대한화학회 생명화학분과 2015 겨울워크샵을 개최하며

2015년 2월 9일, 대한화학회 생명화학분과의 겨울워크샵을 고등과학원에서 개최하면서 여러분과 함께할 수 있게 되어 매우 자랑스럽고 기쁘게 생각합니다. 또한, 바쁘신 와중에도 참석하여 자리를 빛내 주신 김홍석 대한화학회장님과 여러 생명화학분과회원님들께 깊은 감사를 드립니다.

최근 생명화학 분야의 발전은 생물학, 물리학, 공학, 의학을 비롯한 다양한 학문 분야로의 활발한 파급으로 이루어지고 있고 이에 따라 생명화학분과는 새로운 도약을 준비하고 있습니다. 대한화학회 생명화학분과회에서는 화학을 기반으로 다양한 생명 현상을 이해하고, 광범위한 분야의 연구 성과를 상호 교환, 토론하고 있습니다. 2014년 8월 25일에 있었던 여름 워크샵에 이어, 국내 신진연구자 발굴 및 국내 전문 연구자들의 상호 연구교류를 촉진하기 위해 이번에는 겨울 워크샵을 준비하게 되었습니다. 본 워크샵에서는 생명화학분야 연구를 선도하고 계시는 고등과학원 이주영교수님, 서울대학교 박승범교수님, 한양대학교 류성언 교수님 세분의 기조강연과 대사체학, 구조생화학, 화학생물학, 효소화학 등 다양한 생명화학 분야에서 활동하고 계시는 연사 분들께서 관련 내용을 심도 있게 소개해 주실 예정입니다.

아무쪼록 참석해 주신 모든 분들이 본 워크샵의 취지에 공감하고 활발한 의견 교환 및 토론을 통해 유익한 시간이 되시기를 기대합니다. 본 워크샵을 기반으로 국내 생명화학 연구가 상호 협력을 통해 더욱 발전하는 계기가 되기를 바랍니다. 본 워크샵의 성공적인 개최를 위하여 열성적으로 준비하신 모든 운영위원들께 깊이 감사드리며, 본 워크샾을 후원해주신 고등과학원과 항상 관심을 가지고 적극적으로 후원해주시는 관련업체들께도 감사드립니다.

대한화학회 생명화학분과회장

김 양 미 배상

Time Table (2015. 2.9)

Registration / Refreshment (13:00 – 13:20)

Opening Remark (13:20-13:25)

김양미 (생명화학분과회장)

Congratulatory Remark (13:25-13:30)

김홍석 (대한화학회장)

Session I (13:30-15:00) 좌장: 이민재 (경희대)

Plenary Lecture I (13:30-14:00) 이주영(KIAS)

Protein Structure Modeling/Determination by Global Optimization using Ambiguous NOE restraints

OL 1 (14:00-14:20) 김영준(건국대)

Investigating the Regulatory Interaction of Linker Region of *Ciona intestinalis* Voltage-sensitive Phosphatase with Lipid Membrane

OL 2 (14:20-14:40) 황금숙(기초과학지원연구원)

Metabolomics approach for discovering biomarkers and understanding metabolic pathway

OL 3 (14:40-15:00) 서정용(서울대)

Protein–protein interaction that involves coupled unfolding and binding

Coffee Break (15:00-15:15)

Session II (15:15-16:25) 좌장: 김동은 (건국대)

Plenary Lecture II (15:15-15:45) 박승범(서울대)

FITGE-Based Target Identification: New Tool in Chemical Biology

OL 4 (15:45-16:05) 강세병(UNIST)

Engineering Protein Cage Nanoparticle for Biomedical Applications

OL 5 (16:05-16:25) 오상택(국민대)

Dual small molecule modulators of Wnt/β-catenin and p53 signaling

Coffee Break (16:25-16:40)

Session III (16:40-17:50) 좌장: 이 연(서울대)

Plenary Lecture III (16:40-17:10) 류성언(한양대)

Structural proteomics of human protein tyrosine phosphatases

OL 6 (17:10-17:30) 송재경(선문대)

Glycosylation of flavonoids and polyketides using flexible glycosyltransferase

OL 7 (17:30-17:50) 유연규(국민대)

A new approach to study membrane proteins

Closing Remark (17:50)

황광연 (생명화학분과 운영위원장)

Banquet (18:00-20:00)

[PL1]

Protein Structure Modeling/Determination by Global Optimization using Ambiguous NOE restraints

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In the recent CASP (Critical Assessment of Protein Structure Prediction) 11 experiment, a new challenge, the contact assisted category (called Ts target) using simulated sparse NMR contacts was tested. Contacts based on simulations (carried out by the Gaetano Montelione's group) reflect the situation in the initial stage of the NMR experiment. For a fairly large protein (> 160 residues) for NMR, data is typically collected from deuterated samples, which usually results in much spectral overlaps that are difficult to assign properly. The number of simplified spectra straightforward to assign is rather small. Therefore, in the early stage of the protein structure determination by NMR, one is faced with the combinatorial optimization problem to properly assign ambiguous NOE peaks to their corresponding hydrogen atom pairs, which is followed by subsequent structure optimization satisfying all the distance constraint arranged by a given set of the peak assignment. With sparse constraints and the ambiguous distance information, standard NMR structure calculation programs fail to generate accurate protein 3D models, and the protein structure determination in such a situation remains as a challenge. In CASP11, 19 Ts targets with the chain length in the range 108 to 462 residues were tested. We solved the two-level optimization to generate 3D protein models consisent with provided ambiguous restraints, for which we have applied the global optimization method of conformational space annealing. In most of the cases, accurate 3D models were generated typically within 1.0 – 3.0 Å RMSD from the native structure. Proper application of the proposed method can greatly reduce the time and the cost of protein 3D structure determination using NMR data. Finally, a brief discussion on our overall CASP11 performance will be provided.

[1] Keehyoung Joo, InSuk Joung, Jinhyuk Lee, Jinwoo Lee, Weontae Lee, Bernard Brooks, Sung Jong Lee and Jooyoung Lee, Protein Structure Determination by Conformational Space Annealing Using NMR Geometric Restraints (submitted).

[2] Keehyoung Joo, Juyong Lee, Sangjin Sim, Sun Young Lee, Kiho Lee, Seungryong Heo, In-Ho Lee, Sung Jong Lee and Jooyoung Lee, Protein structure modeling for CASP10 by multiple layers of global optimization, Proteins: Structure, Function, and Bioinformatics, 82, 188–195 (2013).

[3] Juyong Lee, Steven P. Gross and Jooyoung Lee, Improved network community structure improves function prediction, Scientific Reports, 3, 2197 (2013).

[4] Juyong Lee, Steven P. Gross and Jooyoung Lee, Modularity optimization by conformational space annealing, Phys. Rev. E, 85, 056702 (2012).

[5] Jooyoung Lee, Harold A. Scheraga, and S. Rackovsky, New Optimization Method for Conformational Energy Calculations on Polypeptides: Conformational Space Annealing, J. Comput. Chem., 18, 1222-1232 (1997).

이 주 영 (Lee, Jooyoung)

Career

1982 B. S. in Physics, Seoul National University

1984 M. S. in Physics, Seoul National University

1987 M. S. in Physics, Brown University

1991 Ph. D. in Physics, Brown University

2000 Professor, School of Computational Science, Korea Institute of Advanced Study

2008 Director, Center for In Silico Protein Science

Research Area / Representative Publications

세계적인 단백질 구조 예측대회에 참여하여 CASP7 부터 시작하여 CASP10 대회까지 4 회 연속으로 단백질 3 차구조 예측 분야에서 최우수 그룹으로 선정되었다. 이로 인하여 강연 초청을 받았으며, Proteins 저널에 초청 논문을 발표하였다. 단백질 3 차 구조 예측 분야에서 세계 최고 수준의 연구 리더로 국제적인 주목을 받고 있다. 최근에는 신물질 디자인 연구에 최적화 방법을 적용하여 불가능하다고 생각했던 Direct bandap silicon 결정 구조의 컴퓨터 디자인 구조를 세계 최초로 발표하였다. 실험만으로는 해결하기 어려운 문제를 실험 결과와 계산 결과를 융합하여 해결하는 연구에 힘쓰고 있다.

Keehyoung Joo, Juyong Lee, Sangjin Sim, Sun Young Lee, Kiho Lee, Seungryong Heo, In-Ho Lee, Sung Jong Lee and **Jooyoung Lee**, Protein structure modeling for CASP10 by multiple layers of global optimization, Proteins: Structure, Function, and Bioinformatics, volume 82, 188–195 (2013)

Juyong Lee, Steven P. Gross and **Jooyoung Lee**, Improved network community structure improves function prediction, Scientific Reports, 3, 2197 (2013)

Keehyoung Joo, Jinwoo Lee, Sunjoong Lee, Joo-Hyun Seo, Sung Jong Lee, and **Jooyoung Lee**, High Accuracy Template Based Modeling by Global Optimization, Proteins: Structure, Function, and Bioinformatics, Vol. 69, 83- 89 Suppl. 8 (2007)

Julian Lee, In-Ho Lee, and **Jooyoung Lee**, Unbiased global optimization of Lennard Jones clusters for N <= 201 by conformational space annealing method, Phys.Rev.Lett., Vol. 91, 080201 (2003)

Jooyoung Lee, Harold A.Scheraga, and S.Rackovsky, New Optimization Method for Conformational Energy Calculations on Polypeptides: Conformational Space Annealing, J.Comput.Chem., Vol. 18, 1222-1232 (1997)

[PL2]

FITGE-Based Target Identification: New Tool in Chemical Biology

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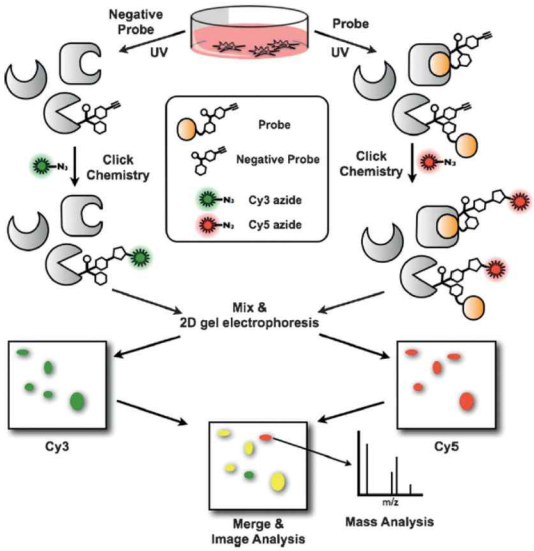
The importance of molecular diversity has been clearly recognized to identify specific bioactive small molecules for the elucidation of mysterious biological processes. The diversity-oriented synthesis (DOS) was introduced for efficient population of molecular diversity in untapped chemical space using complexity-generating synthetic route. To maximize the molecular diversity with high relevance in biological space, we pursued privileged-substructure-based DOS (pDOS) strategy to emphasize the importance of maximized skeletal diversity through the creative reconstruction of core skeletons containing privileged substructures. The efficiency of hit discovery from pDOS libraries was envisioned due to their enhanced relevance to biological space. This is the first systematic study to demonstrate the importance of privileged structures for the construction of molecular diversity through a series of high-throughput screening processes and subsequent biological evaluations. Our divergent pDOS strategy can provide an efficient approach for the discovery of novel small-molecule modulators with excellent specificity in chemical biology and drug discovery. Secondly, a systematic study of Seoul-Fluor will be presented. During our continuous efforts on the construction of drug-like small-molecule libraries using pDOS strategy, we aimed to develop a novel fluorescent core skeleton for the development of bioprobes, applicable for image-based screening. Guiding with computational simulation, we constructed a novel collection of fluorophores, which covers the full-color emission range with predictability. Seoul-Fluor analogs were successfully applied in HCS. Lastly, we developed a new target identification platform, FITGE, which aims to preserve protein-small molecule interactions under the intact cellular environment. After a series of failures using conventional target ID methods, we successfully identified the protein target of anti-proliferative compound with FITGE only under the live cell condition and observed the environment-dependent binding events of a functional small molecule by direct comparison between live cells and cell lysates. Even though it still requires the synthesis of bioactive probes with photo-crosslinker moiety, we believe our FITGE strategy can provide a unique technology platform for target identification in live cells.



[1] Kim, E.; Koh, M.; Lim, B.J.; Park, S.B.* *J. Am. Chem. Soc.,* **2011**, *133,* 6642–6649; Choi, E.; Kim, E.; Lee, Y.; Jo, A.; Park, S. B.* *Angew. Chem. Int. Ed.* **2014** *53(4),* 1346–1350; Kim, E.; Lee, Y.; Lee, S.; Park, S. B.* *Acc. Chem. Res. In press* (Seoul-Fluor).

[2] Park, J.; Oh, S.; Park, S. B.* *Angew. Chem. Int. Ed.* **2012**, *51,* 5447–5451; Koh, M.; Park, J.; Koo, J.Y.; Lim, D.; Cha, M.Y.; Jo, A.; Choi, J.H.; Park, S. B.* *Angew. Chem. Int. Ed.* **2014**, *53(20),* 5102–5106 *(selected as Cover Article); Lee, S.; Nam, Y.; Koo, J.Y.; Lim, D.; Park, J.; Ock, J.; Suk, K.*;* ***Park, S.B.**** *Nature Chemical Biology* **2014** *10(12),* 1055–1060 (FITGE).

[3] Kim, J.; Kim, H.; **Park, S.B.*** *J. Am. Chem. Soc.* **2014** *136(42),* 14629–14638*;* Oh, S.; Park, S.B.* *Chem. Commun.* **2011**, 12754–12761. (pDOS)

[4] Cho, T.-J.‡; Kim, J.‡; Kwon, S.-K.; Lee, D.-S.; Cho, J.; Park, S.B.* *Chem. Sci.* **2012**, *3(10),* 3071–3075; Lee, S; Kim, E.; Park, S.B.* *Chem. Sci.* **2013** *4,* 3282–3287; Jo, A; Park, J.; Park, S.B.* *Chem. Comm.,* **2013** *49(45),* 5138–5140 (Phenotypic Screening).

박 승 범 (Park, Seung Bum)

Career

1993 B. S. in Chemistry, Yonsei University

1997 M. S. in Organic Chemistry, Yonsei University

2001 Ph. D. in Bioorganic Chemistry, Texas A&M University

Representative Publications

- *Target Identification Revealed a Direct HMGB2-binding Small Molecule with an Anti-neuroinflammatory Effect.* Lee, S.; Nam, Y.; Koo, J.Y.; Lim, D.; Park, J.; Ock, J.; Suk, K.*; **Park, S.B.*** *Nature Chemical Biology* **2014** *in press.*
- *Privileged Structures: Efficient Chemical "Navigators" toward Unexplored Biologically Relevant Chemical Space*. Kim, J.; Kim. H.; **Park, S.B.*** *J. Am. Chem. Soc.* **2014** *in press.*
- *Phenotypic Screening to Identify Small-Molecule Enhancers for Glucose Uptake: Target Identification and Rational Optimization of Their Efficacy.* Koh, M.; Park, J.; Koo, J.Y.; Lim, D.; Cha, M.Y.; Jo, A.; Choi, J.H.; **Park, S. B.*** *Angew. Chem. Int. Ed.* **2014**, *53(20),* 5102–5106 *(Cover Article).*
- *Rational Perturbation of Fluorescence Quantum Yields in Emission-tunable and predictable Fluorophores (Seoul-Fluors) by a Facile Synthetic Method Involving C-H Activation.* Choi, E.; Kim, E.; Lee, Y.; Jo, A.; **Park, S. B.*** *Angew. Chem. Int. Ed.* **2014** *53(4),* 1346–1350
- *Discovery of an antiproliferative agent and its target identification in live cells using fluorescence difference in two dimensional gel electrophoresis.* Park, J.; Oh, S.; **Park, S. B.*** *Angew. Chem. Int. Ed.* **2012,** *51(22),* 5447–5451.
- *Emission Wavelength Prediction of a Full-Color-Tunable Fluorescent Core Skeleton, 9-Aryl-1,2-dihydropyrrolo[3,4-b]indolizin-3-one.* Kim, E.; Koh, M.; Lim, B. J.; **Park, S. B.***J. Am. Chem. Soc.* **2011**, *133(17), 6642–6649.*
- *A Two-Photon Tracer for Glucose Uptake*. Tian, Y.S.; Lee, H.Y.; Lim, C. S.; Park, J. ; Kim, H. M.; Shin, Y. N.; Kim, E. S.; Jeon, H.J.; Cho, B.R.*; **Park, S. B.*** *Angew. Chem. Int. Ed.,* **2009**, *48,* 8027–8031.
- *Combinatorial Discovery of Full-color-tunable Emissive Fluorescent Probes Using Novel Core Skeleton*. Kim, E.; Koh, M.; Ryu, J.; **Park, S. B.*** *J. Am. Chem. Soc.*, **2008**, *130*, 12206-12207.

[PL3]

Structural proteomics of human protein tyrosine phosphatases

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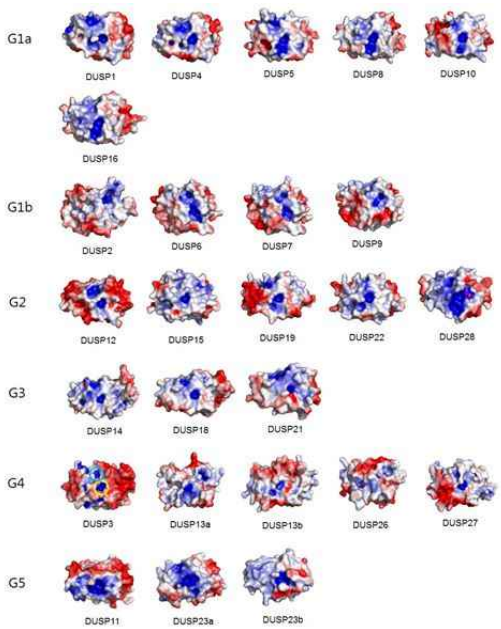
Protein tyrosine phosphatases (PTPs) dephosphorylate the phosphorylated proteins. The PTP-mediated dephosphorylation regulates protein activities either negatively or positively, and play vital roles in various diseases including cancers, vascular diseases, immune diseases and neurological diseases. Although originally characterized PTPs have dephosphorylating-enzyme activities towards phosphor-tyrosines only, there are a number of PTPs that dephosphorylate both phosphor-serines/threonines and phosphor-tyrosines. Mitogen activated protein kinase phosphatases (MAPK phosphatases or MKPs), which are dual-specificity phosphatases, dephosphorylate threonine-X-tyrosine (TXY) motif of MAPKs. They contain a MAPK binding domain (MKB) at their N-termini and a phosphatase catalytic domain at their C-termini. By regulating activity of MAPK signaling pathways, MKPs are pivotal players in cell growth and are implicated in the cell growth-related diseases. Atypical dual-specificity phosphatases (A-DUSPs) were found through their homologies to vaccina virus H1 gene product (VH1). Dual specificity protein phosphatases (DUSPs), which dephosphorylate both phosphor-serines/threonines and phosphor-tyrosines, play vital roles in immune activation, brain function and cell growth signaling. We constructed the family-wide structural library of human DUSPs by experimental structure determination supplemented with homology modeling. The catalytic domain of individual DUSP has characteristic features in the active site and surface charge distribution, indicating substrate interaction specificities. The active site loop-to-strand switch occurs in a subtype-specific manner, indicating that the switch process is needed for the corresponding DUSPs' characteristic substrate interactions. A comprehensive analysis of the activity-inhibition profile and active site geometry of DUSPs reveals a novel role of active pocket structure in the substrate specificity of DUSPs. The structure-based analysis of redox responses indicates that the extra cysteines are important for the protection of enzyme activity. The family-wide structures of DUSPs form a basis for understanding of phosphorylation-mediated signal transduction and the development of therapeutics.



[1] Jeong *et al*. The family-wide structure and function of human dual-specificity protein phosphatases. *Acta Cryst*. **D70**, 421-35 (2014)
[2] Ryu *et al.* Targeting allosteric sites for protein tyrosine phosphatase inhibition. *Biodesign* **2**, 81-90 (2014)
[3] Yu *et al*. Structural basis for the dephosphorylating activity of PTPRQ towards phosphatidylinositide substrates. *Acta Cryst*. **D69**, 1522-9 (2013)
[4] Lee *et al*. Redox regulation of OxyR requires specific disulfide bond formation involving a rapid kinetic reaction path. *Nature Struct. Biol*. **11**, 1179-85 (2004)
[5] Choi *et al*. Structural basis of the redox switch in the OxyR transcription factor. *Cell* **105**, 103-13 (2001)

류 성 언 (Ryu, Seong Eon)

Career

1984 B. S. in Chemistry, Seoul National University

1986 M. S. in Biochemistry, Seoul National University

1991 Ph. D. in Biochemistry, Columbia University

1991-1994 Postdoc, Harvard University

1994-2009 Principal Researcher, Korea Research Institute of Bioscience and Biotechnology

2009-Present Professor, Hanyang University

2012-Present President, Korean Society for Structural Biology

Research Area / Representative Publications

- 탈인산화효소의 구조단백체를 이용한 신약설계

  Jeong *et al*. The family-wide structure and function of human dual-specificity protein phosphatases. *Acta Cryst*. **D70**, 421-35 (2014)

  Yu *et al*. Structural basis for the dephosphorylating activity of PTPRQ towards phosphatidylinositide substrates. *Acta Cryst*. **D69**, 1522-9 (2013)

- 세포스위치단백질의 산화환원 조절

  Lee *et al*. Redox regulation of OxyR requires specific disulfide bond formation involving a rapid kinetic reaction path. *Nature Struct. Biol*. **11**, 1179-85 (2004)

  Choi *et al*. Structural basis of the redox switch in the OxyR transcription factor. *Cell* **105**, 103-13 (2001)

[OL1]

Investigating the Regulatory Interaction of Linker Region of *Ciona intestinalis* Voltage-sensitive Phosphatase with Lipid Membrane

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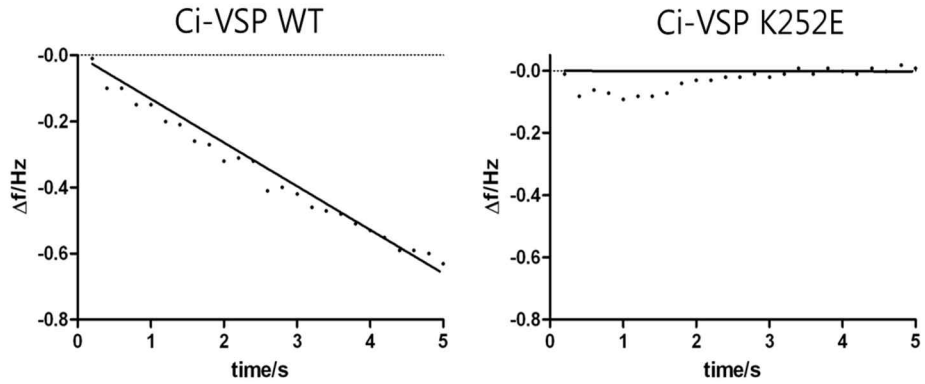
Ci-VSP is a transmembrane enzyme. It has a voltage sensor domain and a phosphatase domain that was originally discovered in *Ciona intestinalis*. Its enzymatic function is induced by cell membrane dislocation and the structural change of the dislocation sensor territory. Depolarization triggers the selective dephosphorylation of phosphoinositides. This enzyme is related to sea squirt of exercise flagellum. TPTE/TPIP, located mainly in the spermatozoa of humans, is similar to Ci-VSP. We studied the construction of His-tagged phosphatase-like domain of Ci-VSP, its recombinant expression and purification, and its enzymatic activity in order to examine the biochemical functions of the Ci-VSP phosphatase domain without interference. We found that Ci-VSP (248-576)-His can be eluted with an elution buffer containing 25 mM NaCl and 100 mM imidazole during His-tag purification. In addition, we found the proper measurement conditions for the kinetic study of Ci-VSP (248-576)-His activity on *p*-nitrophenyl phosphate (*p*NPP). The C-terminus was attached to the 6x His tag in both, Ci-VSP and mutated proteins. The activity change was confirmed by the malachite green assay. Furthermore, to find the binding affinity of the linker site (KRR) and phosphatidylinositol-3,4,5-triphosphate ($PI(3,4,5)P_3$), a quartz crystal microbalance (QCM) was used. In this study, we found that the K252 residue is very important for membrane binding. Our data also suggest that R253 and R254 residues control the structural relationship.



김 영 준 (Kim, Young Jun)

Career

1991 B. S. in Chemistry, Seoul National University

1993 M. S. in Biochemistry, Seoul National University

1993-1998 Senior Researcher, KOLON

2004 Ph. D. in Biochemistry, University of Illinois, Chicago

2008 Postdoc, University of California, San Diego

Research Area / Representative Publications

- 단백질 탈인산화 효소 연구

  CTD phosphatases 구조, 신규 기질 탐색과 생물학적 연구, 진화적 상관성 연구

  Lipid phosphatases 활성화 및 기질 특이성 연구

  나노바이오센서 활용 효소 활성 측정법 연구

Young Jun Kim, Md. Mahbubur Rahman, and Jae-Joon, Lee (2013) “Ultrasensitive and label-free detection of Annexin A3 based on quartz crystal microbalance” Sensors and Actuators B 177:172–177.

Bahk, Young Yil, Bari Mohamed, and Young Jun Kim (2013) “Biomedical application of phosphoproteomics in neurodegenerative diseases” J Microbiol Biotechnol. 23(3):279-88.

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[OL2]

Metabolomics approach for discovering biomarkers and understanding metabolic pathway

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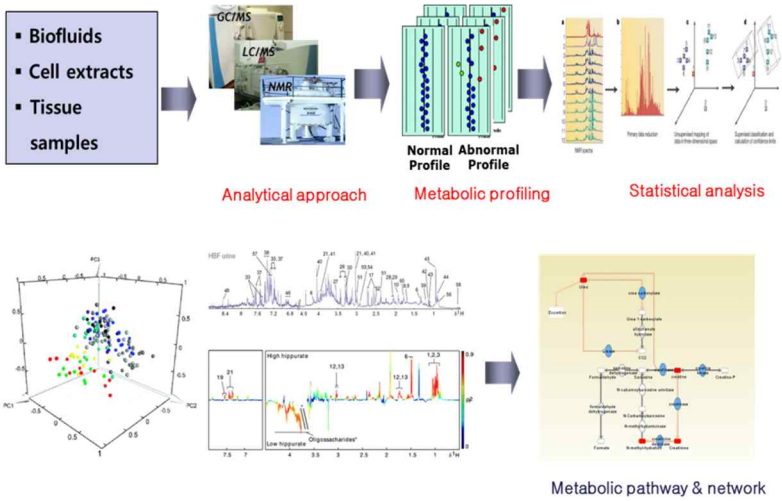
Metabolomics is the study of low molecular weight molecules or metabolites found within cells and biological systems, and profiling and fingerprinting of metabolites in various physiological states. This approach has recently demonstrated enormous potentials in many fields such as genotype discrimination, toxicological mechanism, disease processes, and drug discovery, and has been used to generate comprehensive biochemical profiles of endogenous metabolites for biofluides, cell, and tissue. This metabolic profile is perturbed in a characteristic fashion in disease, toxic process and drug efficacy, and this shift in position can be readily visualized and modeled using chemometric techniques. Understanding the biochemical reason for such a shift in metabolic space leads to the identification of biomarkers of disease or drug efficacy.



^{1}H NMR and Mass spectrometry were used to generate a molecular fingerprint of biofluid, tissue, cell extract samples, and then pattern recognition technique was applied to identity molecular signatures associated with the specific diseases or drug efficiency. Several metabolites that differentiate disease or drug treated samples from the control were thoroughly characterized and the metabolic changes in human and animal model were investigated using ^{1}H NMR and MS. Spectral data were applied to targeted profiling and spectral binning method, and then multivariate statistical data analysis (MVDA) was used to examine in detail the modulation of small molecule candidate biomarkers. The metabolic profiling produces robust models, generates accurate metabolite concentration data, and provides data that can be used to help understand metabolic differences between healthy and disease or drug treated models. Such metabolic signatures could provide diagnostic markers for a disease state or biomarkers for drug response phenotypes, and mechanistic information on cellular perturbations and pathways.

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황 금 숙 (Hwang, Geum-Sook)

Career

1985 B. S. in Chemistry, Kyung Hee University

1992 M. S. in Biochemistry, KAIST

1996 Ph. D. in Biochemistry, KAIST

1996-2000 Senior Researcher, Samsung

2000-2005 Research Fellow, Harvard Medical School

2010-Present Collaborative Professor, Chungnam University

Representative Publications

Noninvasive Diagnosis and Evaluation of Curative Surgery for Gastric Cancer by Using NMR-based Metabolomic Profiling, Jeeyoun Jung, Youngae Jung, Eun Jung Bang, Sung-il Cho, You-Jin Jang, Jung-Myun Kwak, Do Hyun Ryu, Sungsoo Park, Geum-Sook Hwang*, *Annals of Surgical Oncology*. 2014.08 Web Pub.

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^{1}H NMR-Based Metabolite Profiling of Plasma in a Rat Model of Chronic Kidney Disease. Ju-Ae Kim, Hyo-Jung Choi, Yong-Kook Kwon, Do Hyun Ryu, Tae-Hwan Kwon, Geum-Sook Hwang*, *Plos one.* 2014. 9(1), e85445

Serum metabolomics reveals pathways and biomarkers associated with asthma pathogenesis. Jeeyoun Jung, Seung-Hyun Kim, Ho-Sub Lee, Gil Soon Choi, Young-Sang Jung, Do Hyun Ryu, Hae Shim Park, Geum-Sook Hwang*, *Clinical and Experimental Allergy,* 2013.04, 43(4), 425-433

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[OL3]

Protein–protein interaction that involves coupled unfolding and binding

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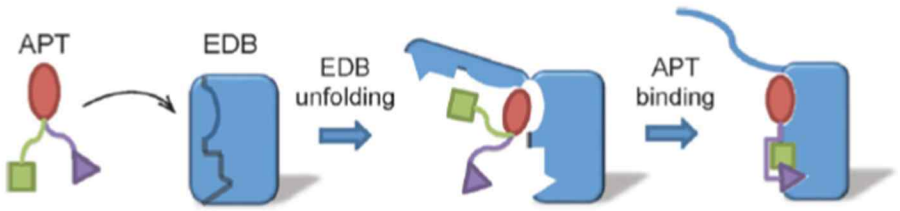
Aptides is a novel class of high-affinity peptides that recognize diverse molecular targets with high affinity and specificity. Here we report the solution structure of an aptide APT specifically bound to fibronectin extradomain B (EDB), a prominent marker of tumor angiogenesis. The complex structure reveals an unusual protein–protein interaction via coupled unfolding and binding. APT binding is accompanied by unfolding of the C-terminal β strand of EDB, permitting APT to interact with fresh-exposed hydrophobic interior surfaces of EDB. The β-hairpin scaffold of APT drives the interaction by a β-strand displacement mechanism, such that an intramolecular β sheet is replaced by an intermolecular β sheet. Binding thermodynamics reveals an enthalpic and entropic balance during the unfolding and binding. Unfolding of EDB perturbs the tight domain association between EDB and FN8 of fibronectin, highlighting its potential use as a scaffold that switches between stretched and bent conformations.



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서 정 용 (Suh, Jeong-Yong)

Career

1993 B. S. in Chemistry, KAIST

1995 M. S. in Chemistry, KAIST

1999 Ph. D. in Chemistry, KAIST

1999-2000 Postdoc, University of Alberta

2000-2004 Senior Researcher, LG Life Science

2004-2009 Visiting fellow, National Institutes of Health

Representative Publications

Yu, T. K., Shin, S. A., Kim, E. H., Kim, S., Ryu, K. S., Cheong, H., Ahn, H. C., Jon, S. & **Suh, J. Y.*** "An Unusual Protein-Protein Interaction through Coupled Unfolding and Binding" (2014) *Angew. Chem. Int. Ed. Engl.* **53** 9784-9787

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[OL4]

Engineering Protein Cage Nanoparticle for Biomedical Applications

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Protein cages, including ferritins, viral capsids, and encapsulins, are biomolecule-based supramolecular polymers and attractive candidates for nano-scale cargo delivery vehicles. While the interior surfaces of the protein cages have been used for encapsulation, attachment and synthesis of organic and inorganic materials, their exterior surfaces have been used for multivalent presentations of molecules, including affinity tags, antibodies, fluorophores, carbohydrates, nucleic acids, and peptides, for molecular targeting and hierarchical structure formation.

We genetically and chemically modified various types of protein cage nanoparticles and functional proteins to use them as multifunctional delivery nanoplatforms and multifunctional modules. The engineered protein cage nanoparticles could acquire various targeting ligands and selectively carry diagnostic or/and therapeutic cargos to target diseases, including cancers, in multiple ways using a mixing-and-matching strategy. Combined with antibody-binding domains and protein cage nanoparticles or functional proteins, antibodies are used as ligands for targeted delivery of therapeutics and/or diagnostics, enrichment of low abundant molecules in complex samples, and specific detections of biomarkers *in vitro* and/or *in vivo.*

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강 세 병 (Kang, Sebyung)

Career

1998 B. S. in Microbial Engineering, Konkuk University

2000 M. S. in Microbial Engineering, Konkuk University

2006 Ph. D. in Biochemistry and Molecular Genetics, University of Alabama, Birmingham

2007-2009 Postdoc, Montana state Univ.

Representative Publications

Moon, H., Lee, J., Min, J., and Kang, S. Developing Genetically Engineered Encapsulin Protein Cage Nanoparticles as a Targeted Delivery Nanoplatform. ***Biomacromolecules***, 2014, 15, 3794-3801

Han, J., Kang, Y. J., Shin, C., Ra J., Shin, H., Hong, S. Y., Do, Y., and Kang, S. Ferritin Protein Cage Nanoparticles as Versatile Antigen Delivery Nanoplatforms for Dendritic Cell (DC)-based Vaccine Development. ***Nanomed-Nanotechnol.*** 2014, 10, 561-569

Min, J., Jung, H., Shin, H-H., Cho, G., Cho, H., and Kang, S. Implementation of P22 Viral Capsids as intravascular MR T1 Contrast Conjugates Via Site-selective Attachment of Gd (III)-chelating agents, ***Biomacromolecules***, 2013, 14, 2332-2339

Kang, H.J., Kang, Y.J., Lee, Y.M., Shin, H., Chung, S.J., and Kang, S. Developing an Antibody-binding Protein Cage as a Molecular Recognition Drug Modular Nanoplatform. ***Biomaterials***, 2012, 33, 5423-5430

Kang, S. and Douglas, T. Some Enzymes Just Need a Room of Their Own. ***Science*** 2010, 327, 42-43.

[OL5]

Dual small molecule modulators of Wnt/β-catenin and p53 signaling

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Both the Wnt/β-catenin pathway and the p53 pathway play important roles in a variety of biological processes, such as cell proliferation, differentiation and homeostasis. Here we used cell-based chemical screening systems to identify ilimaquinone (IQ) and ethylsmenoquinone (ESQ), the marine sponge metabolits, as modulators of the Wnt/ β-catenin pathway and the p53 pathway. IQ and ESQ inhibited β-catenin response transcription (CRT), which had been induced with Wnt3a-conditioned medium (Wnt3a-CM), by down-regulating the level of intracellular β-catenin. Degradation of β-catenin was consistently found in RPMI1890 multiple myeloma (MM) cells after IQ and ESQ treatment. IQ and ESQ repressed the expression of cyclin D1, c-myc and axin-2, which are β-catenin/T-cell factor-dependent genes, and inhibited the proliferation of MM cells by induction of G_0/G_1 cell cycle arrest. On the other hand, IQ and ESQ activated p53 response transcription by stabilizing the p53 protein in both HCT116 and RKO colon cancer cells. Both compounds up-regulate the expression of $p21^{WAF1/CIP1}$, a p53-dependent gene, and suppress proliferation of colon cancer cells. , IQ and ESQ induced G_2/M cell cycle arrest, and increased caspase-3 cleavage and the population of cells that positively stained with AnnexinV-FITC, both of which are typical biochemical markers of apoptosis. Furthermore, autophagy was elicited by both compounds as indicated by microtubule-associated protein 1 light chain 3 (LC3) puncta formations and LC3-II turnover in HCT116 cells. Our findings suggest that IQ and ESQ exert their anti-proliferative activity by inhibition of the Wnt/β-catenin pathway and activation of the p53 pathway and may have therapeutic potential as therapeutic agents.

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오 상 택 (Oh, Sangtaek)

Career

1992 B. S. Sogang University

1994 M. S. Seoul National University

1999 Ph. D. Seoul National University

1999-2001 Postdoc, HHMI/UMDNJ

2001-2003 Principal Investigator, Chemgenomic. Inc., Boston, MA

2004-2011 Assistant Professor, Inje University

Representative Publications

Park S, Yun E, Hwang IH, Yoon S, Kim DE, Kim JS, Na M, Song GY, **Oh S** (2014) Ilimaquinone and Ethylsmenoquinone, Marin Spone Metabolites, Suppress the Proliferation of Multiple Myeloma Cells by Down-regulating the Level of β-Catenin *Marine drugs* 12:3231-3244.

Kim JH, Kim YH, Song GY, Kim DE, Jeong YJ, Liu KH, Chung YH, **Oh S** (2014) Ursolic acid and its natural derivative corosolic acid suppress the proliferation of APC-mutated colon cancer cells through promotion of β-catenin degradation. *Food Chem Toxicol.* 67:87-95

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Gwak J, Oh J, Cho M, Bae SK, Song IS, Liu KH, Jeong Y, Kim DE, Chung YH, **Oh S.** (2011) Galangin Suppresses the Proliferation of β-Catenin Response Transcription-Positive Cancer Cells by Promoting Adenomatous Polyposis Coli/Axin/Glycogen Synthase Kinase-3β-Independent β-Catenin Degradation. *Mol Pharmacol.* 79:1014-22.

[OL6]

Glycosylation of flavonoids and polyketides using flexible glycosyltransferase

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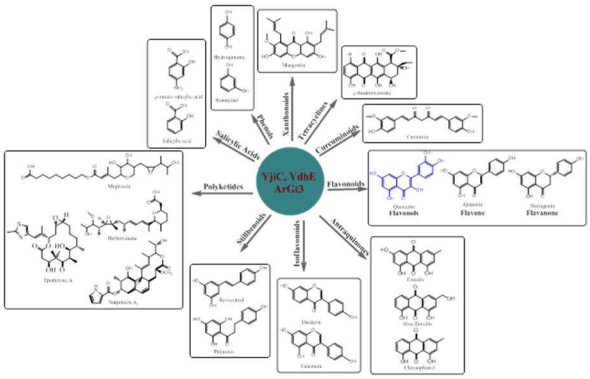
A UDP-glycosyltransferase, YjiC from Bacillus licheniformis DSM13 was exploited for the glycosylation of a number of small molecules. The in-vitro glycosyltransferase assay using YjiC lead to the production of multiple glucosides of polyhydroxyl groups containing aromatic/phenolic as well as aliphatic small molecules exhibiting wide substrate flexibility of the enzyme. We tested the activity of the enzyme with different classes of flavonoids (flavonoid, isoflavonoids, stilbenes, xanthonoids, benzoates) and polyketides (anthraquinone and macrolide). Moreover, we have found the wide donor substrate flexibility of YjiC with different NDP-sugars transferring a range of modified sugars including L- and D-sugars to the selected acceptors which guide to the production of a number of novel derivatives of natural products. But, it is found that YjiC could transfer only at limited positions of the polyhydroxylated compounds with diverse NDP-sugar donors. We further successfully applied YjiC for the in-vivo biotransformation of different flavonoids using engineered E. coli in large scale fermentor to produce glucosylated derivatives. In conclusion, it is found that YjiC has wide donor as well as acceptor substrates flexibility with high catalytic activity. The further exploitation of such glycosyltransferases could help to efficient production of glycosylated derivatives of natural products which might have potential therapeutic as well as cosmetic applications.



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송 재 경 (Sohng, Jae Kyung)

Career

1984 B. S. in Chemistry, Yonsei University

1986 M. S. in Organic Chemistry, Yonsei University

1991 Ph. D. in Biochemistry, Brown University

1994 Postdoc, University of Washington

2012-Present Vice President, Korean Society for Glycoscience

Research Area / Representative Publications

당화반응 및 생합성 과정 연구

Sialyllactose 생산과 유도체 합성

방선균 이차대사물질 생합성 과정 연구 및 신규물질 창출

유전공학에 의한 방선균 이차대사생산 증진 균주 개발

Small molecule glycosylation

효소 기능 연구 및 evolution

Park JW, Park SR, Nepal KK, Han AR, Ban YH, Yoo YJ, Kim EM, Kim D, Sohng JK, Yoon YJ. "Discovery of parallel pathways in kanamycin biosynthesis allows antibiotic manipulation" Nat. Chem. Biol. 2011, 7, 843-852.

Maharjan S, Aryal N, Bhattarai S, Koju D, Lamichhane J, Sohng JK. "Biosynthesis of the nargenicin A1 pyrrole moiety from Nocardia sp. CS682." Appl Microbiol Biotechnol. 2012 Jan;93(2):687-96.

Pandey RP, Malla S, Simkhada D, Kim BG, Sohng JK. “Production of 3-O-xylosyl quercetin in Escherichia coli.” Appl Microbiol Biotechnol. 2013 Mar;97(5):1889-901

Park SR, ParkJW, Ban YH, Sohng JK, Yoon YJ. 2-Deoxystreptamine-containing aminoglycoside antibiotics: Recent advances in the characterization and manipulation of their biosynthetic pathways. Nat.Prod.Rep.2013, 30(1):11-20.

Pandey RP, Parajuli P, Koirala N, Park JW, Sohng JK. "Probing 3-hydroxyflavone for in vitro glycorandomization of flavonols by YjiC" Appl Environ Microbiol. 2013 Nov;79(21):6833-8.

Pandey RP, Kwon HJ, Ahn JS, Osada H, Sohng JK. “The 7th Japan-Korea chemical biology symposium: chemical biology of natural bioactive molecules.” ACS Chem Biol. 2014 May 16;9(5):1070-4.

Le TT, Pandey RP, Gurung RB, Dhakal D, Sohng JK “Efficient enzymatic systems for synthesis of novel α-mangostin glycosides exhibiting antibacterial activity against Gram-positive bacteria.” Appl Microbiol Biotechnol. 2014 Jul 20.

[OL7]

A new approach to study membrane proteins

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Difficulties in the production, extraction of membrane proteins from cell membrane and their solubilization in native conformations have hindered their structural and biochemical analysis. To facilitate high-level expression of membrane proteins in E. coli, a P9 fusion system has been developed. Using this system, a rhodopsin-type GPCR (endothelin receptor) and a ligand gated ion channel (serotonin receptor type 3) have been successfully expressed and purified. Also, an amphipathic polypeptide was synthesized by the conjugation of octyl and glucosyl groups to poly- -glutamic acid (PGA). This polymer, called amphipathic PGA or APG, self-assembles as mono-disperse oligomers with a low critical micelle concentration. Endothelin receptor complexed with APG specifically interacts with endothelin suggesting that the amphipathic polymer stabilized the GPCRs in their active cofnrotmation. The membrane proteins complexed with APG are readily reconstituted in liposomes without disrupting the integrity of lipid bilayer structure.

유 연 규 (Yu, Yeon Gyu)

Career

1985 B. S. in Chemistry, Seoul National University

1987 M. S. in Chemistry, Seoul National University

1993 Ph. D. in Chemistry & Biochemistry, UCLA

1993-1995 Postdoc, UC Berkeley

1995-2005 Senior/Principal Researcher, KIST

Research Area / Representative Publications

막 단백질 구조 및 기능 연구

An amphipathic polypeptide derived from poly-c-glutamic acid for the stabilization of membrane proteins Protein Science (2014) in press

Beta-Amyloid Oligomers Activate Apoptotic BAK Pore for Cytochrome c Release Biophysical Journal (2014) Vol 107, 1601-1608.

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Protein kinase CK2 is inhibited by human nucleolar phosphoprotein p140 in an inositol hexakisphosphate-dependent manner. J Biol Chem. 2006 (12) 281, 36752-36757.

Identification of hNopp140 as a Binding Partner for Doxorubicin with a Phage Display Cloning Method, (2002.) Chemistry & Biology 9, 157-162.