to yield rGO) and this in turn was shown to affect the magnetic behaviour of $Ni(OH)_2$. The ferromagnetic transition temperature (T_c) for $Ni(OH)_2$ decreases as the interlayer distance became shorter, which is opposite to the behaviour observed for the application of hydrostatic pressure to the hybrid sheet. The uniaxial pressure affecting the interlayer of the 2D material, and generated by the reduction of GO to rGO, has the potential to not only influence the behaviour of a range of magnetic materials, but also individual properties of other types of functional materials.

Magnetism in a helicate complexes arising with the tetradentate ligand

H. Ohmagari[*1], M. Nakaya, K. Tanaka[*2], H. Zenno[*2], R. Akiyoshi[*2], Y. Sekine[*2], Y. Zhang[*3], K. S. Min[*4], M. Hasegawa[*1], L. F. Lindoy[*5] and S. Hayami[*2] (*1 Aoyama Gakuin University, *2 Kumamoto University, *3 Australian Nuclear Science and Technology Organization, *4 Kyungpook National University, *5 The University of Sydney)
Dalton Trans. **50**, 494–498 (2021).

The synthesis of [M(dimphen)$(NCS)_2$] (**1**; M = Fe^{II}), (**2**; M = Co^{II}), (**3**; M = Mn^{II}) and [Fe(dimphen)$(NCSe)_2$] (**4**), where dimphen = [1,2-bis (9-methyl-1,10-phenanthrolin-2-yl) ethane], are reported. The crystal packing structures of **1**–**3**, show intermolecular π-π stacking and NCS···SCN interactions. The complex **1** shows ferromagnetic interaction, and the complex **2** displays single-molecular magnet behavior.

EARTH SCIENCE

A Second Specimen of the Crossognathiform Fish *Apsopelix miyazakii* from the Cretaceous Yezo Group of Mikasa Area, Central Hokkaido, Japan

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Paleontological Research, **26** (2) (2022) 213–223.

The specimen collected from the Cretaceous Yezo Group of Mikasa area, central Hokkaido, Japan by T. Matsumoto and T. Omori in 1955, deposited in the University Museum,

the University of Tokyo is determined as a second specimen of *Apsopelix miyazakii*, which is the crossognathid fish described from Teshionakagawa area, northern part of Hokkaido in 2012. Some characters unconfirmed in the holotype, including the dorsoventrally long opercle and subopercle; the well-preserved preopercle having many radial openings of the sensory canal; the sensory canal of the second infraorbital bone having many branches; the presence of the forth infraorbital bone; the large supracleithrum; and the scale-like postcleithrum are preserved in the second specimen. An estimated standard length of the second specimen is more than about 10 cm larger than that of the holotype. The emended diagnosis is proposed for *A. miyazakii* based on the holotype and the second specimen. The discovery of the second specimen extends the range of *A. miyazakii* throughout the Upper Turonian. Also, *Apsopelix miyazakii* possibly lived in a shelf environment near the open ocean.

Non-occlusal dental microwear texture analysis of a titanosauriform sauropod dinosaur from the Upper Cretaceous (Turonian) Tamagawa Formation, northeastern Japan

Homare Sakaki[*1] Daniela. Winkler,[*1] Tai Kubo[*1], Ren Hirayama[*2] Hikaru Uno[*2], Shinya Miyata, Hideki Endo[*1], Kazuhisa Sasaki[*3], Toshio Takisawa[*4], Mugino O.Kubo[*1] (∗1 The University of Tokyo, ∗2 Waseda University, ∗3 Kuji City Office, ∗4 Kuji Amber Museum)
Cretaceous Research, **136**, 2022, 105218.

Sauropod teeth from the Tamagawa Formation of Kuji Group, northeastern Japan, were described and diet of the Kuji sauropod was inferred by dental microwear texture analysis (DMTA). The morphology and slenderness index (SI) of Kuji sauropod teeth indicate they belong to a titanosauriform somphospondyli sauropod and thus confirm the existence of a titanosauriform sauropod at the coastal area of East Asia during the late Turonian. Dental microwear texture (DMT) of the Kuji sauropod is compared with extant lepidosaurs with known dietary preferences, indicating a higher degree of oral food processing in the Kuji sauropod than in extant lepidosaurs. The Kuji sauropod fed on materials less resistant and softer than molluscan shells or exoskeletons of insects and likely relied on plant materials. Considering what is known about the paleoflora of the Tamagawa Formation, the most likely diet was ferns and gymnosperms. These initial results encourage future applications of DMTA to various sauropods, which could help to reveal the evolution of their feeding ecology and whether the increase of SI is associated with dietary change.

The first choristoderan record from the Upper Cretaceous of Asia, Tamagawa Formation, Kuji Group, Japan

Ryoko Matsumoto[*1], Ren Hirayama[*2], Shinya Miyata, Masataka Yoshida[*3] d, Shunsuke Mitsuzuka[*4], Toshio Takisawa[*5], Susan E. Evans[*6] (∗1 Kanagawa Prefectural Museum of Natural History, ∗2 Waseda University, ∗3 The University of Tokyo, ∗4 Nippon Koei Co., Ltd. ∗5 Kuji Amber Museum,∗6 University College London)
Cretaceous Research, **129**, (2022) 104999.

Choristoderes are freshwater diapsid reptiles that are distributed through Laurasia in Jurassic-Miocene deposits. The group shows great diversity in the Early Cretaceous of Asia, with all recognized morphotypes recorded from that region. However, there is then a substantial gap in the Asian record until choristoderes are reported from the Paleocene of Kazakhstan. This gap has raised questions as to whether the group became extinct in Asia during the Late Cretaceous, with subsequent reinvasion from either North America or Europe. Here we report the discovery of vertebrae attributable to Choristodera indet. from the lower Upper Cretaceous (Turonian) of the Tamagawa Formation, Kuji City, Iwate Prefecture, Japan. This is the first record of Choristodera from the Upper Cretaceous of Asia, and may imply that the group persisted in this region from the Jurassic to the Paleocene. The challenge for the future will be to recover a more complete record of Choristodera in the Upper Cretaceous of Asia.

2. Books, Reviews and Other Printings

MATHEMATICS

MathSchiNet Mathematical Reviews（https://mathscinet.ams.org/mathscinet）
・MR 4153158（reviewer : Masatoshi Iida）
・MR 4211870（reviewer : Masatoshi Iida）
・MR 4181782（reviewer : Masatoshi Iida）
・MR 4400123（reviewer : Masatoshi Iida）
・MR 4430933（reviewer : Masatoshi Iida）

エルミート・アダマール不等式の精密化とその応用
柳　研二郎
京都大学数理解析研究所講究録，vol. **2194**, 2021, pp. 120-131

Python による音源分離－情報数理体験講座 2021 の報告－
清水優祐
城西情報科学研究，**29**(1), pp. 1-7, 2022.

CHEMISTRY

機械学習と化学の関わり
寺前裕之
埼玉新聞，2022 年 3 月 19 日

PubChem のデータを用いた分子座標の作成―データベースを用いて Gaussian16 の入力ファイルを作成する方法―
寺前裕之
城西情報科学研究，**29**, 15-26 (2022).

2020 年度前期，理学部化学科のオンライン講義を振り返って
佐野香織，宇和田貴之，見附孝一郎
城西大学教職課程センター紀要，**5**, 19-26 (2021).

「子ども大学にしいるま」への化学科の取り組み
橋本雅司，宇和田貴之，秋田素子，石黒直哉，見附孝一郎，阪田知巳，森田勇人，石川　満
城西大学教職課程センター紀要，**5**, 53-59 (2021).

Structure and RNA Recognition Mechanism of RRM Domain in Cyano-bacterial RNA Binding Protein, RbpD from *Anabaena variabilis*
Eugene Hayato Morita, Yuki Tanaka, Hidenori Hayashi, Naoki Sato, Kyoko Furuita, Naohiro

Kobayashi, Toshihiko Sugiki, Chojiro Kojima
Proceedings of 22nd International Society of Magnetic Resonance Conference, 9th Asia-Pacific NMR Symposium (APNMR9), 60th Annual Meeting of the Nuclear Magnetic Resonance Society of Japan, and 60th Annual Meetings of the Society of Electron Spin Science and Technology. 22-27 Aug 2021, P1-2-2 (2021).

Structure and dynamics of LaIT2, a toxic peptide from Japanese scorpion, *Liocheles australasiae*
Maiki Tamura, Eugene Hayato Morita, Shinya Ohki
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Rare-earth based tetrapyrrolic sandwiches: chemistry, materials and applications
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Synthesis of $KNbO_3$/$LiTaO_3$ Piezoelectric Film by Hydrothermal Method
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3. Oral Presentations

MATHEMATICS

クラスター代数に潜む概均質ベクトル空間
Takeyoshi Kogiso
2020 年度表現論ワークショップ online，2021 年 1 月

連分数の q- 変形のいくつかの応用と PV との接点
小木曽岳義
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連分数，Conway-Coxeter frieze, Cluster 代数，有理結びの関係
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Takeyoshi Kogiso
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Dodgson-Desanot-Jacobi identity と Fricke identity から見えてくる数字とその q- 変形,
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小木曽岳義
青山数理セミナー，青山学院大学，2022 年 9 月

連分数とその q- 変形から見える数学
小木曽岳義
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Prehomogeneous Vector spaces coming from Multivariate Resultants and Veronese embeddings
小木曽岳義
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A unified family of P_J -hierarchies（J=I,II,IV,34）with a large parameter
梅田陽子
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多重スケール解析によるインスタントン解構成法
梅田陽子
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Genus two curves associated with the autonomous 4-dimensional Painlevé-type systems,
中村あかね
Web-seminar on Painlevé Equations and related topics，2021 年 9 月

Nonlinear to linear- introduction to the Painlevé equations through elliptic/hyperelliptic functions
中村あかね
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エルミート・アダマール不等式の精密化とその応用
柳研二郎
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「非線形解析学と凸解析学の研究」，オンライン講演，2021 年 3 月 2 日

エントロピー及び相対エントロピーの上界・下界の精密化とその応用
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N 型エルミート・アダマール不等式とノルム不等式への応用
柳研二郎
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微小拡散過程を用いた感染症数理モデルのパラメータ推定
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部分空間同定法によるカルマンフィルタを用いた逐次予測
川内陽平，清水優祐
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CHEMISTRY

分子軌道エネルギーと機械学習による BZP 系不安薬の薬効予測
寺前裕之，玄美燕[*1]，山下　司[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
日本コンピューター化学会 2021 年春季年会（オンライン），2021 年 6 月，講演要旨集 2014

分子軌道エネルギーと機械学習による薬物物性の予測
寺前裕之，玄美燕[*1]，山下　司[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
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Prediction of Molecular Properties with Machine Learning and Molecular Orbital Energies
Hiroyuki Teramae
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分子軌道エネルギーと機械学習による分子物性の予測
寺前裕之，玄美燕[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
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フェルラ酸の抗酸化作用の置換基効果に関する機械学習
寺前裕之 , 玄美燕[*1]，高山　淳[*1]，岡﨑真理[*1]，坂本武史[*1]（*1 城西大薬）
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色素分子から酸化チタンナノ粒子への電子注入反応の速度論
伊得 和音，見附 孝一郎
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モノリシックペロブスカイト太陽電池の界面形態と発電性能
内田美雪，見附孝一郎

第 16 回分子科学討論会（横浜），2022 年 9 月，講演要旨集，4P-048

ITO-PEN を基板とする色素増感型またはペロブスカイト型フレキシブル太陽電池
ヴー ティ リン，見附孝一郎
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Morphology and performance of monolithic perovskite solar cells studied by FESEM and electrochemical analyses
Miyuki Uchida, Tomoyo Nihashi, Koichiro Mitsuke
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Sub-nanosecond time-resolved fluorescence spectroscopy for relaxation kinetics of photoexcited dye molecules
Kanon Ie, Rina Watanabe, Koichiro Mitsuke
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Flexible solar cells based on a nanocrystalline TiO_2 layer deposited on an ITO-PEN film
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Dispersion state of C_{60} in a thin film of C_{60}-fatty acid mixture at the air-water interface
Nanako Ozawa, Yuri Tanuma, Koichiro Mitsuke
36th Symposium on Chemical Kinetics and Dynamics（Online），2021 年 6 月，Book of Abstracts, 2P11

（2-カルボキシエチル）ジフェニルホスフィンを配位子とするヨウ化銅（I）錯体をドープした DNA-脂質複合体膜の発光
髙澤頼昌，森田勇人，阪田知巳
第 68 回応用物理学会春季学術講演会（オンライン），2021 年 3 月，講演要旨集 16a-P02-6

ナノエレクトロニクス用分子ワイヤーに向けた金属イオンと DNA から成る M-DNA 複合体の作製
内山健斗，森田勇人，阪田知巳
第 82 回応用物理学会秋季学術講演会（オンライン），2021 年 9 月，講演要旨集 22p-P04-10

（2-カルボキシエチル）ジフェニルホスフィンを配位子とするヨウ化銅（I）錯体をドープした DNA-脂質複合膜の光学特性
髙澤頼昌，森田勇人，阪田知巳
第 38 回「センサ・マイクロマシンと応用システム」シンポジウム（オンライン），2021 年 11 月，講演要旨集 10P3-SSP-2

ヤエヤマサソリ由来毒素 LaIT2 の溶液構造に基づく殺虫 / 抗菌活性発現機構解析
達城智遥，田村真生，大木進也，森田勇人
第 94 回日本生化学会大会（横浜；オンライン），2021 年 11 月

パルスエレクトロポレーション法によるゲノム編集に適したアフリカツメガエル受精卵の表面処理
角田夏美，水出光哉，森田勇人
第 44 回日本分子生物学会年会（横浜；パシフィコ横浜），2021 年 12 月

ナノエレクトロニクス用分子ワイヤーに向けた亜鉛（II）イオンと DNA から成る M-DNA 複合体の作製
内山健斗，森田勇人，阪田知巳
第 69 回応用物理学会春季学術講演会（相模原），2022 年 3 月，講演要旨集 24p-P02-14

ナノエレクトロニクス用分子ワイヤーに向けたコバルト-DNA 複合体の作製
大須田竜樹，森田勇人，阪田知巳
第 83 回応用物理学会秋季学術講演会（仙台），2022 年 9 月，講演要旨集 21p-P17-15

ナノエレクトロニクス用分子ワイヤーに向けた M-DNA（M=Zn, Co）複合体の作製
大須田竜樹，森田勇人，阪田知巳
第 39 回「センサ・マイクロマシンと応用システム」シンポジウム（徳島），2022 年 11 月，講演要旨集 15P2-P-2

アホロートルのネオテニーに対するヨウ素の形態学的影響
久保田恵，宮崎友理，森田勇人
第 45 回日本分子生物学会年会（横浜；パシフィコ横浜），2022 年 12 月

エレクトロポレーションによる両棲類卵ゲノム編集用セルの 3D プリンタによる作製
角田夏美，水出光哉，森田勇人
第 45 回日本分子生物学会年会（横浜；パシフィコ横浜），2022 年 12 月

一次元希土類フタロシアニン錯体が持つ一次元空孔を利用したイオン脱挿入挙動の解明
佐藤　鉄，B. K. Breedlove，高石慎也，山下正廣，加藤恵一
日本化学会第 101 回春季年会（千葉 オンライン），2021 年 3 月，講演要旨集，A13-3am-03.

Challenge to continuous filling control using phthalocyanine complexes and crystals
佐藤　鉄，B. K. Breedlove，高石慎也，山下正廣，加藤恵一
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フタロシアニン錯体単結晶を用いたイオン挿入挙動の解明
佐藤　鉄，B. K. Breedlove，高石慎也，山下正廣，加藤恵一
第 15 回分子科学討論会（茨城 オンライン），2021 年 9 月，講演要旨集，4P027.

Electro-Conductive Single-Molecule Magnet Composed of a Phthalocyaninato Double-Decker Complex with Magnetoresistance

Tetsu Sato, Brian K. Breedlove, Shinya Takaishi, Masahiro Yamashita, Keiichi Katoh ACCC (Taiwan online), Oral-05, 2022 年 8 月

反射スペクトル測定によるフタロシアニン希土類錯体のフィリング制御の研究

佐藤　鉄，郭紫荊，宮本辰也，高石慎也，山下正廣，加藤恵一，岡本　博
日本物理学会 2022 秋季大会（東京），2022 年 9 月，講演要旨集，13pW611-8.

Sonochemical reaction to control the near-infrared photoluminescence proper- ties of single-walled carbon nanotubes

Y. Konno[*1], A. Nishino[*1], M. Yamada[*1], Y. Maeda[*1], Y. Miyauchi[*2], K. Matsuda[*2], J. Matsui[*3], M. Mitsuishi[*4], M. Suzuki（*1 Tokyo Gakugei University, *2 Kyoto University, *3 Yamagata University, *4 Tohoku University）
NT21: International Conference on the Science and Application of Nanotubes and Low-Dimensional Materials (Virtually hosted from Rice University Houston, USA), 2021 年 6 月 , C115.

Benzaldehyde Derivative Obtained from Hypoxylon truncatum NBRC 32353 Treated with Hygromycin B

H. Kamauchi[*], M. Suzuki, K. Takao[*], Y. Sugita[*]（* Faculty of Pharmacy and Pharmaceutical Science, Josai University）
The 11th JCK Joint Symposium on Pharmacognosy, (Tokyo), 2021 年 9 月，講演要旨集，P3-24.

イリジウム錯体光増感剤，チオウレア，アゾ化合物の協働作用が可能とするテトラヒドロキノリン誘導体合成

伊藤謙之介[*1]，長尾駿一[*1]，徳永　健[*1]，水口貴章[*1]，唐木文霞[*1]，平山重人[*1]，鈴木光明，橋本雅司，藤井秀明[*2]（*1 北里大，*2 工学院大）
日本化学会第 101 春季年会（オンライン），2021 年 3 月，講演要旨集，A21-2pm-11.

可視光により誘起される芳香族イミンと N,N N′,N′ - テトラメチルジアミノメタンの形式的 [3+2] 付加環化反応によるイミダゾリジン合成

伊藤謙之介[*1]，石井七彩[*1]，高篠諄史[*1]，原　彩[*1]，今　聡[*1]，水口貴章[*1]，唐木文霞[*1]，平山重人[*1]，長井賢一郎[*1]，佐藤倫子[*1]，徳永　健[*3]，鈴木光明，橋本雅司，藤井秀明[*1]（*1 北里大，*2 工学院大）
第 50 回複素環化学討論会（オンライン），2021 年 10 月，講演要旨集，30-19.

イリジウム(III)錯体光増感剤存在下における 1,2,5-オキサジアジナン誘導体の合成

伊藤謙之介[*1]，篠　諄史[*1]，原　彩[*1]，水口貴章[*1]，唐木文霞[*1]，平山重人[*1]，長井賢一郎[*1]，佐藤倫子[*1]，鈴木光明，橋本雅司，石川春樹[*1]，石田　斉[*2]，藤井秀明[*1]（*1 北里大，*2 関西大）
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新規のオキシム誘導体の合成
内田勝也，鈴木光明
日本化学会第 101 春季年会（オンライン），2021 年 3 月，講演要旨集，P03-2am-05.

新規ベンゾジアゼピンの合成
金子遥香，鈴木光明，富田惇輝
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菌糸-バイオフィルム形成阻害をターゲットとした真菌由来天然物の誘導体合成
鎌内　等*，木村　由*，牛渡美琴*，關　大志*，鈴木光明，平田桃香*，高尾浩一*，杉田義昭*
（*城西大薬）
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ピリジル基をもつベンゾジアゼピン誘導体の合成
金子遥香，鈴木光明
日本化学会第 102 春季年会（オンライン），2022 年 3 月 23 日，講演要旨集，P1-1am-24.

ハト Scale ケラチン遺伝子のクローニング
高橋理恵子
第 94 回 日本生化学会大会（オンライン），2021 年 11 月，講演要旨集，P-667

ハト Scale ケラチン遺伝子のクローニング
高橋理恵子
第 95 回 日本生化学会大会（名古屋），2022 年 11 月，講演要旨集，P-263

ギフチョウにおける化合物結合タンパク質（CSP）遺伝子クラスターの解析
北川浩子
第 94 回日本生化学会，2021 年 9 月，P-669

ギフチョウ属の前脚ふ節における食草選択関連遺伝子の同定
北川浩子
第 95 回日本生化学会（名古屋），2022 年 11 月，1P-264

環境 DNA 分析による入間川支流のホトケドジョウの生息地調査
石黒直哉，加藤優斗，中澤秀道
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モバイル PCR 装置を用いた簡便かつ迅速なアベサンショウウオ（*Hynobius abei*）の環境 DNA 検出手法の確立
日和佳政*1，戸井田和希，石黒直哉（*1 合同会社ローカル SD クリエーション）
日本 DNA 多型学会第 31 回学術集会（金沢），2022 年 11 月

環境 DNA を用いた滑川町におけるドブガイ類の生息する谷津沼
石黒直哉，石田美咲乃
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魚類の卵膜は先に形成されたものほど最外層側になる～そのメカニズムの解明～
渡邊花菜，神田真司，佐野香織
第 7 回ユニーク会（東京），2021 年 9 月

トウガラシの種間におけるカプサイシン合成効率の違い
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