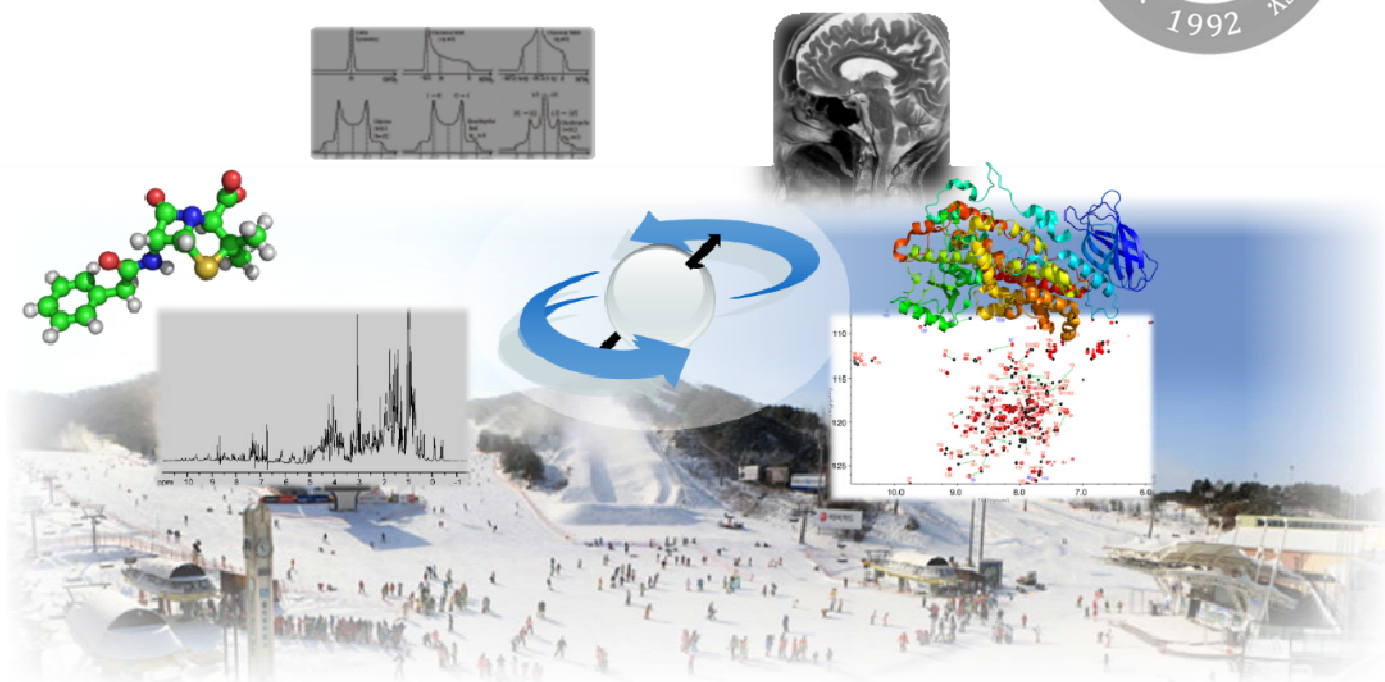


# 2021 한국자기공명학회 하계 학술대회 및 총회



**일시 : 2021년 6월 24일 (목) ~ 26일 (토)**

**장소 : 웰리힐리파크 (강원도 횡성군)**

**후원 :**

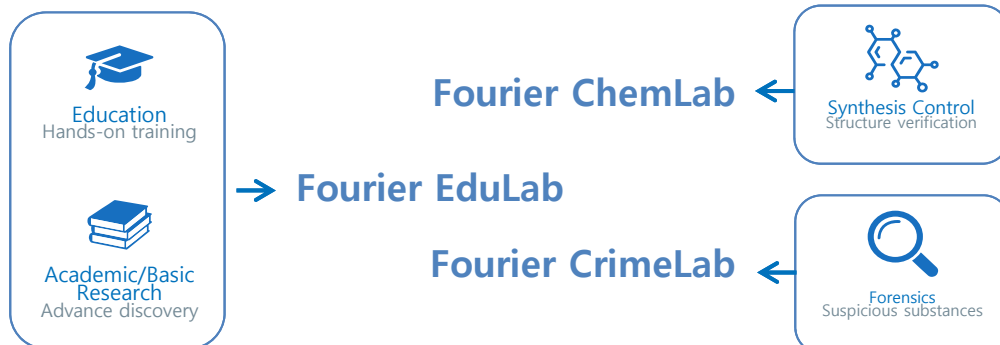
한국기초과학지원연구원, 브루커바이오스핀코리아,  
지올코리아, BK인스트루먼트, 한국과학기술연구원,  
티앤제이테크, SCIEX Korea, 마스터 코리아,  
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## ▶ 인사 말씀 ◀

한국자기공명학회 회원 여러분, 안녕하십니까?

날씨가 점점 더워지고 있지만 모두 건강하시고, 회원님들의 연구와 학업에 큰 성취가 있기를 기원합니다.

한국자기공명학회에서는 2021년 6월 24일~26일 강원도 횡성 웰리힐리 파크에서 제53회 정기총회 및 하계 학술발표회를 현장과 온라인으로 개최합니다. 코로나19의 국가적인 엄중한 시기로 인해 학회 회원과 자기공명분야에 관심을 가지신 분들 중 연구책임자 중심으로 소규모로 현장 참여를 권장하며 일정상 참여가 어려우신 연구자님과 학생회원님의 온라인 참여로 진행하고자 합니다.

이번 학술발표회에서는 생체분자 NMR 연구분야에 국내 최고 석학이신 고려대학교 전영호교수님, 서울대학교 박성혁교수님, 경상대학교 이준화교수님, 콜로라도대학교 이웅희교수님, 충북대학교 김지훈교수님, DGIST 김진해교수님, GIST 박진주교수님, 제주대학교 김도희교수님, 한국표준과학연구원 심정현박사님께서 초청강연을 해주실 예정입니다. 또한 Biomolecular NMR, MR imaging, Metabolomics, solid state NMR등 다양한 분야의 젊은 국내 학자들의 강연이 준비되었습니다. 교육 세션에서는 최신 NMR 관련 기기개발 동향 및 측정기법 다양한 연구방법이 소개하고자 하오니 많은 관심과 참여 부탁드립니다.

아울러 학회의 발전을 위해 늘 후원을 아끼지 않으시는 기관(한국기초과학지원연구원, 한국과학기술연구원) 및 기업(브루커바이오스핀코리아, 지올코리아, 비케이인스트루먼트, 티앤제이테크, SCIEX Korea, 마스터코리아, 인성크로마텍, 동인바이오텍, KoreaLabs)에 깊은 감사를 드리며, 학회를 준비하는 이사진과 스태프분들께 깊은 감사를 드립니다.

코로나19의 힘든 시기에 늘 건강 챙기시고 이번 53회 정기 학술발표회를 통해 학문의 발전과 많은 정보가 공유되는 유익한 시간 되시길 기원합니다.

2021년 6월 24일

(사) 한국자기공명학회장  
한양대학교 화학분자공학과 원호식

2021년 한국자기공명학회 실행이사진  
총무이사 서정용 (서울대학교)  
학술이사 안희철 (동국대학교)  
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편집이사 오석훈 (한국기초과학지원연구원)

## DAY-1: Jun. 24, 2021 (Thursday)

**14:00~14:45** Registration

**14:45~15:00** Opening Ceremony

**15:00~16:30 Education Session: Sponsor Companies** 좌장: 류경석 박사 (KBSI)

15:00~15:30 ES1. BRUKER Korea Session

15:30~16:00 ES2. JEOL Korea Session (동영상)

16:00~16:30 ES3. BKI Session (동영상)

**16:30~17:00** Break

**17:00~18:10 Scientific Session-A: JEOL 학술상** 좌장: 김낙균 박사 (KIST)

17:00~17:10 시상식 및 Photo Time – 수상: 원호식 KMRS 회장 (한양대)

17:10~17:40 SC-A1. 박성혁 교수 (서울대) – Live NMR metabolomics for realtime monitoring of metabolism

17:40~18:10 SC-A2. 이준화 교수 (경상국립대) – A Long Journey with NMR and Z-DNA

## DAY-2: Jun. 25, 2021 (Friday)

**09:00~09:30** Registration

**09:30~11:00 Special Lecture: POKY & AI in NMR** 좌장: 안희철 교수 (동국대)

09:30~10:10 SL1. 이웅희 교수 (U. of Colorado Denver) – POKY: a software suite for multidimensional NMR and 3D structure calculation of biomolecules

10:20~11:00 SL2. 이웅희 교수 (U. of Colorado Denver) – AI-assisted NMR automation in the POKY suite

**11:00~12:00 Scientific Session-B: BKI 신진연구자상** 좌장: 안희철 교수 (동국대)

11:00~11:10 시상식 및 Photo Time – 수상: 원호식 KMRS 회장 (한양대)

11:10~11:35 SC-B1. 김지훈 교수 (충북대) – Structural studies on the membrane protein, Caveolin3, using NMR

11:35~12:00 SC-B2. 김진해 교수 (DGIST) – Quaternary dynamics of transthyretin modulates its physiological and pathological features

**12:30~13:00** Lunch



**13:00~14:00 Poster Session (동영상 및 학회 홈페이지 PDF)**

**14:00~15:00 Scientific Session-C: Bruker 젊은과학자상** 좌장: 이준화 교수 (경상국립대)

14:00~14:15 시상식 및 Photo Time – 수상: 원호식 KMRS 회장 (한양대)

SC-C1. 최서리 박사과정 (경상국립대, PI 이준화 교수) – NMR Study of target DNA recognition of human TALE transcription factor, MEIS1

발표 15분 SC-C2. 조혜영 박사 (고려대, PI 전영호 교수) – Structural study of the interaction between AIMP2-DX2 and HSP70 on the cancer development

SC-C3. 안소영 박사 (서울대, PI 서정용 교수) – Intrinsic disorder is essential for Cas9 inhibition of anti-CRISPR AcrIIA5

**15:00~16:30 Scientific Session-D**

좌장: 이봉진 교수 (서울대)

15:00~15:15 시상식 및 Photo Time – 수상: 원호식 KMRS 회장 (한양대)

15:15~15:40 SC-D1. 박진주 교수 (GIST) – Selective DNA recognition and protein-protein interactions of the human transcription factor FOXO4

15:40~16:05 SC-D2. 김도희 교수 (제주대) – Structure-based design of peptides that trigger Streptococcus pneumoniae cell death

16:05~16:30 SC-D3. 심정현 박사 (KRISS) – Dynamic nuclear polarization system with or without cryogen toward hyperpolarized MRI

**16:30~17:00 Break**

**17:00~18:00 Bruker 이조웅학술상 시상 및 강연**

17:00~17:10 시상식 및 Photo Time – 수상: 원호식 KMRS 회장 (한양대)

17:10~18:00 수상강연: 전영호 교수 (고려대) – Interactions of the aminoacyl tRNA synthetases: protein-protein interactions suggesting a new way to suppress cancer

**18:00~18:30 총회**

**18:30~20:00 Dinner**

## **DAY-3: Jun. 26, 2021 (Saturday)**

**10:00~11:30 Round Table Discussion**

- 학회 발전 방향 및 연구 방향 자유 토의
- AI in NMR

**11:30~12:00 Closing Ceremony**



# 안 내

## 등록

- 사전등록: <http://www.kmrs.or.kr>, 사전등록 마감 (2021년 6월 22일 화), **현장등록 없음**
- 등록비: 정회원 14만원 (온라인 7만원), 학생회원 2만원 (온라인 참석만 가능)
- 숙소: 웰리힐리파크 (강원도 횡성군) 1544-8833, 학회 할인 예약은 은지원 지배인에게 개인적으로 연락해서 예약바랍니다 (연락처: 010-3555-5196).

## 오시는길

- 강원도 횡성군 둔내면 고원로451 웰리힐리파크 마루홀
- KTX 둔내역



## 문의처

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## **Interactions of the aminoacyl tRNA synthetases: protein-protein interactions suggesting a new way to suppress cancer**

Hye Young Cho<sup>1</sup>, Ameer Ull Mushtaq<sup>1</sup>, Ji Seon Kim<sup>1</sup>, Dae Gyu Kim<sup>2</sup>, Semi Lim<sup>2</sup>, Jin Young Lee<sup>2</sup>, Nam Hoon Kwon<sup>2</sup>, Sunghoon Kim<sup>2</sup>, Young Ho Jeon<sup>1</sup>

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Aminoacyl-tRNA synthetases (ARSs) are enzymes to catalyze the ligation of amino acids to cognate tRNAs in translation. ARSs as a house keeping gene are pivotal role to exact transfer the amino acids for protein synthesis. Among 20 mammalian ARSs, 9 ARSs form the macromolecular complex, multi-tRNA synthetase complex (MSC), with three non-enzymatic factors for efficient translation. Among the three non-enzymatic factors in MSC, aminoacyl-tRNA synthetase-interacting multi-functional protein2 (AIMP2) is the major scaffolding molecule to stabilize the MSC for enhancing the efficiency of translation, and KRS shows the strong binding to AIMP2 in MSC. Here, we show that a component of MSC, the lysyl-tRNA synthetase enhances cell migration and tumor metastasis through the binding with 67kDa laminin receptor (67LR), dimerized form of p40/37LRP which is one of the ribosomal components. In addition, a splicing variant of AIMP2 lacking exon 2, referred as AIMP2-DX2 (or simply DX2) is oncogenic, and the cellular stability of AIMP2-DX2 is increased by the binding with HSP70, resulting in AIMP2-DX2-mediated cell proliferation and lung cancer progression. Our results suggest that specific modulation of protein-protein interaction of the ARSs and MSC components may offer a way to control tumor growth and metastasis while avoiding the toxicities associated with inhibition of the normal functions of ARSs.

## Live NMR metabolomics for realtime monitoring of metabolism

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Recent studies point out the link between altered metabolism and various diseases, but metabolic monitoring of biological systems have mostly been performed at fixed time points on extracted material. As NMR is a non-destructive technique, we applied heteronuclear 2D NMR to living or functional biological systems. At the protein level, we present a triple resonance NMR-based approach for specific detection of glutaminase activity using stable-isotope labeled glutamine in live cells. Compared to conventional methods involving coupled enzyme assays, the proposed approach is direct because it detects the presence of the H–N–CO amide spin system. The approach was applied to investigating the effects of a glutaminase inhibitor and the inhibitory effects of glucose on glutamine metabolism in live cells. The approach can be extended to other enzymes targeting carbon bonds using HCACO. At the organelle level, we monitored the mitochondrial metabolism in real time. We used  $^{13}\text{C}$  pyruvate as a tracer to monitor its metabolism in isolated and functional human mitochondria. We found acetyl phosphate synthesis from pyruvate in live human mitochondria which has been largely forgotten since its first description about 70 years ago in bacteria. The kinetic profile of acetyl phosphate formation was biphasic, and its transient nature suggested its role as a metabolic intermediate. The method also allowed for the estimation of pyruvate dehydrogenase (PDH) enzyme activity through monitoring of the acetylCoA formation, independent of competing cytosolic metabolism. We also detected lactate production from pyruvate in live mitochondria which is modulated by p53, a well-known tumor suppressor. Although lactate production has been known only in cytosol, the mitochondrial formation was confirmed with the recovery of lactate formation upon treatment of specific inhibitor of mitochondrial pyruvate carrier followed by a membrane permeabilizer. At the cell level, the live metabolomic method allowed for metabolomic differentiation between cancer and normal cells on the basis of time dependent changes in metabolite concentrations. Cancer cells were found to have large in- and out-flux of pyruvate as well as increased net production of alanine and acetate. The method also enabled evaluation of the metabolic effects of galloflavin whose anticancer effects have been attributed to its specific inhibition of lactate dehydrogenase. Our approach

revealed previously unknown functional targets of galloflavin, which were further confirmed at the protein levels. How the live metabolomic method can be expanded to other hierarchical biological systems will be also presented.



## A Long Journey with NMR and Z-DNA

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It has been 50 years since left-handed Z-DNA was found in a polymer of alternating d(CG)<sub>n</sub> under high salt condition. Z-DNA binding proteins (ZBPs) have been identified in an RNA editing enzyme (ADAR1), DNA-dependent activator of interferon-regulatory factor (DAI, also known ZBP1 and DLM1), the viral E3L protein and a fish ZBP-containing protein kinase (PKZ). The crystal structures of ZBPs in complex with 6-base-paired (6-bp) DNA duplex showed that two molecules of ZBP bind to each strand of double-stranded Z-DNA with 2-fold symmetry with respect to DNA helical axis. NMR study of Z $\alpha$  domain of human ADAR1 (hZ $\alpha$ <sub>ADAR1</sub>) complexed 6-bp Z-DNA suggest an *active* B-Z transition mechanism in which the hZ $\alpha$ <sub>ADAR1</sub> first binds to B-DNA and then converts to Z-DNA, a conformation that is then stabilized by the additional binding of a second hZ $\alpha$ <sub>ADAR1</sub>. Similar results were observed for the h Z $\alpha$  domain of yatapoxvirus E3L (yabZ $\alpha$ <sub>E3L</sub>). In the case of non-CG-repeat DNA, the hZ $\alpha$ <sub>ADAR1</sub> exhibits the sequence preference of d(CGCGCG)<sub>2</sub> >> d(CACGTG)<sub>2</sub> > d(CGTACG)<sub>2</sub> through multiple sequence discrimination steps during the B-Z transition. Chemical shift perturbation and relaxation dispersion experiments on hZ $\alpha$ <sub>ADAR1</sub> upon binding to Z-DNA as well as Z-RNA. Our study demonstrates the unique dynamics of hZ $\alpha$ <sub>ADAR1</sub> during the A-Z transition of RNA, in which the hZ $\alpha$ <sub>ADAR1</sub> forms a thermodynamically stable complex with Z-RNA, similar to Z-DNA, but kinetically converts RNA to the Z-form more slowly than DNA. NMR study on the complexes of various hZ $\alpha$ <sub>ADAR1</sub> mutants with a 6-bp Z-DNA showed that single mutations at residues K169, N173, or Y177 cause unusual conformational changes in the hydrophobic faces of helices  $\alpha$ 1,  $\alpha$ 2, and  $\alpha$ 3, which dramatically decrease the Z-DNA binding affinity, whereas single mutations at residues K170, R174, T191, P192, P193, or W195 slightly affected the Z-DNA binding affinity. In the NMR study of Z $\alpha$  domain of goldfish PKZ (caZ $\alpha$ <sub>PKZ</sub>), global analysis of chemical shift perturbation data found that increasing [NaCl] from 10 to 100 mM reduced the binding affinity of caZ $\alpha$ <sub>PKZ</sub> for both B-DNA (600-fold) and Z-DNA (25-fold) and decreased its B-Z transition activity (4.6-fold). This study suggested that the structure of the intermediate complex formed by caZ $\alpha$ <sub>PKZ</sub> and B-DNA is modulated by varying salt concentration and thus it could be used as a molecular

ruler to determine the degree of B-Z transition

## **POKY: a software suite for multidimensional NMR and 3D structure calculation of biomolecules**

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The need for an efficient and cost-effective method is compelling in biomolecular NMR. To tackle this problem, we have developed the Poky suite, the revolutionized platform with boundless possibilities for advancing research and technology development in signal detection, resonance assignment, structure calculation, and relaxation studies with the help of many automation and user interface tools<sup>1</sup>. This software is extensible and scalable by scripting and batching as well as providing modern graphical user interfaces and a diverse range of modules right out of the box. Poky is freely available to non-commercial users at <https://poky.clas.ucdenver.edu>.

### References

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## AI-assisted NMR automation in the POKY

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Methods to solve long-awaited challenges have been devised by the activation of multidisciplinary studies. Especially, adapting artificial intelligence (AI) technologies from computer science to basic sciences is the crowning achievement. For instance, deep learning, one area of machine learning, has astonished the field by exhibiting the top-level accuracy in the global CASP (the critical assessment of protein structure prediction) competition two times in a row <sup>1,2</sup>. Our group has also achieved many outstanding results by interfacing AI techniques to the nuclear magnetic resonance (NMR) spectroscopy that enables investigating structures and functions of biomolecules at the atomic-level <sup>3–8</sup>. In this talk, I will present AI-assisted NMR automation methods available in our POKY suite <sup>9,10</sup>.

### References

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## Structural studies on the membrane protein Caveolin3 using NMR

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Membrane proteins (MPs) represent ~ 30% of all proteins in living organisms. They play many important roles in a wide range of cellular functions such as transport, transmission of cell signaling and scaffold support. Due to their significant participation in physiological processes, MPs constitute ~60% of drug targets and are the most attractive object of research in the pharmaceutical industry. Therefore, knowledge about the structure of MP is decidedly important for efficient drug design. Nevertheless, structure determination of transmembrane protein is still a challenging area even though recently the number of deposited structures of membrane protein in the PDB were rapidly increased by the efforts using X-ray crystallography, electron microscopy, solid and solution nuclear magnetic resonance (NMR) technology. Among these technologies, solution NMR is a powerful tool for studying on protein-protein, protein-ligand and protein dynamics at the wide range of time scale as well as structure determination of membrane proteins.

Caveolins mediate the formation of caveolae, which are small omega-shaped membrane invaginations involved in a variety of cellular processes. There are three caveolin isoforms, the third of which (Cav3) is expressed in smooth and skeletal muscles. Mutations in Cav3 cause a variety of human muscular diseases. In this work, we characterized the secondary structure, dynamics, and topology of the monomeric form of the full-length lipidated protein. Cav3 consists of a series of membrane-embedded or surface-associated helical elements connected by extramembrane connecting loops or disordered domains. Our results also reveal that the N-terminal domain undergoes large scale pH-mediated topological rearrangement between soluble and membrane-anchored forms and several interplays were observed among residues in the flexible N-terminal. Considering that roughly one-third of pathogenic mutations in Cav3 influence charged residues located in this domain, we hypothesize that this transition is likely to be relevant to the molecular basis of Cav3-linked diseases. These results provide insight into the structure of Cav3 and set the stage for mechanistic investigations of the effects of pathogenic mutations.

## Quaternary dynamics of transthyretin modulates its physiological and pathological features

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Transthyretin (TTR), in its native tetrameric state, is an essential transporter of thyroxine and holoretinol binding protein for human. However, its dissociation into the mis-folded monomer facilitates abnormal aggregation of TTR, causing deposition of TTR aggregates typically in the peripheral nervous system or in the heart. Although numerous studies were conducted to elucidate heterogeneous quaternary features of TTR, it is still elusive to appreciate atomistic details of multiple quaternary structures and correlate these structural dynamics with its physiological and pathological behaviors. Here, we determined with nuclear magnetic resonance (NMR) spectroscopy the three-dimensional structures of the two TTR monomeric variants: amyloidogenic monomeric TTR and its less-amyloidogenic variant, T119M. We observed that Hsp90 interacts with monomeric TTR more strongly than with tetrameric TTR. In addition, by employing T119M monomeric variant, we were able to stabilize and characterize the dimeric state of TTR, whose detailed NMR spectroscopic investigation is currently on-going. Finally, we also reported that thyromimetic molecules, whose physicochemical properties resemble with thyroid hormones, can suppress the amyloidogenic propensity of TTR by stabilizing its tetrameric state. Taken together, we believe that our results provide detailed information for quaternary dynamics of TTR structures, as well as novel and promising therapeutic strategies for TTR amyloidosis.

## **NMR Study of target DNA recognition of human TALE transcription factor, MEIS1**

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Transcription factors are proteins that bind specific sites or elements in regulatory regions of DNA, known as promoters or enhancers, where they control the transcription or expression of target genes. MEIS1 protein is a DNA-binding domain present in human transcription factors and plays important roles in various biological functions. This gene encodes a homeobox protein belonging to the TALE ('three amino acid loop extension') family of homeodomain-containing proteins. TALE proteins are distinguished by the presence of three extra amino acids in the loop binding the first to the second alpha helix of the homeodomain. . The highly conserved DNA-binding TALE proteins define the family and is responsible for specific recognition of a common sequence motif, [5'- TGAC- 3'].

In order to characterize the molecular recognition of DNA by MEIS1, we performed <sup>1</sup>H/<sup>15</sup>N HSQC experiment and imino proton NMR experiments between MEIS1 and consensus MEIS1 target DNA. We also studied perturbations in the backbone of MEIS1 upon binding to DNA. The exchange rate constants of the imino protons for the wild type and mutant were measured by using water magnetization experiment. We compared to the dynamics of both wild type and mutant and characterized MEIS1 target DNA recognition.



## **Structural study of the interaction between AIMP2-DX2 and HSP70 on the cancer development**

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Aminoacyl-tRNA synthetase-interacting multifunctional protein 2 (AIMP2), which is a crucial component for a Multi-synthetase complex (MSC), is well known to separates from the complex and acts as a potent tumor suppressor. Recently, it was revealed that an exon 2 deleted splicing variant of AIMP2 (AIMP2-DX2) is often upregulated in diverse cancers, and 70kda heat-shock protein (HSP70) is critical to determine the cellular level of AIMP2-DX2. Although the biological implication of the interaction between AIMP2-DX2 and HSP70 has been suggested, the structural aspect of the interaction remains elusive. Here, we studied structural details of the interaction between AIMP2-DX2 and HSP70 by using X-ray crystallography and NMR spectroscopy. It was found that both N-terminal flexible region and GST domain of AIMP2-DX2 are involved in the interaction with the substrate-binding domain of HSP70, which results in the stabilization of AIMP2-DX2 by preventing the AIMP2-DX2 from Siah1-dependent ubiquitination and progression to tumorigenesis. It was confirmed that inhibiting the interaction between the AIMP2-DX2 and HSP70 by chemical compound, BC-DXI-495, suppressed cancer cell growth. Structural modeling in which BC-DXI-495 is docked into the hydrophobic pocket of AIMP2-DX2 was performed and this hydrophobic pocket is close to the HSP70-binding surface, suggesting an inhibitory effect of BC-DXI-495 on HSP70-AIMP2-DX2 binding. These results will provide crucial structural information to elucidate the molecular mechanism of oncogenic activity of DX2 on cancer development.

## Intrinsic disorder is essential for Cas9 inhibition of anti-CRISPR AcrIIA5

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Clustered regularly interspaced short palindromic repeats (CRISPRs) and CRISPR-associated (Cas) proteins provide bacteria with RNA-based adaptive immunity against phage infection. As a countermeasure, phages have developed anti-CRISPR (Acr) proteins that neutralize the bacterial CRISPR immunity. AcrIIA5, encoded by *Streptococcus thermophilus* strongly inhibits the host Cas9 and orthologs *in vivo*, but the molecular mechanism underlying the Cas9 inhibition remains unknown. Here we report the solution structure of AcrIIA5 that reveals a novel  $\alpha/\beta$  fold connected to an N-terminal intrinsically disordered region (IDR).

Remarkably, truncation of the N-terminal IDR abrogates the inhibitory activity against Cas9, revealing that the IDR is essential for Cas9 inhibition by AcrIIA5. Progressive truncations and mutations of the IDR illustrate that the disordered region not only modulates the association between AcrIIA5 and Cas9–sgRNA, but also alters the catalytic efficiency of the inhibitory complex. The length of IDR is critical for the Cas9–sgRNA recognition by AcrIIA5, whereas the charge content of IDR dictates the inhibitory activity. Conformational plasticity of IDR may be linked to the broad-spectrum inhibition of Cas9 homologs by AcrIIA5. The results reveals unique structural and functional features of AcrIIA5, suggesting its distinct mode of action and the diversity of the inhibitory mechanisms employed by Acr proteins.

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**Selective DNA recognition and protein-protein interactions of the human transcription factor FOXO4**

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Forkhead box O4 (FOXO4) is a human transcription factor (TF) that involves in cell homeostasis. While the structure and DNA binding properties of the forkhead domain (FHD) have been thoroughly investigated, how the transactivation domain (TAD) regulates the DNA binding properties of the protein remains elusive. Here, we investigated the interaction between FHD and TAD and its implication to DNA binding properties using solution NMR spectroscopy. We found that TAD and DNA share the same surface of FHD for binding. Furthermore, TAD-FHD interactions affect differently kinetic function of FHD depending on the type of DNA. We also studied FOXO4 interaction of p53, which promote cellular senescence. Our data showed that dual binding sites between two proteins mediate the interaction. Our works demonstrate the complexities of protein interactions and provide new perspectives on the FOXO4 function.

## Structure-based design of peptides that trigger *Streptococcus pneumoniae* cell death

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Toxin–antitoxin (TA) systems regulate key cellular functions in bacteria. Here, we report a unique structure of the *Streptococcus pneumoniae* HigBA system and a novel antimicrobial agent that activates HigB toxin, which results in mRNA degradation as an antibacterial strategy. In this study, protein structure–based peptides were designed and successfully penetrated the *S. pneumoniae* cell membrane and exerted bactericidal activity. This result represents the time during which inhibitors triggered *S. pneumoniae* cell death via the TA system. Furthermore, we found that the HigBA complex shows a crossed–scissor interface with two intermolecular  $\beta$ –sheets at both the N and C termini of the HigA antitoxin. Our biochemical and NMR titration studies provided valuable information regarding the transcriptional regulation mechanisms associated with the structural variability of HigAs. An inhibition study with peptides additionally proved that peptide binding may allosterically inhibit HigB activity. Overall, our results provide insights into the molecular basis of HigBA TA systems in *S. pneumoniae*, which can be applied for the development of new antibacterial strategies.

## Dynamic nuclear polarization systems with or without cryogen toward hyperpolarized MRI

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Hyperpolarization of nuclear spins provides a substantial enhancement in signal-to-noise ratio, which may enable background-free magnetic resonance imaging with nuclei other than proton. Hyperpolarized nanoparticles (HPNP) having endogenous polarization agents and biocompatibility have been emerged as a candidate overcoming the short  $T_1$  limit of hyperpolarized  $^{13}\text{C}$  pyruvates. Here, I first introduce a fully home-built dynamic nuclear polarization (DNP) system working at 3.3 K and 5 T. The system can be exploited versatilely for hyperpolarizing silicon nanoparticles or nanodiamonds. *In vivo*  $^{29}\text{Si}$  MR images obtained from HPNP-injected mouse will be presented.

Second, as an alternative to the cryogenic DNP system, an optical DNP system functioning at room temperature has developed at KRISS. In diamond, optically-induced electronic polarization can be transferred to  $^{13}\text{C}$  nuclei. A  $^{13}\text{C}$  nuclear polarization higher than 0.1 % was achieved only at 0.018 T via multi-frequency irradiation. Its potential as a low-cost and mobile polarizer will be discussed as well.

## Substrate binding studies of single mutant adenylate kinase from mycobacterium tuberculosis (AKmtE122K) by NMR

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Adenylate kinase (AK) is an enzyme that catalyzes the  $Mg^{2+}$  ion mediated high energy phosphorylation ( $Mg^{2+}$ -ATP + AMP  $\leftrightarrow$   $Mg^{2+}$ -2ADP) process producing two ADPs by forming ATP and AMP complexes with substrates, and these processes are known to be involved in energy metabolism and nucleotide synthesis. Although AK1 from eukaryotes and AK (AKmt) from mycobacterium tuberculosis has high homology in amino acid sequences of enzyme active site, the activity of AKmt is about 10% of AK1. Based on the charged amino acids of AK1 has carried an important role in enzyme activity and substrate affinity, we carried out genetic recombination and cell culture to produce  $^{13}C$ ,  $^{15}N$ -labeled wild type AKmt and its mutant protein (AKmtE122K) that has similarity to the amino acid sequence of AK1. The mutant was substituted with the negatively charged Glu[122] of LID domain into the positively charged Lys[122] and The activity of single mutant AKmtE122K were observed to be 2 fold higher than that of AKmt. In order to understand the substrate binding mechanism, complete NMR signal assignments were accomplished for single and double mutants by using 2D and 3D multinuclear multidimensional NMR experiments and molecular dynamics simulations. The structural changes of the loop and the domain are important in the mechanism and function of enzyme. The structural relocation of LID domain and AMP binding domain changing from the open form into the close form during the catalytic process was observed by NMR. Dissociation constant associated with active binding sites were measured with ATP, AMP titration. NMR measurements and molecular dynamic studies showed that ATP saturation to AKmtE122K gave rise to a structural change in LID domain with 0.5  $\mu M$  strong binding strength than that of AKmt whereas AMP saturation provide with 0.1  $\mu M$  strong binding strength and enabled the AMP binding site to change from the open form into the closed form. In a substrate binding, the saturation may induce structural stabilization of binding site and finally improve the substrate binding. It implies that the dynamic behavior of protein has important in its activity.

## Mechanistic studies on the interaction between lipid vesicles and the $\alpha$ -synuclein isoforms.

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Lewy body and Lewy neurite are well-known neuropathological lesions of Parkinson's Disease(PD). The main component of these hallmark lesions is alpha-synuclein( $\alpha$ S). Accumulating evidence tells us that pathologic oligomerization and aggregation of  $\alpha$ S is strongly related to the pathogenesis of PD. Through alternative splicing, the  $\alpha$ S gene (SNCA) encodes at least 4 different  $\alpha$ S isoforms: the canonical isoform that consists of 140 amino acid residues and the other three that lack exon4, exon6, or both. Such splicing of the SNCA gene is assumed to alter  $\alpha$ S aggregation properties, and previous studies have suggested that the expression levels of  $\alpha$ S isoforms in brain tissues show a marked difference between healthy controls and PD patients. However, while a large number of studies have been carried out on the canonical full-length  $\alpha$ S, barely no research is performed on the other three isoforms. It has been shown that the aggregation propensity and the function of  $\alpha$ S is heavily related to how  $\alpha$ S interacts with lipid membranes. Therefore, the main purpose of our research is to identify the mode and mechanism of the interaction between lipid vesicles and the  $\alpha$ S isoforms. We used circular dichroism(CD) and solution NMR to quantify their lipid-binding affinity. Change in the CD signal of the  $\alpha$ S isoforms was measured at 222 nm as a function of [ESC (DOPE:DOPS:DOPC=5:3:2) lipid] / [ $\alpha$ S isoform] ratios. Furthermore, <sup>1</sup>H-<sup>15</sup>N HSQC and DOSY experiments were performed for  $\alpha$ S protein isoforms in the presence of ESC lipid vesicles with negatively charged headgroups. Relative peak intensities and linewidths were plotted as a function of  $\alpha$ S residue number. Based on these data, it was identified that the lipid-binding affinity of N-terminus increases in the absence of C-terminal exon6. Our data also indicates the multiple distinct lipid-binding modes of  $\alpha$ S isoforms.

## **Characterization of protein structure and long-term stability of anti-CRISPR AcrIIA8**

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The clustered regularly interspaced short palindromic repeats (CRISPR) and CRISPR-associated (Cas) systems provides adaptive immunity against invading phages in bacteria and archaea. To overcome against CRISPR-Cas systems, phages have acquired anti-CRISPR (Acr) proteins that interfere with CRISPR-Cas activity. AcrIIA8 is one of the recently discovered Acr proteins that can mediate inhibition of Cas9 from *Streptococcus pyogenes* activity. To elucidate the AcrIIA8 of structural characteristics, we purified the recombinant protein and analyzed its structure using NMR spectra. During this process, We learned that AcrIIA8 protein was unstable with increasing degradation and also aggregations over time. We show that addition of a protease inhibitor cocktail and higher salt concentration helped long-term protein stability and solubility of AcrIIA8. Structure determination of AcrIIA8 is currently in progress.



## Protein engineering of recombinant position-specific lipase enzymes

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Lipase catalyzes the hydrolysis of triacylglycerol into the glycerol and fatty acids. Lipase can act on a diverse kind of lipid substrates and plays a crucial role in digestion and processing of dietary lipids, such as triglycerides, fats, and oils. The lipases are used a lot in biotechnological application such as a modification of lipids, production of biodiesel and synthesis of bioactive esters. When we overexpressed the Cml (*Cordyceps militaris* lipase) and Bba (*Beauveria bassiana*) lipases using the prokaryotic system, the proteins were mainly produced as an inclusion body. We then tried different expression vectors and induction temperatures to obtain soluble proteins. We also co-expressed chaperon proteins with lipases to facilitate folding during induction. Producing functional lipases in the prokaryotic system would save costs with increases yield, promising potential biotechnological applications.

## Investigation of a dual inhibitor against the type I-E and I-F CRISPR-Cas systems

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Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)-Cas are widely distributed in bacteria and archaea, and can provide adaptive immune defense systems against invading phages and plasmids. Phages evolved counter-defense systems to neutralize the host CRISPR-Cas machinery, which are known as anti-CRISPR (Acr) proteins. To date, Acr proteins have been discovered for various type I (subtypes I-D, I-E, and I-F) and type II (II-A and II-C). The Acr proteins interact with different components of Cas proteins in a specific manner. Recently, an Acr protein inhibiting both I-E and I-F CRISPR-Cas systems have been reported, and the domain analysis indicated a chimera of previously identified AcrIE4 and AcrIF7 (AcrIE4-F7). We prepared the individual and combined versions of AcrIE4 and AcrIF7, obtained their  $^1\text{H}$ - $^{15}\text{N}$  HSQC spectra, and examined their binding with the Cas targets.

## NMR-based structural characterization of Tid1-JD and Tid1-eJD

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Heat shock protein 40 (Hsp40) are important co-chaperones of heat shock protein 70 (Hsp70). Hsp70 chaperone machines are ubiquitously present in all living organisms and play critical roles in protein homeostasis by temporarily interacting to many different substrates, via an adenine nucleotide-dependent cycle. Hsp40s are essential for this process. Hsp40s stimulate the hydrolysis of ATP bound to Hsp70 and stabilize the interaction with substrate poly peptides. In humans, Hsp40s compose a variety of family with more than 40 different members<sup>2</sup>, which vary in their substrate selectivity and in the structural compositions. Interestingly, although Hsp40s share similar structure, the functions of Hsp40s are diverse in the cell. Every Hsp40s possess the J-domain which is key region to interact with an Hsp70 and the other distinct regions which may cause the particularity in the targeting of Hsp70 chaperones to specific substrates. Based on the structural components, Hsp40 family is divided into three subclasses, class A, B and C. The J-domain of class A and class B members is located at the N-terminus like DnaJ which was firstly described member in the literature, whereas this domain exists anywhere in the protein belonging to the class C members. In Hsp40 class A members, the J-domain is followed by a glycine/phenylalanine (G/F)-rich region, two homologous  $\beta$ -barrel domains, a zinc-finger-like region, and a C-terminal dimerization domain. Class B members have similar structural components except a lack of a zinc-finger-like region. Class C members includes proteins with the functional J-domain that do not belong to Class A or Class B. They may have various other domains or functional motifs in the protein. In the present study, we designed two different constructs, one contains only J domain and the other contains J domain and extra residues from G/F rich domain in the C-terminus, called Tid1-JD and Tid1-eJD, respectively. The structure of Tid1-JD was determined by using solution NMR, and binding experiments of Tid1-JD and Tid1-eJD to peptide from P53 and full-length p53 were carried out using NMR. HSQC spectra comparison between Tid1-JD and Tid1-eJD show that (G/F) rich region was bound to J-domain not like Hsp40 A2 class, which suggests that (G/F) rich region may play a important role in regulation of binding between J-domain and other binding partner.

## **Elucidation of the structure and binding interactions of *Acinetobacter baumannii* ACP with $\beta$ -ketoacyl ACP synthase III as a potential potent antibacterial target**

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Fatty acids are critical to the survival of all organisms as they are used for storing energy and forming cell membranes, while also functioning as intermediates in various signaling pathways. Thus, fatty acid synthases (FASs) represent effective targets for antibiotics. Nevertheless, multidrug-resistant bacteria, including the human opportunistic bacteria, *Acinetobacter baumannii*, are emerging threats. Meanwhile, the FAS pathway of *A. baumannii* is relatively unexplored. Considering that acyl carrier protein (ACP) has an important role in the delivery of fatty acyl intermediates to other FAS enzymes, we elucidated the solution structure of *A. baumannii* ACP (AbACP) and, using NMR spectroscopy, investigated its interactions with  $\beta$ -ketoacyl ACP synthase III (AbKAS III), which initiates fatty acid elongation. Results show that AbACP comprises four helices, while  $\text{Ca}^{2+}$  reduces the electrostatic repulsion between acid residues, and the unconserved F47 plays a key role in thermal stability. Moreover, AbACP exhibits flexibility near the hydrophobic cavity entrance from D59 to T65, as well as in the  $\alpha 1\alpha 2$  loop region. Further, F29 and A69 participate in slow exchanges, which may be related to shuttling of the growing acyl chain. Additionally, electrostatic interactions occur between the  $\alpha 2$  and  $\alpha 3$ -helix of ACP and AbKAS III, while the hydrophobic interactions through the ACP  $\alpha 2$ -helix are seemingly important. Our study provides insights for development of potent antibiotics capable of inhibiting *A. baumannii* FAS protein-protein interactions.

## Substrate Specificity of Fatty Acid Synthases of *Propionibacterium acnes*

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*Propionibacterium acnes* (*P. acnes*) is a representative bacterium that causes acne vulgaris which is a serious skin inflammatory disease from adolescents to adults. Recently, it has been reported that *P. acnes* is also involved in the various inflammatory response such as an infection of surgery for artificial joints and the importance of developing antibiotics against *P. acnes* has emerged. Fatty acid synthesis (FAS) is essential for bacterial viability and *P. acnes* exhibits special cell membrane features to control membrane fluidity by branched-chain fatty acids (BCFAs). To gain effective control of *P. acnes*, a deeper understanding of the cellular metabolism mechanism, we have solved the structure of  $\beta$ -ketoacyl ACP synthase III (PaKAS III) which initiates the fatty acid elongation process. Conformation-sensitive urea polyacrylamide gel electrophoresis and tryptophan fluorescence quenching experiments confirmed that PaKAS III prefers isobutyryl-CoA as the acetyl-CoA, and the unique shape of the active site cavity complies with incorporation of branched-short chain CoAs. In this study, we determined the solution structure of acyl carrier protein (PaACP) which is a cofactor in FAS. Furthermore, we investigated the substrate specificity of PaACP for branched-chain fatty acid in comparison with that of *E. coli* ACP. Chemical shift perturbation (CSP) and spin relaxation data revealed that PaACP accommodates branched isobutyryl chain while *E. coli* ACP cannot. Unconserved C50 and I46 as well as flexibility of  $\alpha 2\alpha 3$  loop provide wider hydrophobic cavity for PaACP to shuttle branched acyl cargos compared to those of other bacterial ACP. This study clearly illustrates how BCFA synthesis is achieved in *P. acnes* and the unique shape of the cavity in PaKAS III and PaACP required for the branched-chain primer and can give insight to design novel inhibitors which target FAS enzymes of *P. acnes* specifically.

## **NMR Study of the specific DNA Sequence Recognition Mechanism of DLX3**

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Transcription factors (TFs) are proteins involved in the regulation of gene expression at the transcriptional level. They interact with DNA in a sequence-specific manner through their DNA-binding domains (DBDs), which are used to classify TFs into structural families. The DNA binding homeodomain of Dlx3 transcription factor bind to consensus TAATT sequence found on the promoter region of osteogenic genes including osteocalcin, Runx2 bone sialoprotein and regulate their transcription. For gene transcription to occur, transcription factors must bind to specific sequences of DNA. The highly conserved DLX3 is responsible for specific recognition of a common sequence motif, [5'- TAATTG-3']. To understand the molecular mechanisms of specific DNA recognition of DLX3, We performed 1H-15N HSQC titration with WT-DNA and T5G-DNA. The exchange rate constants of the imino protons for the wild type DNA, and TF-DNA complex were measured by using water magnetization experiment.

## **NMR studies of transcription factor HOXA1 complexed with its target DNA**

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In molecular biology, a transcription factor (TF) is a protein that controls the rate of transcription of genetic information from DNA to mRNA, by binding to a specific DNA sequence. Homeobox (Hox) genes encode a conserved family of transcription factor proteins that are critically important in vertebrate development. In humans, the Hox genes are distributed into four linkage groups (HOXA, HOXB, HOXC, and HOXD) comprising 39 genes located on chromosomes 7, 17, 12, and 2. Specifically, the HOXA1 may be involved in the placement of hindbrain segments in the proper location along the anterior-posterior axis during development. In this study, to understand this molecular mechanism of the HOXA1 with specific target DNA, we performed NMR experiments that HSQC titrations on HOXA1 complexed with 10-bp DNA duplex, d(5'- CGTAATGGCC -3')/d(5'- GGCCATTACG -3'), (wt-hx1DNA) and G5T mutant DNA. Our study will provide DNA recognition pathway of HOXA1.

## **NMR Study of target DNA recognition of Transcription Factor protein PBX4**

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Transcription factors (TFs) are proteins that bind specific sites or elements in regulatory regions of DNA, known as promoters or enhancers, where they control the transcription or expression of target genes. The three amino acid loop extension (TALE) homeodomain proteins are a family of transcription factor including the mammalian PBX, MEIS and PREP proteins. The PBC subclass comprises the proteins PBX1, PBX2, PBX3 and PBX4 in mammals. The TALE-HD differs from the classical HD by the insertion of three additional amino acids. These three amino acids are almost always a proline-tyrosine-proline (PYP) motif and are located between the first and second helix of the HD. The highly conserved DNA-binding TALE proteins define the family and is responsible for specific recognition of a common sequence motif. In prior studies, packing of spiral 4 for the rest of the PBX homo-domain has been shown to be able to stabilize spiral 3 and maintain the optimal form for binding to DNA. To understand the molecular mechanisms of specific DNA recognition of PBX4, we performed NMR experiments on PBX4 complexed with 10-bp DNA duplex, d(CGATGATTGA)/d(TCAATCATCG), (wt-pxDNA) and its mutants using NMR. We studied the PBX4-DNA interactions using imino proton and HSQC titrations. We also performed the <sup>15</sup>N relaxation dispersion and imino proton exchange experiments to study the kinetics of target-specific DNA binding of PBX4.



## Inhibition of tau and A $\beta$ <sub>42</sub> aggregation by ortho-catechol containing isoflavone

Ji-Na Yoo<sup>1</sup>, Jong Kil Lee<sup>2</sup>, Nam-Jung Kim<sup>2</sup>, Min-Duk Seo<sup>1\*</sup>

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Alzheimer's disease (AD) is a neurodegenerative disorder that accompanies memory loss and cognitive impairment characterized at the molecular level by two lesions: the intracellular neurofibrillary tangles (NFT) and extracellular amyloid plaque [1]. The tangles and plaque are caused by deposition of abnormal aggregation of microtubule-associated protein tau and fibrous assemblies of amyloid beta peptide. Recently, a series of polyhydroxyisoflavones were identified as novel therapeutic scaffolds for AD [2]. We here designed an isoflavone containing *ortho*-catechol moiety which is known to be crucial for inhibiting pathological protein aggregation both NFT and amyloid plaque [3]. To determine whether the *ortho*-catechol containing isoflavone is effective in preventing the aggregation of tau and A $\beta$ <sub>42</sub>, <sup>1</sup>H-<sup>15</sup>N heteronuclear single quantum coherence (HSQC) nuclear magnetic resonance (NMR) spectroscopy, thioflavin T (ThT) fluorescence and transmission electron microscopy (TEM) analysis was performed. Through the results, we identified that this compound could affect the aggregation process of tau and A $\beta$ <sub>42</sub>. Our results would contribute to understanding the mode of action of the catechol containing isoflavone during fibril formation, which will provide us perspicacity for new potential therapeutics development for AD.

## **NMR structural studies of human melanocortin-4 receptors and the syndecan-4**

Ji hong Wang, Hyunjin Ko, Minseon Kim, and Yongae Kim\*

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Email: dhkdwlgld@naver.com, hyuniee0830@naver.com

Human transmembrane proteins (hTMPs) are playing an important role in the biological system like gateways to permit the transport of a specific substance. Transmembrane proteins act as receptors, channels, and pumps between cells to transport various ions and nutrients, and they have been implicated in several diseases. It can also lead to loss of function as a carrier of substances and failure of signal transmission systems.

Among them, human melanocortin-4 receptor (hMC4R), which is expressed in the pituitary gland and functions to maintain energy homeostasis, will be dealt with. Studies of melanocortin-4 receptors, which play an important role in appetite control and energy homogeneity, is valuable because it is directly related to the direction of genetic problem-solving for human obesity. This study mainly deals with the process of expression, purification, and optimization, a process to obtain high yield wt/m-hMC4R-TM2 protein for NMR structure studies. The expressed proteins focus on investigating the structural differences of the wt/m-hMC4R-TM2 proteins by obtaining high yields and high purity. The resulting wt/m-hMC4R-TM2 protein was applied to various spectroscopy methods, including solution-state NMR spectroscopy and solid-state NMR spectroscopy.

Syndecan-4 (Syd4) performs a variety of functions, including cell-to-cell interactions, extracellular matrix interactions, cancer progression, and cell proliferation. Syndecan-4 is a type of transmembrane protein and transmits stimulation into cells through PIP<sub>2</sub> (phosphatidylinositol-(4, 5)-bisphosphate) phospholipids. Syndecan-4 (Syd4) dimerization is important for signal transduction. Thus, we demonstrated an optimized method for recombinant expression and purification of syndecan-4(Syd4). For efficient research, wild-type Syd4-TM

(wSyd4), Syd4-eTC (ecto-, TM, Cyto-) and mutant Syd4-TM (mSyd4) were studied to show dimer formation by the amino acid sequence GxxxG motif. Dimers were shown to be formed by the GxxxG motif, where wild-type Syndecan-4 TM was a dimer and mutant Syndecan-4 TM was a monomer. They were also investigated by solution/solid NMR spectroscopy to confirm their structures and interactions with PIP<sub>2</sub>.

## **The NMR structural and mechanistic studies of novel antimicrobial peptides, LPcin**

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Naturally derived antimicrobial peptides (AMPs) that can be considered a novel type of antibiotics being studied for bacteria resistant to antibiotics. AMPs are substances produced to defend against invasion of external bacterial, and many cationic AMPs have been isolated therefrom. Lactophorin-I (LPcin-I) is also a cationic amphiphilic AMP of the C-terminal region 113-135 of proteose-peptone, a protein derived from cow's milk. It has antimicrobial activity against Gram-positive bacteria and Gram-negative bacteria. Based on the amino acid sequence of LPcin-I, candidate peptides with better antimicrobial activity were designed through peptide engineering and antimicrobial activity experiments were conducted. Through this, the selected candidate LPcin analog peptides were expressed in large quantities through a gene recombination technique and obtained with high purity through an optimized purification method.

The secondary structure of the LPcin analogs were measured by CD, and the three-dimensional structure and orientation in the presence of a lipid bilayer were measured through solution/solid-state NMR spectroscopy. In order to identify the topology of the LPcin analogs and study the mechanism of action, a solid NMR probe for  $^1\text{H}$ - $^{15}\text{N}$  measurement and  $^1\text{H}$ - $^{31}\text{P}$  measurement were manufactured in our laboratory. In addition, the actual antimicrobial activity of the LPcin analogs in the actual bacteria were confirmed through SEM. Through this study, it will be possible to contribute to the establishment of a new AMP development system and provide an academic basis for AMP research.

## Validation of anti-inflammatory properties of tIK peptide and structural study through NMR

Jinhee Jeong, Minseon Kim and Yongae Kim\*

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Rheumatoid arthritis, an autoimmune disease, becomes inflamed the synovial membrane around the joint and destroys the ligaments and cartilage. This inflammation spreads to the skins and blood vessels, causing anemia, vasculitis, and headaches. Imbalance of pro- and anti-inflammatory cytokines is one of the causes of this disease. A recent study found that truncated-IL-18 (tIK) protein inhibits the expression of inflammatory cytokines. Therefore, we conducted research to develop anti-inflammatory peptides using only the inflammatory portion of the tIK amino acid sequence. We investigated the phosphorylation pattern in macrophages of tIK transgenic mice and found that the tIK protein phosphorylates the tyrosine 496<sup>th</sup> of the interleukin (IL)-10 receptor subunit alpha, and the inflammation disappears. To find the base sequence of a specific part of the tIK protein that phosphorylated the IL-10 receptor, the structure of tIK was predicted using sequence homology modeling using IL-10 and the sequence of 4 epitopes was assumed. The anti-inflammatory activity of each epitope was examined through the T<sub>H</sub>17 cell differentiation test, and the peptide consisting of 18 amino acids with the best anti-inflammatory effect was named tIK 18-mer. Referring to the sequence of this peptide, shorter, anti-inflammatory 9-mer and 14-mer were also found.

Peptide expression was performed by culturing *E. coli*, and peptides uniformly labeled with <sup>15</sup>N were analyzed through MALDI-TOF and NMR. It was confirmed that the experiment was successfully performed, and the experimental procedure was optimized. The secondary structure of the peptide was confirmed using CD and 2D NMR, and chemical shift perturbation was studied to confirm the interaction between the receptor and the anti-inflammatory peptide. Finally, an anti-inflammatory test was performed to prove the anti-inflammatory effect of the purified peptide.

## Metabolic changes of Flatfish Infected with *Streptococcus parauberis* using HR-MAS NMR-Based Metabolomics

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The interests of marine organisms have been increased as aquaculture industry developed rapidly. However, there are many kinds of infectious diseases that cause financial damage. The infectious diseases expand at a rapid rate in the fish farms because of the small area and dense population of fish. There is a great need for the rapid diagnosis and treatment. This study will be utilized for the base data of development diagnostic and therapeutic methods by observing the changes of metabolic profiles. In this study, flatfish (*Paralichthys olivaceus*) was infected with *Streptococcus parauberis* for 1 week. Control group (0 day) and infected groups (3 day and 7 day) were compared to each other using NMR-based metabolomics. *Streptococcus* is a mortal pathogen in fish cause serious economic losses for the aquaculture industry. Serum and liver of flatfish were measured with HR-MAS (high resolution-magic angle spinning) NMR. Spectral binning was performed at the Chenomx NMR suite 7.1 (Chenomx Inc., Edmonton, AB, Canada) and the binning data were analyzed by the Principal component analysis (PCA), Partial least squares discriminant analysis (PLS-DA) and Orthogonal Partial Least Squares discriminant analysis (OPLS-DA) using the SIMCA-P<sup>+</sup> 12.0 software (Umetrics, Umeå, Sweden). The metabolites were assigned using the Chenomx 600 MHz library database. In serum and liver, PCA, PLS-DA and OPLS-DA score plots showed the clear separation between control group and infected groups. Acetoacetate, proline, pyruvate and myo-inositol in serum and acetoacetate, creatine, fumarate, glucose, methionine, O-phosphocholine, phenylalanine, succinate and uridine in liver were significantly increased.

## **Metabolomics profiling of *Vibrio harveyi* and WSSV Infection in Whiteleg Shrimp, *Litopenaeus vannamei*, using HR-MAS NMR**

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*Department of Chemistry and Chemistry Institute for Functional Materials, Pusan National University, Busan 46241, Republic of Korea*

E-mail: suhkmann@pusan.ac.kr

The shrimp industry in Korea is thriving as to meet the demands. However, there is a growing concern over the industry that infectious disease causes a massive economic loss. It is necessary to set up new strategy to prevent the disease. Among the infectious disease in white leg shrimp (*Litopenaeus vannamei*), White spot syndrome virus (WSSV) and *Vibrio harveyi* was studied in this research. In this study, white leg shrimp was infected with WSSV and *Vibrio harveyi* for a week. The blood and the hepatopancreas of white leg shrimp were analyzed by High Resolution Magic Angle Spinning Nuclear Magnetic Resonance (HR-MAS NMR) based Metabolomics. Spectral binning was performed at the Chenomx NMR suite 7.1 (Chenomx Inc., Edmonton, AB, Canada) and the binning data was analyzed by the Principal component analysis (PCA), Partial least squares discriminant analysis (PLS-DA) and Orthogonal Partial Least Squares discriminant analysis (OPLS-DA) using the SIMCA-P<sup>+</sup> 12.0 software (Umetrics, Umeå, Sweden). The metabolites were assigned using the Chenomx 600 MHz library database. With the multivariate analysis, choline and uracil was the most significant metabolite in the study. This was supported by the Variable Importance Projection (VIP) Score that the score was over 2.0. In the result of the correlation analysis, glycine-serine-threonine metabolism was affected.





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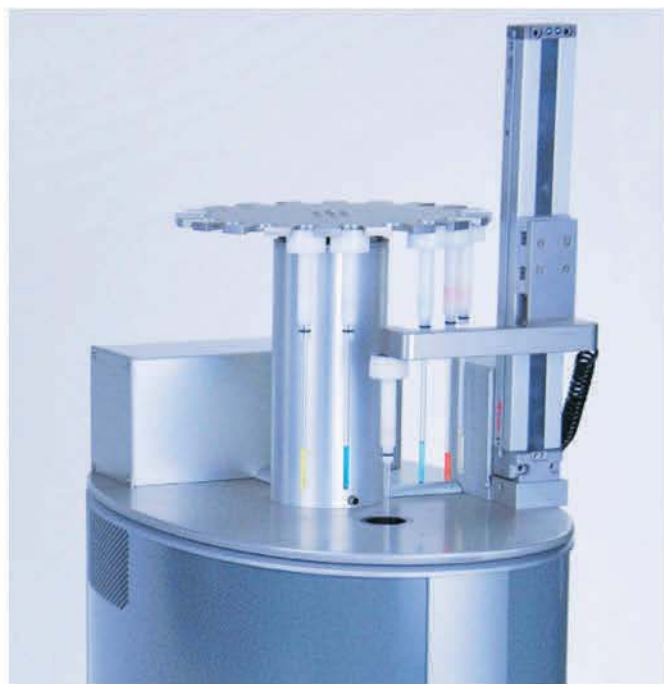


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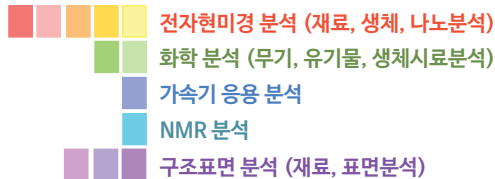
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TEM-sampling 재료

6972

TEM-sampling 생물/폴리머

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SEM-sampling 생물

4933

FE-SEM (Inspect F)

4944

FE-SEM (Inspect F50)

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FE-SEM (Regulus)

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E-SEM

5972

FE-SEM (Nova-SEM)

5972

FE-SEM (Teneo VS)

5540

FIB (Helios)

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FIB (Nova)

5985

FIB (Quanta 3D)

6973

APT (Atom Probe)

4946

Raman

4944

EPMA

5540

AAS, DMA(Hg), ICP/OES

5967~8

ICP/MS

5967~8

HPLC-ICP/MS

5967~8

fsLA (Laser Ablation) system

5967~8

원소기반 습식분석 (Silica,PH-meter)

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UV-Vis/NIR

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EA (CHNS, O)

5998

TG-DTA, DSC

5998

HPLC

5963

IC

5963

LC/MS/PK (비밀상)

5920

LC-HR/MS (UPLC-Q-ToF)

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(micro) FT-IR

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GC, GC-ToF-MS

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800MHz NMR(액체)

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AES (Auger)

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ToF SIMS

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D-SIMS

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XPS/UPS

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XAFS

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X-ray PDF

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XRD (박막, 벌크)

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HR-XRD (고분해능)

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XRD (분말)

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- 표적 단백질의 발현을 위한 다양한 벡터 클로닝 및 과발현 시스템 구축
- 박테리아 (E.coli) 시스템을 이용한 단백질 생산 최적화 및 고순도 대량 생산

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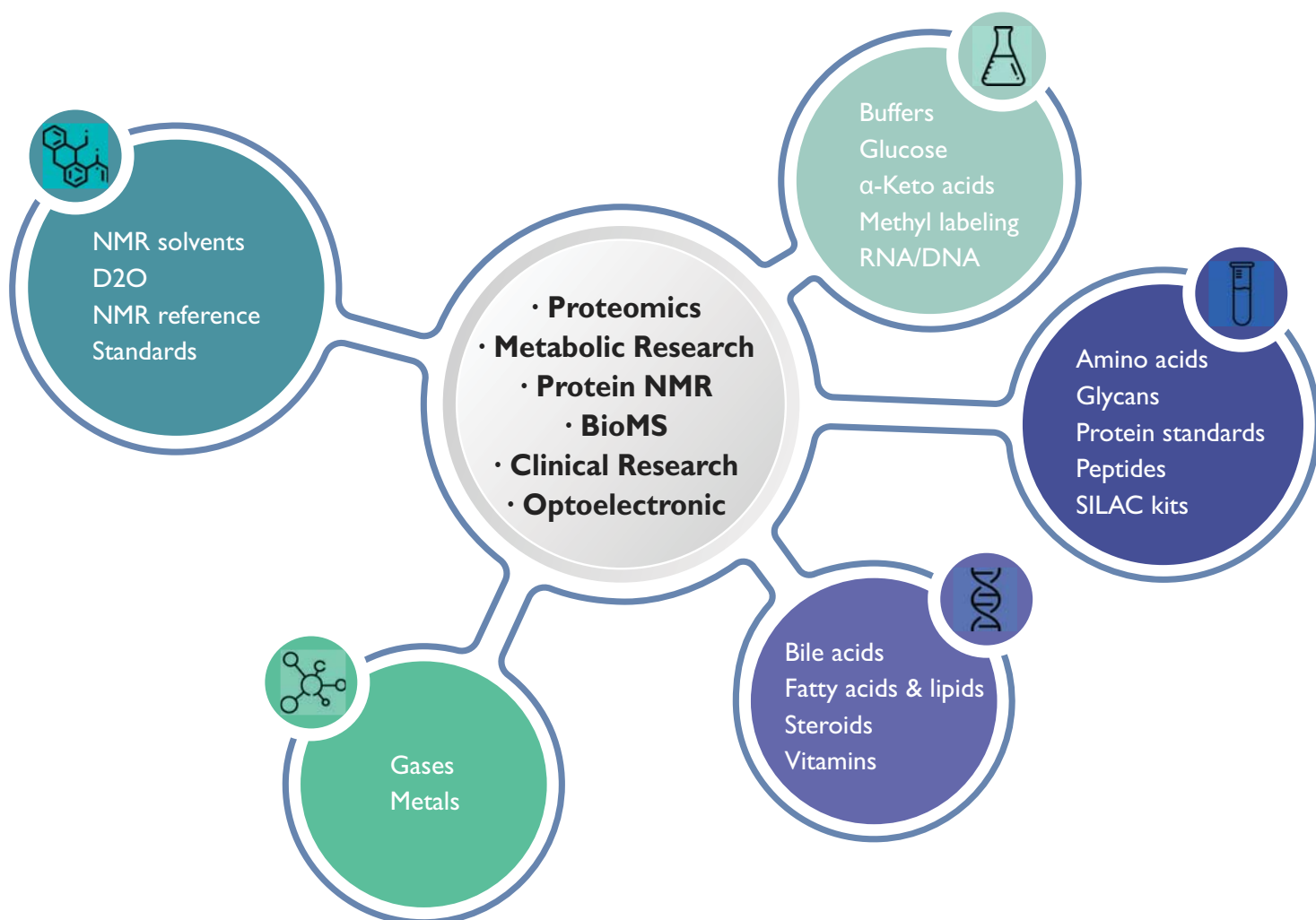
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Kinetics of protein  
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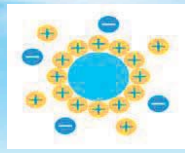
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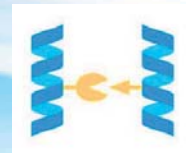
Molar Mass



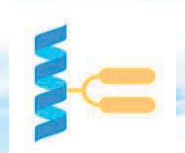
Size



Charge



Interaction



Conjugate

## 단백질 특성 분석 솔루션 I

### Light Scattering Technology

- ▶ Multi Angle Light Scattering (MALS) - DAWN
  - SEC-MALS, FFF-MALS 를 통한 단백질의 특성 및 구조 분석.
  - 절대분자량(Absolute molar mass)
  - Size (Rg size)
  - Conformation
  - Conjugation ratio(접합체 분자량 비율)

- ▶ Dynamic Light Scattering(DLS) - Dynapro Nanostar
  - Size(Rh) 및 Size distribution
  - Molar mass
  - Aggregation and stability(Tm, Tagg, KD, A2)
  - Purity or contamination

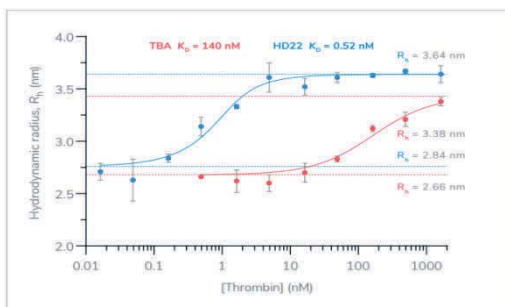
- ▶ HT-DLS(High Throughput DLS) - Dynapro PlatereaderIII
  - 96,386,1536 웰 플레이트를 이용한 고효율 처리 DLS 시스템.



## 단백질 특성 분석 솔루션 II

### MDS Technology

- ▶ Fluidity One-W : microfluidic diffusional sizing(MDS) 기술을 이용하여, 단백질의 Rh 사이즈와 affinity 를 분석.
- ▶ 5ul 의 샘플 볼륨으로 Rh 사이즈와 Kd 값을 동시에 분석.



- ▶ 라벨링을 통한 Fluorescence 검출로 타겟 단백질을 분석할 수 있으며, 농도와 오염에 민감하지 않아 막단백질의 계면활성제 및 단백질의 응집물 등이 결과에 영향을 미치지 않음.



fluidity one-w

\* Fluidity One-W Serum 버전으로 COVID-19 관련 중화항체 분석 가능.



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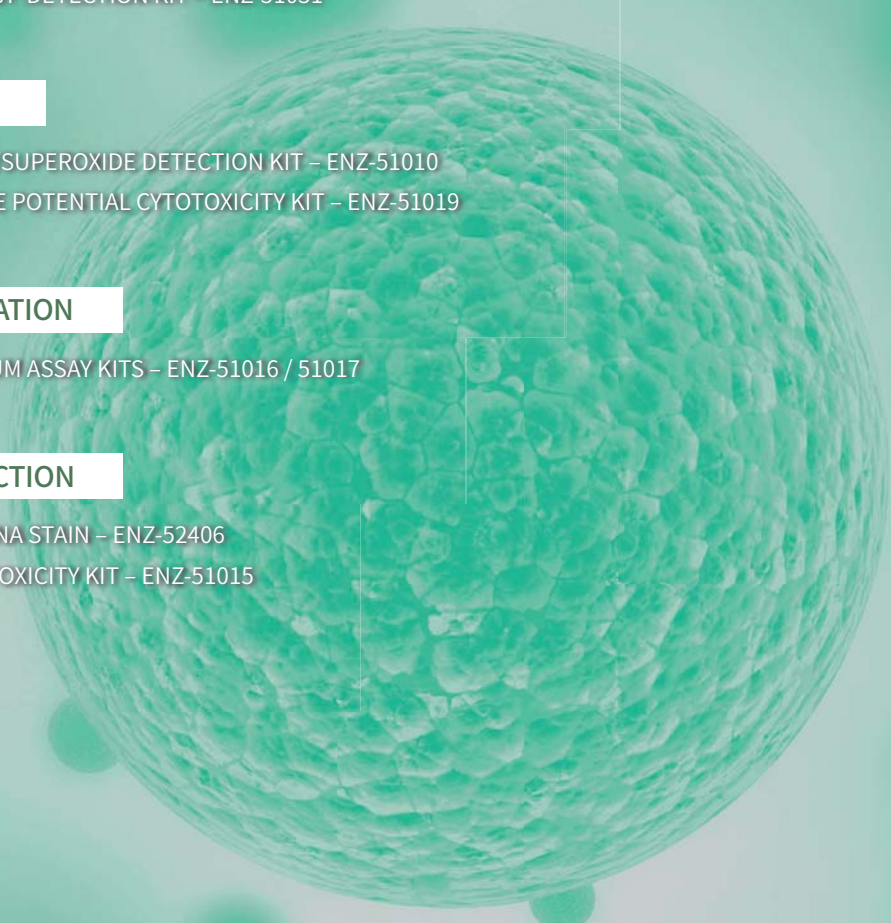
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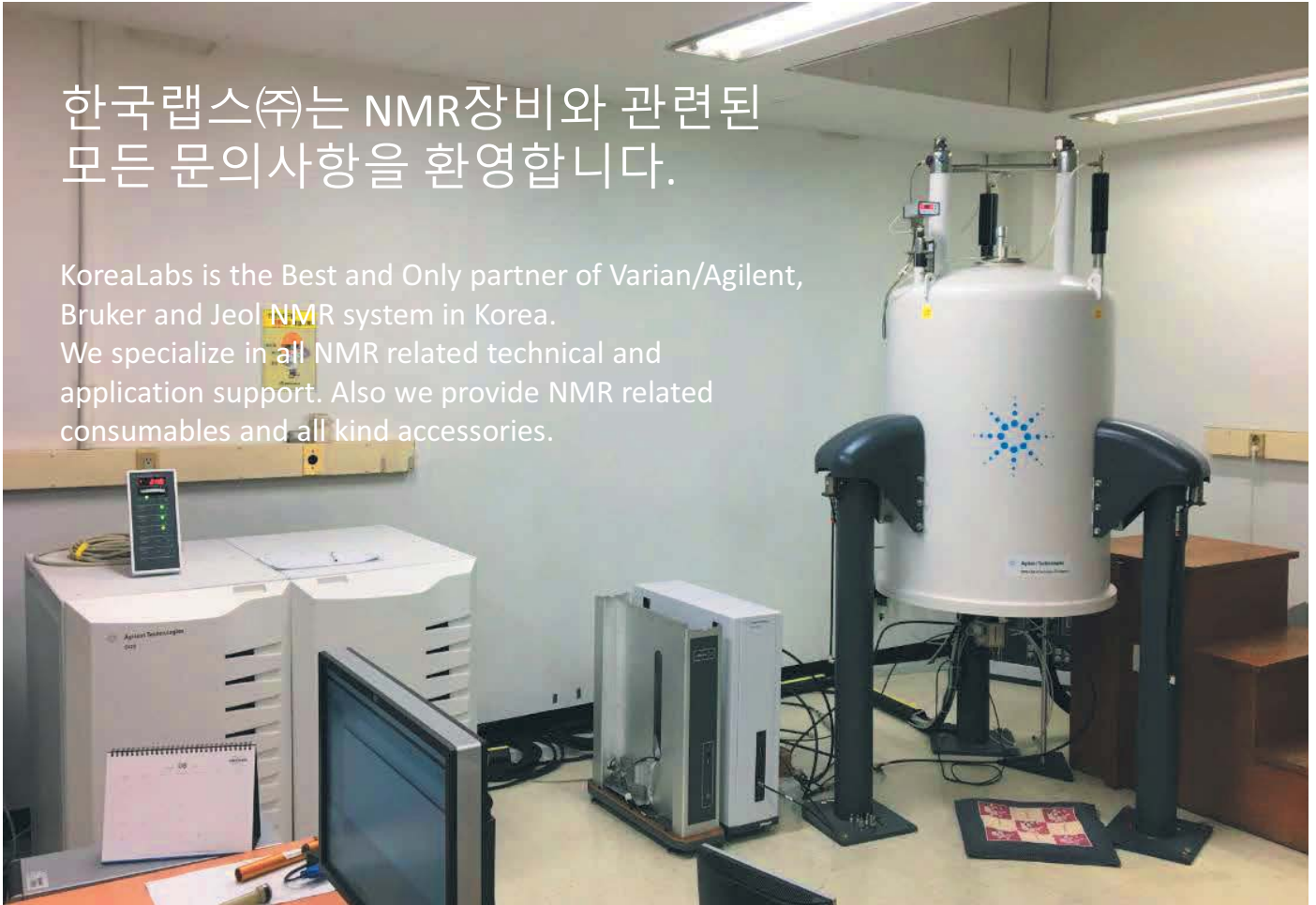
- NUCLEAR-ID® RED DNA STAIN – ENZ-52406
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한국랩스(주)는 NMR장비와 관련된 모든 문의사항을 환영합니다.

KoreaLabs is the Best and Only partner of Varian/Agilent, Bruker and Jeol NMR system in Korea.  
We specialize in all NMR related technical and application support. Also we provide NMR related consumables and all kind accessories.



- **NMR 장비유지보수**

NMR 주요 시스템과 관련 부속장비 및 부품들을 보호하고 최상의 기기 상태를 유지하기 위하여 다양한 종류의 서비스 계약을 제공합니다. NMR콘솔, 소프트웨어, Probe는 물론 주변장치들 전반의 원활한 운영을 위하여 장비를 설치 초기 수준의 점검으로 수행하고 정기적인 현장 방문 검사와 필요한 부분을 수리합니다.

- **NMR 교육 및 분석지원**

Varian/Agilent NMR 장비를 운영중인 사용자를 위한 교육 프로그램으로 NMR의 기본조작부터 고급실험 운영까지 종합적인 범위의 맞춤 교육 서비스를 제공합니다.

- **NMR 튜브,시약 및 관련 전 부품**

NMR에 사용되는 튜브와 시약 및 관련제품을 제공하며 장비 운영 시 문제가 발생한 파트에 대하여 상담하고 신속하게 공급합니다.

- **NMR 헬륨 충전 서비스**

NMR 시스템의 Magnet사양과 상태를 세밀하게 파악하여 알맞은 헬륨 충전주기의 일정 계획을 세우고 사전에 연락을 취하여 서비스 일정에 맞추어 액체 헬륨을 충전합니다.





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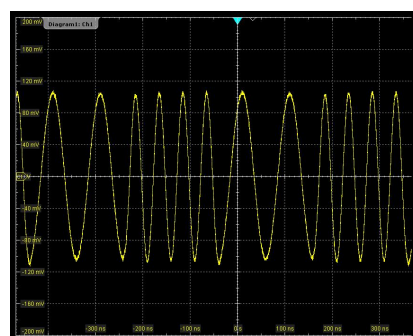
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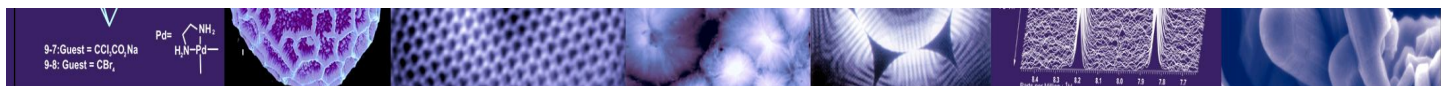


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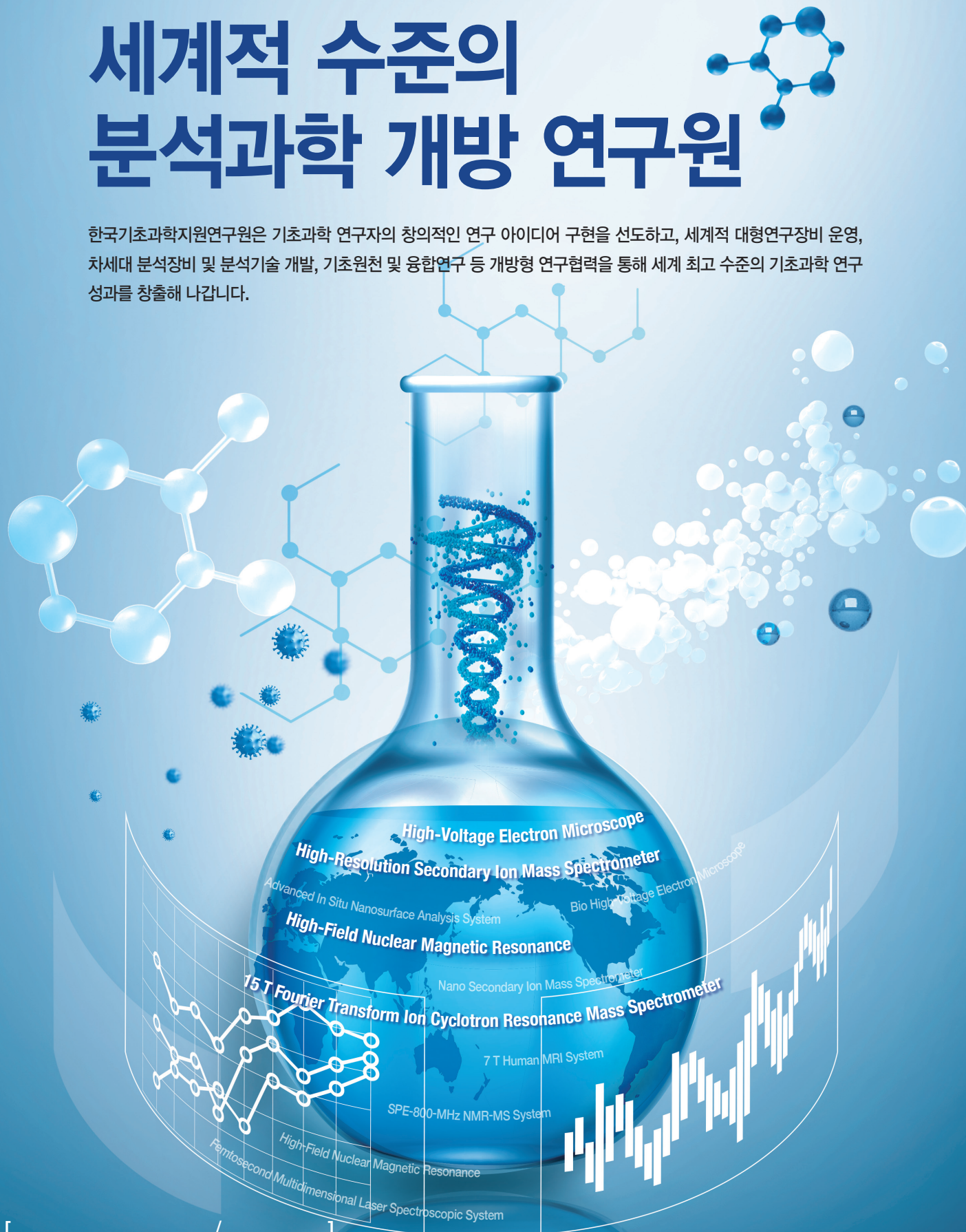
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# 세계적 수준의 분석과학 개방 연구원

한국기초과학지원연구원은 기초과학 연구자의 창의적인 연구 아이디어 구현을 선도하고, 세계적 대형연구장비 운영, 차세대 분석장비 및 분석기술 개발, 기초원천 및 융합연구 등 개방형 연구협력을 통해 세계 최고 수준의 기초과학 연구 성과를 창출해 나갑니다.



[ NMR : 900/800/700/400 MHz NMR + 1.2GHz NMR (2024~25 )  
MRI : 7.0/3.0 T Human MRI, 4.7 T/9.4 T Animal MRI (2022~23 )