2018 한국질량분석학회

겨울심포지움

2018 14th KSMS Winter Symposium

2018 . 2. 2. (금)

서울 KIST 국제협력관(1F) 컨벤션 홀

KSMS 한국질량분석학회
Korean Society for Mass Spectrometry

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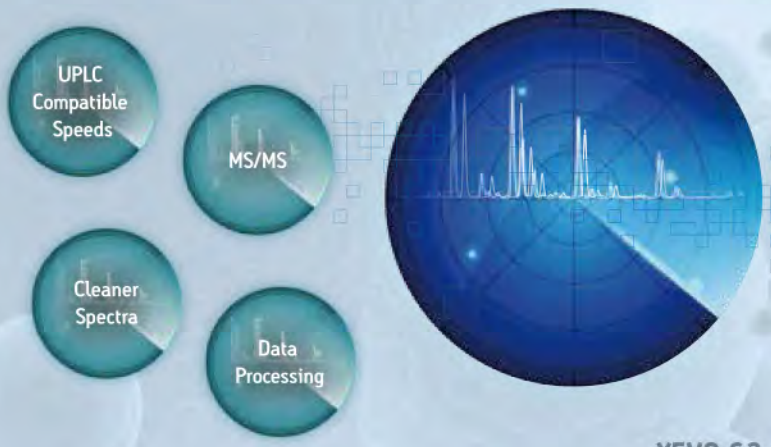

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성공을 위한 개인 맞춤형 교육

1 일반적인 교육 프로그램이 실패하는 이유

문제

- 교재가 오래됨
- 한 번에 과도한 정보량
- 개인 맞춤형 교육이 아님

결과

- 교육생이 관심을 갖지 못함
- 교육을 잊어버림

2 일관된 교육이 중요한 이유

이점

- 분석법 문제 직접 해결
- 기초 장비 직접 유지보수
- 새 직원에 대한 일관된 온보딩 프로세스

결과

- 생산성 증가
- 성공 및 경력 개발

3 SCIEX**University**만의 차별화 방법

이점

- 개인 맞춤형 학습 경로 및 새로운 콘텐츠
- 신청한 교육에 대한 적극성인 참여 의식
- 독자적인 반복 학습 방식*

결과

- 교육생의 관심 향상
- 지식 보유 향상

SCIEX**University**가 연구실 성과를 더욱 향상시키는 방법에 대해서는 sciex.com/kr/education을 참조하십시오.

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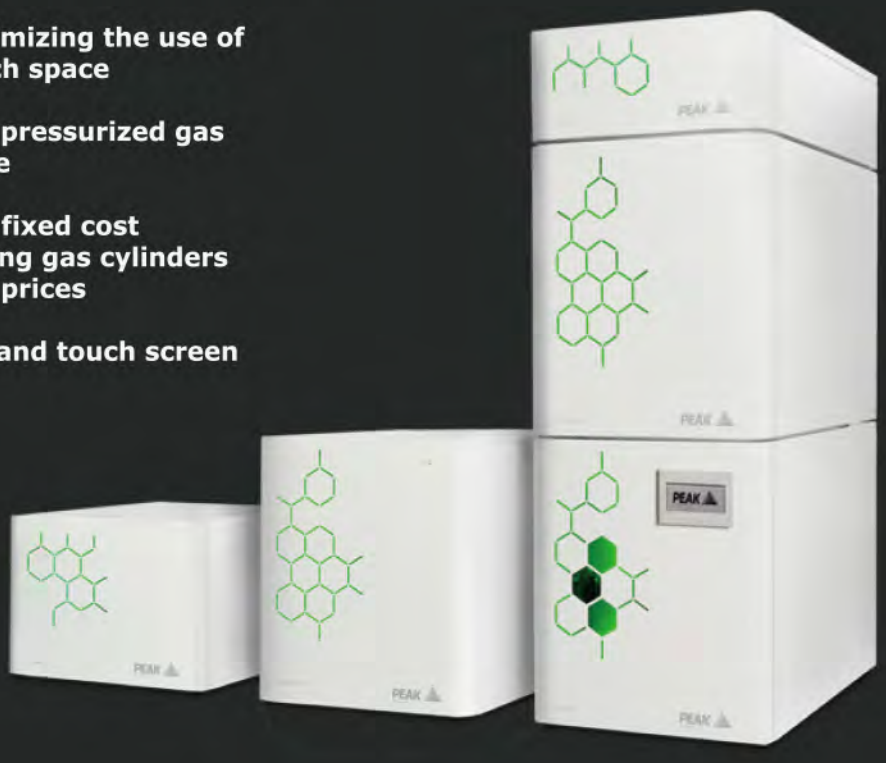

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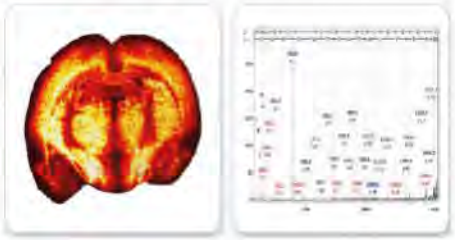
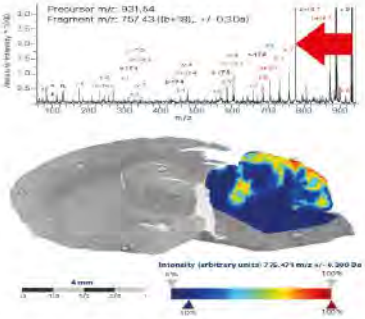
현존하는 MALDI-TOF/TOF 중 가장 빠른 데이터 획득 속도와 안정성을 갖춘 최첨단 시스템 Bruker rapifleX!

rapifleX

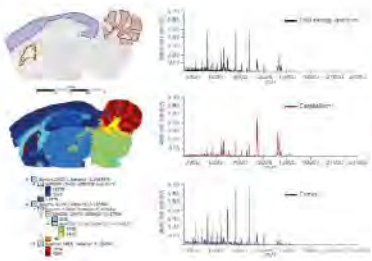
- Speed – 최대 10kHz의 laser repetition rate 와 50 pixels/초의 속도로 높은 데이터 처리량(약 5-20배 정도)을 제공
- Robustness – 새로운 ion source로 매우 간편한 self source cleaning 가능
- Definition – 최소 <5μm의 pixel size로 정밀한 이미징 가능 (고해상도)
- Confidence – 넓은 MS 분석을 위한 이동식 MS/MS Ion optics
- Reproducibility – 새로워진 Smartbeam™ 3D laser는 향상된 픽셀간 재현성을 제공



✓ 조직에 직접 trypsin digestion하여 이미징 및 LC-MS를 통한 바이오마커 동정 가능



✓ 손상된 쥐 두뇌 섹션에서 얻은 Intact protein 단백질 MALDI 이미징
✓ acquisition time: 기존장비에 비해 14배 빠른 속도



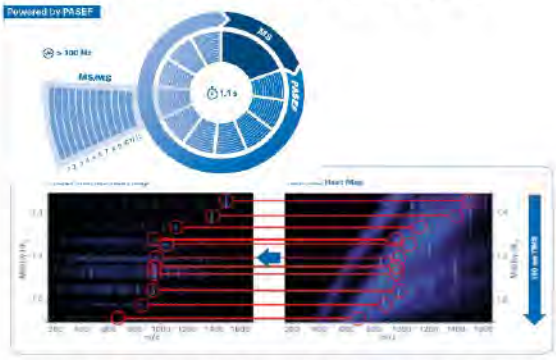
✓ MS 스펙트럼을 통한 소뇌 및 피질 맵핑을 통해 분자 유사성 해석 제공

Trapped Ion Mobility technology 를 이용한 Shotgun Proteomics의 새로운 패러다임, Bruker timsTOF Pro!

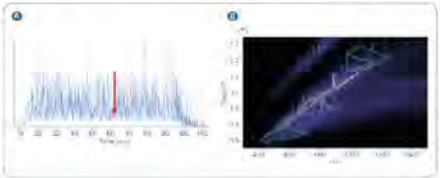
timsTOF Pro

- PASEF(parallel accumulation serial fragmentation)를 이용하여 전구체 이온 선택의 최적화를 통해 최대 10배 빠른 획득 속도를 제공 (100ms 이내에 평균 12개 전구체 MS 분석 가능)
- 적은 샘플 양으로도 높은 감도 및 처리량으로 분석 가능
  (ex – 200ng HeLa sample, 90 min gradient 이내 분석 가능, 기존 분석법(180분)과 비교하여 ID 개수 동등 이상)
- Collisional Cross Section(CCS – 충돌 단면적)으로 이성질체 분석에 대한 신뢰성을 제공

✓ Trapped Ion Mobility 와 PASEF 를 이용한 전구체 이온 치적화 및 분석 시간 단축



✓ 전구체 선택 시간 단축을 위한 스케쥴링으로 감도저하 없이 더 많은 MS/MS 스캔 제공



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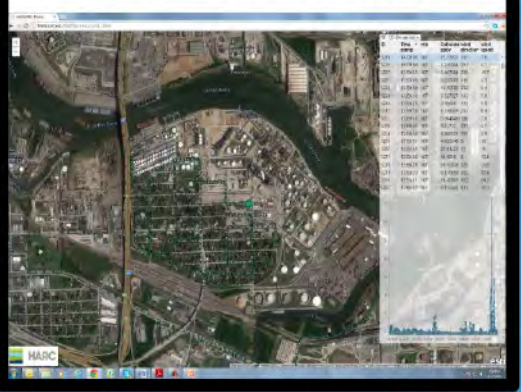

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2018 년 한국질량분석학회 겨울심포지움
일 시 : 2018 년 2 월 2 일 (금), 10:00 ~ 18:30
장 소 : 서울 KIST 국제협력관(1F) / 컨벤션 홀

목 차

안내사항

2018년 한국질량분석학회 겨울심포지움에 참가하신 회원 여러분 환영합니다

■ **현장 등록 시간 및 장소**

- 시 간 : 2018 년 2 월 2 일 (금) 10:00 ~ 18:30
- 장 소 : 서울 KIST 국제협력관(1F) 컨벤션 홀

■ **한국질량분석학회 2018 년 연회비 및 겨울심포지움 등록비 안내**

회원구분	연회비	사전등록비	현장등록비
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정회원	40,000	40,000	50,000
학생회원	20,000	20,000	30,000
비회원			90,000

1. 심포지움 등록은 2018 년도 연회비 납부자만 가능합니다.
2. 등록 내용
   - 식사 제공(중식/석식권 제공)

■ **포스터 게시 및 발표**

- 장소 및 게시 시간 : KIST 국제협력관 1F lobby / 2018 년 2 월 2 일 (금) 10:00~
  (포스터 부착 가능 시간: 2 월 2 일(금) 09:00~)
- 게 시 : 2018 년 2 월 2 일 (금) 10:00 ~ 18:00
- 발 표 : 2018 년 2 월 2 일 (금) 12:10 ~ 14:00 (포스터 번호는 Poster Seesion: P.41 참고)
  홀수: 12:10 ~ 13:00 발표
  짝수: 13:00 ~ 13:50 발표
- 철 거 : 2018 년 2 월 2 일 (금) 18:00 ~
- 포스터 일련번호를 부착하였으니, 해당 번호에 포스터를 부착하고 발표 시간에 배석하시기 바랍니다.

■ **공지사항**

- 행사 기간 내 이름표를 꼭 패용해 주시기 바랍니다.
- 세션 중에는 핸드폰 벨소리를 진동 혹은 무음으로 해 주십시오.
- 세션 중에는 발표가 방해되지 않도록 개인적인 사진촬영은 자제하여 주십시오.

■ **겨울심포지움 현장 안내**

- 심포지움 행사장: 국제협력관 1F (10번)
- 심포지움 중식: 대식당 - 본관 (1번 건물 내)
- 심포지움 석식: 외빈식당
  국제협력관 2F (10번 건물 내)

- KIST 출입 안내소
  - 22번: 북문 안내소
  - 21번: 준문 안내소

※ 지하철 6호선 이용자
: 22번 북문 안내소 이용가능

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- 지하철 : 6 호선 > 상월곡역(한국과학기술연구원역) → 4 번출구 → 한국과학기술연구원 (도보 5 분 소요)
  1 호선 > 청량리역 (2 번출구) → 현대코아 정류장 → 간선버스 201 번 승차 → 세종대왕기념관 앞 하차
- 버 스 : 청량리 방면 : 현대코아 정류장→ 간선버스 201 번 승차 → 세종대왕기념관 앞 하차 →
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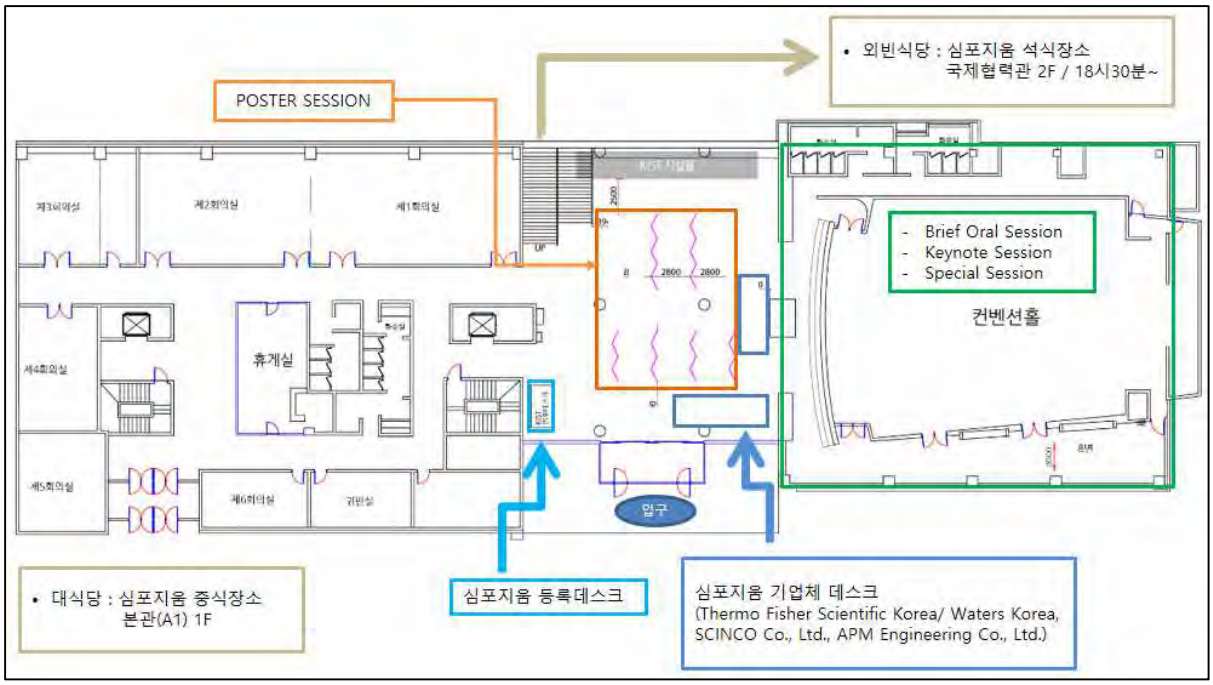
■ **겨울심포지움 세션장소 안내**



■프로그램 안내

February 2 (Friday)

TIME	PROGRAM	
10:00~	**등 록**	
10:20~10:30	**개회사 (회장: 임용현)**	
10:30~12:10	**Brief Oral Session** 조직책임자/좌장: 조 건 (한국기초과학지원연구원) / 이도엽 (국민대학교) 17명 각 5분 발표 (대상자: 석·박사 학위과정 학생)	
12:10~14:00	**중식 및 Poster Session** 조직책임자/좌장: 김민식 (경희대학교) / 장경순 (한국기초과학지원연구원)	
14:00~16:00	**Keynote Session** 조직책임자/좌장: 김광표 (경희대학교) / 김성환 (경북대학교) 질량분석분야 중량급 연구자 4분 초청 / 분야별 overview를 포함 각 30분 발표	
14:00~14:30	이유진 (서울대학교)	**Mass spectrometry on protein-protein complexes -The good and The bad**
14:30~15:00	최만호 (한국과학기술연구원)	**Bringing Mass Spectrometry-Based Steroid Signatures into Translational Research**
15:00~15:30	김병주 (한국표준과학연구원)	**Development of Food Certified Reference Materials for Nutrients Analysis and Establishing Isotope Dilution Mass Spectrometry as Higher-Order Methods**
15:30~16:00	유병용 (한국과학기술연구원)	**Accelerator mass spectrometry and its applications**
16:00~16:10	**Coffee Break**	
16:10~18:15	**Special Session** (Recent technologies for MS) 최근 2년내 MS 분야 최신 분석기술 관련 논문을 발표한 젊은 과학자 5분 초청/각 25분 발표 조직책임자/좌장: 한상윤 (가천대학교) / 김태영 (광주과학기술원)	
16:10~16:35	김정아 (한국기초과학지원연구원)	**Microfluidic lipid extraction technology for mass spectrometry**
16:35~17:00	나동희 (중앙대학교)	**MALDI-TOF MS Characterization of the Reversed-phase Chromatographic Behavior of PEGylated Peptides**
17:00~17:25	차상원 (한국외국어대학교)	**Analytical Strategies for Exposomics Research with Deciduous Teeth**
17:25~17:50	김진영 (한국기초과학지원연구원)	**Computational Method for Glycosylation Analysis by Tandem Mass Spectrometry**
17:50~18:15	김혜정 (오송첨단의료산업진흥재단)	**In-depth analysis of plasma proteome for discovery of age-related macular degeneration biomarkers**
17:50~18:15	**우수 포스터 시상 및 폐회식**	
18:30 ~	**만 찬**	

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SYMPOSIUM

세부프로그램

FEBRUARY 2

BRIEF ORAL SESSION

10:30 – 12:10

컨벤션 홀

Organizer/ Chairs: 조 건 (한국기초과학지원연구원) / 이도엽 (국민대학교)

10:30–10:35	MATLAB-based statistical analysis software for screening of edible oils and establishing 3D statistical models 손민희 (서강대학교)
10:35–10:40	On-line proteolysis and glycopeptide enrichment with thermo-responsive porous polymer membrane reactors (TPPMR) and nLC-ESI-MS/MS 양준선 (연세대학교)
10:40–10:45	Quantitative profiling of cervicovaginal fluid proteome using a 2D-nLC-ESI-MS/MS for early detection of preterm birth 김권성 (서강대학교)
10:45–10:50	Korean whole saliva proteome, ethnically-different human saliva proteome 조하라 (단국대학교)
10:50–10:55	Analysis of total uranium and thorium in naturally occurring radioactive materials using standard addition method combined with inductively coupled plasma mass spectrometry 김휘진 (과학기술연합대학원대학교/한국표준과학연구원)
10:55–11:00	Discovery of specific common fragments on trimethylsilylated PDE-5 inhibitors for their rapid screening and confirmation by GC-MS/MS combined with extracted common ion chromatogram 박나현 (경희대학교)
11:00–11:05	Quantification of glycated hemoglobin in dried blood spot using isotope dilution HPLC-MS/MS 트란흐엉 (과학기술연합대학원대학교/한국표준과학연구원)
11:05–11:10	Stable carbon isotope analysis of organic sediments. Is it possible to analyze at the molecular level? 손승우 (경북대학교)
11:10–11:15	Determination of fumonisins in maize using isotope dilution-liquid chromatography tandem mass spectrometry 아리스티아완 요시 (과학기술연합대학원대학교/한국표준과학연구원)
11:15–11:20	Effect of temperature on microwave-assisted tryptic digestion of protetins 김여선 (충남대학교)
11:20–11:25	Study of cross-interaction between amyloid-β 1-42 and 1-40 in the early stage of fibrillation using ESI-MS 허채은 (고려대학교)
11:25–11:30	Proteomics Analysis of Individual Serum Samples of Large Artery Atherosclerosis Stroke Patients and Healthy Subjects 문소라 (을지대학교)
11:30–11:35	Discovery of plasma metabolite biomarker cluster for discriminating graves' disease and its subtypes by using integrative GC-MS and LC-MS analysis. 지동윤 (국민대학교)

11:35–11:40 Construction of mouse brain glycome library using LC/MS and MS/MS
윤재경 (충남대학교 분석과학기술대학원)

11:40–11:45 Site-specific characterization of N- and O-glycoproteins in human and mouse plasma using LC-MS/MS and I-GPA search system
이현경 (한국기초과학지원연구원/충남대학교 분석과학기술대학원

11:45–11:50 Integrative multi-omic analysis of Th1 differentiation
김민정 (경희대학교)

11:50–11:55 Proteomics and phosphoproteomics studies of cell lines with CRISPR-Cas9 edited kinases for cancer disease.
한빛나라 (경희대학교)

KEYNOTE SESSION

14:00 – 16:00

컨벤션 홀

Organizer/ Chairs: 김광표 (경희대학교) / 김성환 (경북대학교)

14:00–14:30	Mass spectrometry on protein-protein complexes-The good and The bad 이유진 (서울대학교)
14:30–15:00	Bringing Mass Spectrometry-Based Steroid Signatures into Translational Research 최만호 (한국과학기술연구원)
15:00–15:30	Development of Food Certified Reference Materials for Nutrients Analysis and Establishing Isotope Dilution Mass Spectrometry as Higher-Order Methods 김병주 (한국표준과학연구원)
15:30–16:00	Accelerator mass spectrometry and its applications 유병용 (한국과학기술연구원)

SPECIAL SESSION

16:10 – 18:15

컨벤션 홀

Organizer/ Chairs: 한상윤 (가천대학교) / 김태영(광주과학기술원)

16:10–16:35	Microfluidic lipid extraction technology for mass spectrometry 김정아 (한국기초과학지원연구원)
16:35–17:00	MALDI-TOF MS Characterization of the Reversed-phase Chromatographic Behavior of PEGylated Peptides 나동희 (중앙대학교)
17:00–17:25	Analytical Strategies for Exposomics Research with Deciduous Teeth 차상원 (한국외국어대학교)
17:25–17:50	Computational Method for Glycosylation Analysis by Tandem Mass Spectrometry 김진영 (한국기초과학지원연구원)
17:50–18:15	In-depth analysis of plasma proteome for discovery of age-related macular degeneration biomarkers 김혜정 (오송첨단의료산업진흥재단)

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BRIEF ORAL SESSION

Brief Oral Session-1

MATLAB-based Statistical Analysis Software for Screening of Edible Oils and Establishing 3D Statistical Models

Minhee Son, Han Bin Oh*

Dept of Chemistry, Sogang University, Baekbum-ro 35, Seoul 04107, Korea

In this study, we made a software that designed to be able to project and classify unknown edible oil mass spectra on 3D PCA / PLS-DA model by importing mass analysis data of unknown edible oil by using different amount and composition if lipids such diacylglycerols (DAGs) and triacylglycerols (TAGs) according to kinds of edible oil. For the statistical analysis model, 9 kinds of edible oil were used, such as sesame, perilla, olive, canola, grape-seed, sunflower-seed, corn, soybean, coconut oils, and the equipment was Tinkerbell MALDI-TOF (Asta, Korea). In addition to the existing statistical analysis models, we have built models directly based on user data and made the models available for classification or screening of samples.

Brief Oral Session-2

On-line proteolysis and glycopeptide enrichment with thermo-responsive porous polymer membrane reactors (TPPMR) and nLC-ESI-MS/MS

Joon Seon Yang[1], Juan Qiao[2], Jin Yong Kim[1], Liping Zhao[2], Li Qi[2,*] and Myeong Hee Moon[1,*]

[1]Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea
[2]Beijing National Laboratory for Molecular Sciences; Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Acedemy of Sciences, No. 2 Zhongguancun Beiyijie, Beijing, 100190, China

Protein N-glycosylation, one of post-translational momdifications (PTMs), is a process that glycans attach covalently to nitrogen atom in asparagine (asn, N) amino acid. Since several glycosylated proteins are known as biomarkers of disease such as cancers, it is important to analyze glycoproteins in biological samples. In this study, dual micro-scale thermo-sensitive porous polymer membrane reactor (TPPMR) was developed for on-line proteolysis and glycopeptide enrichment prior to nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS/MS).

PS-MAn-NIPAM (PNPAm) is thermo-sensitive porous polymer membrane which is synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization and is coated on nylon membrane by breath figure method. Trypsin and lectin mixtures (ConA and WGA) can be immobilized on the coated membrane for proteolysis and glycopeptide enrichment, respectively, and each of membrane is inserted in TPPMR module. Dual TPPMR modules are directly connected to nLC-ESI-MS/MS system and proteolysis efficiency in proteolysis and glycopeptides enrichment were evaluated by varying temperature. The developed method demonstrates that on-line proteolysis and glycopeptide enrichment can be performed with only about 1.5 μL human plasma sample with the successful identification of 155 glycoproteins.

Brief Oral Session-3

Quantitative Profiling of Cervicovaginal Fluid Proteome Using a 2D-nLC-ESI-MS/MS for Early Detection of Preterm Birth

Kwonseong Kim[1,2], Young Eun Kim[2], Sun Young Lee[2], Han Bin Oh[1], Dukjin Kang[2]

[1]Department of Chemistry, Sogang University, Seoul 04107, Korea
[2]Center for Bioanalysis, Division of Chemical and Medical Metrology,
Korea Research Institute of Standards and Science, Daejeon, 34113, Korea

Occurring preterm birth (PTB) before 37 weeks of pregnancy is one of major causes, resulting in perinatal mortality and neonatal morbidity. Nevertheless, the proteomic study on the development of biomarker(s) for early detection of PTB, unfortunately, has not been matured. In this study, we performed shotgun proteomic analysis of the cervicovaginal fluid (CVF) samples from PTB and its normal counterpart, so as to unveil the protein biomarkers using two dimension-nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (2D-nLC-ESI-MS/MS). The quantitative assessments of CVF proteome from both PTB and control were carried out through an isobaric labeling approach with iTRAQ. Out of 1044 proteins identified, 1009 proteins were able to be in common quantified in PTB/control CVF samples. From MS/MS-based isobarically quantitative determination, 30 proteins from PTB were twofold or more upregulated, compared to that of control ones, while 59 proteins were measured to be twofold decreased. Based on the bioinformatic analyses (*e.g.*, Gene Ontology and KEGG), we found that 18 proteins, having the different expression levels between PTB and control, were implicated in immune response in cell. Resultingly, both of up-/down-regulated proteins identified in this study might be applicable to the development of biomarker(s) having the potential in the clinical diagnosis of PTB.

Brief Oral Session-4

Korean whole saliva proteome, ethnically-different human saliva proteome

Ha Ra Cho[1], Han Sol Kim[1], Jun Seo Park[1], Seung Cheol Park[2], Kwang Pyo Kim[2], Troy D. Wood[3], Yong Seok Choi[1,*]

[1]College of Pharmacy, Dankook University, Cheonan, Chungnam, South Korea
[2]Department of Applied Chemistry, The Institute of National Science, College of Applied Science, Kyung Hee University, Yongin, Kyoungki, South Korea
[3]Department of Chemistry, The State University of New York at Buffalo, Buffalo, New York, The United States of America

While more than 3,000 salivary proteins have been identified since the early 2000s, there has not been any trial to build Korean saliva proteome. Additionally, ethnic differences in the human plasma proteome were recently reported, but there was not any report on this aspect in the human saliva proteome, yet. Thus, here, the Korean whole saliva (WS) proteome was constructed for the first time and it was characterized by the comparison with the integrated human saliva protein dataset for the determination of ethnic differences in the human saliva proteome. A total of 674 proteins were indexed in the catalogue by the nLC-Q-IMS-TOF analyses of WS samples collected from 11 healthy South Korean adult male volunteers and 11 healthy South Korean adult female volunteers. Among 674 proteins, 358 proteins were not found in the integrated human saliva protein dataset. Also, the significant uniqueness of the Korean WS proteome was observed in gene ontology. Since the inter-platform reproducibility of the nLC-Q-IMS-TOF system was confirmed, these observations are strong evidences to support ethnic differences in the human saliva proteome. Additionally, since 47 out of the 358 distinct Korean WS proteins were found to be associated with the top 10 deadliest diseases in South Korea, the potential of ethnicity-specific human saliva proteins as biomarkers for diseases highly prevalent in that ethnic group was confirmed. Finally, the present Korean WS protein catalogue is expected to be used as the first level reference for future Korean saliva proteome studies.

Brief Oral Session-5

Analysis of total uranium and thorium in naturally occurring radioactive materials using standard addition method combined with inductively coupled plasma mass spectrometry

Hwijin Kim[1,2], Jong Wha Lee[2], Yeongran Lim[2], Sang Han Lee[3], Jung-Suk Oh[3], Yong-Hyeon Yim[2], Sung Woo Heo[2], Kyoung-Seok Lee[2,*]

[1]Department of Bio-Analytical Science, University of Science and Technology (UST), Daejeon, 34113, Korea

[2]Center for Analytical Chemistry, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea

[3]Center for Ionizing Radition, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea

Radioactivity from naturally occurring radioactive materials (NORMs) are potentially harmful to human health. Regulation and quality control of NORMs are important to prevent hazards from these materials. Certified reference materials (CRMs) of NORMs are typically certified for radioactivity of the constituent elements using alpha spectrometry. However, the mass fractions of the radioactive elements are indirectly obtained by conversion of the radioactivity data using specific activities. In this study, we measured the mass fractions of radioactive elements uranium and thorium in environmental samples zircon, bauxite, and phosphogypsum and compared the results obtained using alpha spectrometry. As the unavailability of isotopically enriched materials prohibits the use of isotope dilution inductively coupled plasma mass spectrometry (ID-ICP-MS), standard addition was used to determine the mass fractions in the samples using ICP-MS. The samples were processed by alkali fusion employing lithium tetraborate/lithium bromide flux and recovered in dilute nitric acid. Standard uranium and thorium solutions were spiked into the sample solutions by appropriate amounts along with thalium as an internal standard, resulting in ten measurement solutions. The determined mass fractions of uranium and thorium were 0.9–300 mg kg^{-1}, and the expanded uncertainties (at a 95% level of confidence) were estimated to be less than 3.4%. Good agreement was observed between the values from ICP-MS and alpha spectrometry, supporting the validity of the measurement results. The analytical procedure developed in this study is expected to be a basis of future research for certification of radioactive elements in NORMs.

Brief Oral Session-6

Discovery of specific common fragments on trimethylsilylated PDE-5 inhibitors for their rapid screening and confirmation by GC-MS/MS combined with extracted common ion chromatogram

Na-Hyun Park, Myoung Eun Lee, Jisu Hur, Bum Hee Kim, Jongki Hong*

College of Pharmacy, Kyung Hee University, Seoul 02447, Korea

PDE-5 inhibitor counterfeit drugs have been increasingly adulterated in supplement diets and widely distributed through internet markets and underground routes. In this study, GC-MS/MS method was developed for the screening and confirmation of 63 erectile dysfunction drugs in supplements. The trimetylsilyl (TMS) derivatization of PDE-5 inhibitors produced the characteristic fragments within similar structural moiety for sildenafil, tadalafil, and vardenafil analogues. Specific common fragments enabling to reflect their structural characteristics were observed as m/z 383, 384, and 265 for sildenafil analogues, m/z 334 and 241 for tadalafil analogues, and m/z 476, 384, for vardenafil analogues. These ions were formed through the cleavage of piperazinosulfonamide or piperazine ring for sildenafil and vardenafil analogues, and the successive losses of benzodioxole and diketopiperazine for tadalafil analogues. For the rapid screening of multiple classes of the PDE-5 inhibitor adulterants, extracted common ion chromatograms (ECICs) based on specific fragments of similar molecular moieties were attempted. These ECICs of specific ions could effectively cover PDE-5 inhibitor adulterants and new emerging counterfeit drugs. Especially, selected reaction monitoring (SRM) mode in GC-MS/MS could offer high sensitivity and selectivity for erectile dysfunction drugs derivatives in complicate matrix samples. The established method was successfully applied for the monitoring of several types of dietary supplements to protection of public health and consumer safety.

Keywords: PDE-5 inhibitors; supplement diets; screening; trimethylsilylation; extracted common ion chromatogram; GC-MS/MS

Brief Oral Session-7

Quantification of glycated hemoglobin in dried blood spot using isotope dilution HPLC-MS/MS

Thi Thanh Huong Tran[1,2], Ji-Seon Jeong[2,*]

[1]*Department of Bio Analytical science, University of Science and Technology (UST), Daejeon, Republic of Korea*

[2]*Center for Bioanalysis, Division of Metrology for Quality of Life, Korea Research Institute of Standards and Science (KRISS), Daejeon, Republic of Korea*

The collection of patient whole blood on paper, known as dried blood spot (DBS), was introduced in 1963 for the screening of inherited metabolic diseases in neonates. Compared with conventional venous blood sampling, DBS sampling is less invasive method, and easy to keep and transport samples. In this study, an isotope dilution-ultra performance liquid chromatography–tandem mass spectrometry (ID-LC-MS/MS) was investigated to quantify glycated hemoglobin (HbA_{1c}) in DBS. HbA1c has been widely used to assess glycemic control in diabetes mellitus. We used only one disc of 3.2-mm diameter for quantification of HbA1c, and that is about 3 μL of whole blood.

The bias factor caused by underestimation of area was strictly investigated and revised with area calculation software. The results were compared with areas by manual technique using ruler, or nominal value of puncher. The accuracy and precision of measurement showed sufficient results in the optimized sample treatment conditions. The variations of different position within a spot showed acceptable results (<3 %). As some unstable compounds in blood are easily susceptible to harsh environmental conditions, we examined the short-term effect of temperature (1-50 ºC) and humidity (<30% and 30- 70%) during a period of 10 days on the sample stability. The optimized analytical method was applied to real blood samples, and results showed excellent comparability with those of venous methods. This study provides reliability to constitute a practical procedure for a rapid measurement of $HbA_{1c.}$

Brief Oral Session-8

Stable carbon isotope analysis of organic sediments. is it possible to analyze at the molecular level?

Seungwoo Son, Donghwi Kim, Sunghwan Kim*

Department of Chemistry, Kyungpook National University, Daegu, Republic of Korea

Stable carbon isotope ratio ($^{13}C/^{12}C$) has been widely used in geochemistry, paleoclimatology and paleoceanography researches. It is well known that C_3 and C_4 plants have different isotope signatures. The reason for the difference can be attributed to difference in reaction rates differs caused by mass difference of ^{13}C and ^{12}C containing molecules. The stable carbon isotope ratios of organic sediments have been used to study geochemical origin and correlation between different area. Generally, stable isotope analysis of carbon is performed by burning an aliquot of material and analyzing the generated CO_2 gas by using specially designed sector mass spectrometry. Quantitative isotope ratio data can be obtained by using this method. However, the method is limited to obtain the ratio at the molecular level. Therefore, in this study, ultra-high resolution mass spectrometry has been evaluated for feasibility of molecular level ^{13}carbon isotope analysis. For the evaluation of crude oils, they were analyzed by (+) atmospheric pressure photo ionization Fourier transform ion cyclotron resonance mass spectrometry (APPI FT-ICR MS). And For the evaluation of humic acids, they were analyzed by (-) electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (ESI FT-ICR MS). In crude oils data, isotope ratio of sulfur class compounds were evaluated by using the equation, as well as humic acid data isotope ratio of oxygen compounds were evaluated by using same method. The obtained data were compared between organic sediments originated from different locations. The isotope ratio calculated from FT-ICR MS data were compared with the bulk ratio obtained with Elemental Analyzer–Isotope ratio mass spectrometry (EA-IRMS).

Brief Oral Session-9

Determination of fumonisins in maize using isotope dilution-liquid chromatography tandem mass spectrometry

Yosi Aristiawan[1,2], Kihwan Choi[1,*], Byungjoo Kim[1,*]

[1]*Center for Analytical Chemistry, Korea Research Institute of Standard and Science, Daejeon, 34113, Korea*

[2]*Department of Bio-Analytical Science, University of Science & Technology (UST), Daejeon, 34113, Korea*

Fumonisins are mycotoxins from a few species of fungi in the genus Fusarium causing a variety of diseases of both animals and humans. These fungi are commonly found in corn through systematic transfer from their roots. To detect fumonisin occurrence in corn or corn-based food, proper and decent analytical methods are required. In this study, we developed an analytical method for the determination of three types of fumonisins (FB_1, FB_2, and FB_3) in corn flour based on isotope dilution-liquid chromatography tandem mass spectrometric (ID-LC/MS/MS) method. Fumonisins were extracted from corn flour and the extracts were purified with immunoaffinity column before introduced to LC/MS/MS instrument. The experimental parameters, such as kind of extraction solvent, clean-up column, and solvent-to-sample ratio were studied. Solubility and extraction efficiency was better when phosphate buffered saline (PBS) was used as extractant compared to acetonitrile-water or methanol-water solutions. A post-column infusion system was used to investigate the clean-up efficiency of immunoaffinity columns. The amount of fumonisins bound to corn flour matrix could be extracted with PBS. Thus, hydrolysis was not necessary for fumonisin analysis in this study. Selected reaction monitoring (SRM) was employed in the mass spectrometer at m/z 706.5 ⟶ 334.4 (FB_1) and m/z 706.4 ⟶ 336.3 (FB_2 and FB_3). Through the gradient elution of 5 mM ammonium formate in water containing 0.1% formic acid and 5 mM ammonium formate in methanol containing 0.1% formic acid on C18 column, FB_1, FB_2, and FB_3 were successfully separated. The proposed method provided a detection limit range from 0.4 to 0.5 μg/kg and a limit of quantification range from 1.2 to 1.9 μg/kg. Following validation of the developed method, fumonisin level was investigated with additional corn-based products.

Brief Oral Session-10

Effect of temperature on microwave-assisted tryptic digestion of protetins

Yeoseon Kim, Dabin Lee, Sol Han, and Jeongkwon Kim*

Department of Chemistry, Chungnum National University, Daejeon, 34134, Korea

Protease is used in protein digestion. Trypsin, one of the most common proteases, cleaves exclusively at C-terminus of amino acid Lysine and Arginine in proteins. Moreover, organic solvents are often added for the trypsin digestion to modify native proteins to denatured proteins, and this tendency makes it effective to digest proteins. In this study, we investigate the digestion efficiency of trypsin for the digestion of bovine serum albumin and horse skeletal muscle myoglobin. Sample solutions were prepared with different amounts (0 %, 10 %, and 20 %) of acetonitrile and digested using trypsin with a help of microwave irradiation. Digested peptides were analyzed using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry and the sequence coverage and the intenstiy or the protein peak were used as indicators of trypsin activity.

Brief Oral Session-11

Study of cross-interaction between amyloid β 1-42 and 1-40 in the early stage of fibrillation using ESI-MS

Chae-Eun Heo, Hugh I. Kim

Dept of Chemistry, Korea University, Seoul 02841, Republic of Korea

Amyloid-β 1-42 (Aβ42) and 1-40 (Aβ40) peptides, whose self-assembly process has been linked with the formation of amyloid plaques in Alzheimer's disease, exist as a mixture in human fluids. For this reason, heteromeric self-assembly of Aβ42 and Aβ40 has been widely investigated to understand the influence of this mixture in Aβ fibrillation. However, understanding the role of heteromeric self-assembly in Aβ fibrillation is a challenge owing to the heterogeneous cross-interactions between Aβ42 and Aβ40. Herein, we demonstrated the influence of the cross-interaction of Aβ42 and Aβ40 in the early stage of fibrillation using electrospray ionization mass spectrometry (ESI-MS) and drift tube ion mobility spectrometry (DTIMS) along with solution small-angle X-ray scattering (SAXS) and molecular dynamics (MD) simulations. In the mixture of Aβ42 and Aβ40, Aβ42 has a slight preference for homo-oligomerization versus hetero-oligomerization with Aβ40 (1~2 fold) when forming small oligomers (from dimer to tetramer) in the early stage of the fibrillation. However, the cross-interaction is gradually attenuated as oligomerization proceeds because of the different conformations in Aβ42 and Aβ40 assemblies. Consequently, the competitive self-assembly of Aβ42 and Aβ40 can disturb homo-oligomerization of Aβ42 in the early stage of fibrillation, whereas Aβ42 and Aβ40 species prefer the independent self-assembly after the early stage.

Brief Oral Session-12

Proteomics Analysis of Individual Serum Samples of Large Artery Atherosclerosis Stroke Patients and Healthy Subjects

Jiyeong Lee[1], Arum Park[1], Sora Mun[2], You-Rim Lee[2], AeEun Seok[1], Hyo-Jin Kim[2], Yoo-Jin Lee[2], Hee-Gyoo Kang[1,2]

[1]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Korea.

[2]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, Korea.

Ischemic stroke is classified into several subgroups based on causes. Large artery atherosclerosis is known as a major cause of ischemic stroke. Many studies have been reported that large artery atherosclerosis is closely associated with inflammation and several inflammation markers were also increased in patients with large artery atherosclerosis. However, there is no exact diagnostic marker for large artery atherosclerostic stroke. Most of studies have analyzed to identify novel biomarker in various disease using pooled serum samples. However, these studies can lead to biased results. Our aim is to analyze individual serum sample instead of pooled serum sample. 52 patients and 43 healthy subjects are used for biomarker of large artery atherosclerosis stroke. Quantification of identified 514 serum proteins were performed by SWATH-MS acquisition. As a result, differentially expressed proteins by more than 2 fold were 149. The result of functional analysis showed that the differentially expressed proteins are associated with alternative complement pathway-related immune response and positive regulation of tolerance induction to nonself antigen. The comparative analysis of serum proteins in patients with large artery atherosclerosis stroke and healthy subjects helps to understand pathophysiology of large artery atherosclerosis. We expect that inflammation-related proteins will distinguish subtype of stroke from healthy subjects.

Brief Oral Session-13

Discovery of plasma metabolite biomarker cluster for discriminating Graves' disease and its subtypes by using integrative GC-MS and LC-MS analysis.

Dong Yoon Ji[1], Soo Jin Park[1], Se Hee Park[2,3], Eun Jig Lee[2,4] and Do Yup Lee[1,*]

[1]*The Department of Bio and Fermentation Convergence Technology, BK21 PLUS project, Kookmin University, Seoul, Republic of Korea*

[2]*Division of Endocrinology and Metabolism, Department of Internal Medicine, Yonsei University College of Medicine, Seoul, Republic of Korea*

[3]*Graduate School, Yonsei University College of Medicine, Seoul, Republic of Korea*

[4]*Institute of Endocrine Research, Yonsei University College of Medicine, Seoul, Republic of Korea*

Autoimmune disease is a condition that arises from abnormal immune responses to self-antigen, which leads to damage of tissues or dysfunction of biological system. Graves' disease (GD) is an autoimmune disorder that affects thyroid, and frequently results in hyperthyroidism. It often develops to an enlarged thyroid and eye bulging, Graves' ophthalmopathy (GO) with 25% frequency of GD. Since there is no specific molecular indicator for the disease, biomarker based on blood metabolite can be an effective and powerful tool for diagnosis, and suggest putative therapeutic target. In this study, a gas chromatography coupled time-of-flight mass spectrometry was employed to characterize primary metabolic profiles from plasma of GD (n=20), GO (n=27), and healthy control (n=32). Multivariate statistical analysis were applied to identify the metabolic phenotype of Graves' disease compared to health control. The most significant alteration was found in glycolysis and branched chain amino acids. The subsequent biomarker model consisting of 1,5-anhydroglucitol, proline, glucose and pyruvate showed excellent discrimination power. Area under the curve (AUC) values by receiver operating characteristic (ROC) analysis were 0.94 (control vs others), 0.87(GO vs others) and 0.86(GD vs others), respectively. In addition, lipid profiling revealed the dramatic alteration of sphingolipids and phospholipids in the disease, which included oleoyl-LPA and sphingosine 1-phosphate.

Brief Oral Session-14

Construction of mouse brain glycome library using LC/MS and MS/MS

Jaekyung Yun[1,2], Jua Lee [1,2], and Hyun Joo An[1,2,*]

[1]Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea
[2]Graduate School of Analytical Science and Technology,
Chungnam National University, Daejeon, Korea

Glycosylation on neuronal cell surface plays an important role in neuro-biological functions including synaptic plasticity and memory formation. Despite its biological importances, molecular-level investigation into brain glycome has remained in relative uncertainty due to the lack of effective analytical methods. In this study, a highly sensitive MS-compatible method for glycan/glycolipid extraction from brain tissue was combined with structure-specific nano-LC/MS and MS/MS to build up brain glycome library including N- and O-glycans and gangliosides. Briefly, N-glycans were enzymatically released by PNGaseF, while O-glycans were concentrated by beta-elimination method. Gangliosides were extracted based on modified Folch method. Purified and enriched glycans and gangliosides by SPE were identified and quantified by positive ion mode of nano-LC PGC Chip/Q-TOF MS and negative ion mode of nano-LC C18 Chip/Q-TOF, respectively. The biosynthetic library of mouse brain glycome was constructed using about one hundred glycans and 70 gangliosides with brain-specific glycans characterized by tandem MS using diagnostic fragment ions. The constructed library of mouse brain glycome was applied for monitoring glycome alteration in various neurobiological environments including different developmental stages and KO conditions (Maneal, Galnt13, St8sia3) with high speed and accuracy. This approach could be useful as the informative data for glycome study related the specific neurodiseases.

Keyword: Glycans, Ganglioside, LC/MS, Mouse brain

Brief Oral Session-15

Site-specific characterization of N- and O-glycoproteins in human and mouse plasma using LC-MS/MS and I-GPA search system

Hyun Kyoung Lee[1,2,*] Ju Yeon Lee[1], Gun Wook Park[1], Jin Young Kim[1] and Jong Shin Yoo[1,2]

[1]Korea Basic Science Institute, O-chang Cheongju, Korea
[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea

Mouse has been used as an animal model for scientific research owing to its physiological similarity to human. However, their N- and O-glycosylation of glycoproteins showed many differences between mouse and human. Usually glycosylation is directly involved in various biological process and plays crucial role in human diseases due to their unusual biological sensitivity. Therefore, the site-specific characterization of glycosylation in model mouse is necessary in order to investigate progression of disease.

This study provided comparison of the site-specific N- and O-glycosylation between human and mouse plasma using LC-MS/MS with I-GPA (Integrated GlycoProteome Analyzer) search system[1]. The site-specific glycosylation between human and mouse has three differences in plasma. First, the sialic acid of N- and O-glycopeptides was almost entirely Neu5Gc in mouse plasma, while in human plasma was Neu5Ac. Second, O-acetylated NeuGc of N-glycopeptides was identified in mouse plasma only. Third, antennal HexNAc-NeuGc of N-glycopeptides was specifically identified from several glycoproteins in mouse plasma only. In conclusion, our study has provided a comprehensive overview of the site-specific N- and O-glycosylation of human and mouse in plasma.

Reference

1. Gun Wook Park and Jin Young Kim et al., *Scientific Reports*, 6:21175 (2016)

Brief Oral Session-16

Integrative multi-omic analysis of Th1 differentiation

Min Jung Kim, Kwang Pyo Kim and Min-Sik Kim*

Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea

Naïve CD4+ T cells can be differentiated into T helper cells through several rounds of division, and these differentiated T helper cells are essential for human immune activities such as infection, allergic responses, macrophages and also mediate direct antiviral function. Here, we analyzed the proteins involved in signal transduction of early T cell differentiation by setting each time point divided into 6 time points. The samples were labeled by using TMT-reagent after digestion and the labeled peptides were subjected to LC-MS/MS analysis. After integrating RNA-seq, global and phosphorylated proteome profiling, we characterized the network of early signaling pathways for T cell differentiation. Through the analysis of transcriptomes based on RNA-seq, we classified networks of transcription factors of T cell differentiation. And we identified 847 differentially phosphorylated peptides from phosphoproteomic analysis and 755 differentially expressed proteins from global proteomics. All DEPs (fold changes>3) among each analysis were identified in the abundance of each time point to perform gene ontology and pathway analysis. In conclusion, our results and future experiment will be able to identify the modeling of drugs related to CD4 activation and T cell differentiation and also identify autoimmune diseases caused by T cell mutation.

Brief Oral Session-17

Proteomics and phosphoproteomics studies of cell lines with CRISPR-Cas9 edited kinases for cancer disease.

Bitnara Han[1], Hyeong Min Lee[1], Jae Min Lim[1], Jin-Soo Kim[2,3], Kwang Pyo Kim[1]

[1]Department of Applied Chemistry, College of Applied Sciences, Kyung Hee University, Yongin 446-701, Republic of Korea
[2]National Creative Research Initiatives Center for Genome Engineering, Seoul National University, Seoul, South Korea
[3]Department of Chemistry, Seoul National University, Seoul, South Korea.

As an important key to cancer treatment, signlaing pathways regulated by kinasses are the targets of most cancer drugs. However, targeted anticancer agents are facing limitations due to their resistance and low popularity and efficiencies. The kinase genes were edited using CRISPR-Cas9 technology and target deconvolution was performed by screening from various omics perspectives to find an aberrantly activated signaling pathway and an unintended target of kinase inhibitor.

Four kinases (ERK2, PIK3CA PLK1, and PAK4) of HCT116 cells, were knocked out using CRISPR-Cas9 to obtain cell lines. Proteins were extracted from these knockout cell lines and tryptic digestion followed by labeling using TMT reagent. We performed global profiling and phosphopeptides enrichment using IMAC method for the labeled proteins. As a result, a total of 7,500 proteins, 4200 phosphoproteins and 10877 phosphosites were identified by LC-MS / MS.

Results of GOBP enriched for DEPs (Differentially Expressed Proteins) and DPPs (Differentially Expressed Phosphoproteins) in each knockout cell line were obtained and a model of protein-protein interaction network was established.

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KEYNOTE SESSION

Keynote Session-1

Mass spectrometry on protein-protein complexes-The good and The bad

Eugene C. Yi

Dept of Molecular Medicine and Biopharmaceutical Sciences Seoul National University

Mass spectrometry, recognized as a primary tool for the study of the life sciences, has been well suited for both the areas of characterization of small and maceromolecules and the determination of the entire set of proteins in a cell, an organism or a tissue at a defined time point and under defined conditions. Integrating various front-end sample manipulation methods and the back-end bioinformatics tools enable to expand the mass spectrometry platform for investigating more complex celluar functions, which involve the coordinated action of several proteins. Defining the complete set of macromolecular protein complexes via immunoaffinity mass spectrometry (IP-MS) approach has contributed to the field of functional proteomics. As the protein interactions are often of a transient nature, it is difficult to detect correct molecular entities in the protein complexes. In this presentation, we will highlight the importance of detailed experimentation at the molecular level to discover correct molecular entities of cells and to decipher how proteins interact in the given cellular functions.

Keynote Session-2

Bringing Mass Spectrometry-Based Steroid Signatures into Translational Research

Man-Ho Choi

Molecular Recognition Research Center, KIST, 5 Hwarang-ro 14-gil, Seoul 02792, Korea

The term translational refers to the "translation" of basic scientific findings in a laboratory setting into potential treatments for disease. Translational research is an interdisciplinary branch of the biomedical field supported by three main pillars: bench-side, bedside and community. Owing to controversy over the effects of steroids on disease pathophysiology, comprehensive quantification of steroid hormones has been extensively considered for disease diagnosis / prognosis and the identification of novel bio-signature and molecular mechanisms of biomedical pathphysiology. To promise exact quantification of steroid levels in complex biological specimens, further emphasis should be made on the efficient separation by chromatography, such as gas and liquid chromatography, prior to mass spectrometric detection. Recent advances in mass spectrometry-based bioanalytical techniques enable accurate estimation of circulating as well as localized steroids, allowing these assays to be more powerful in translational research.

Keynote Session-3

Development of Food Certified Reference Materials for Nutrients Analysis and Establishing Isotope Dilution Mass Spectrometry as Higher-Order Methods

Byungjoo Kim*[,1], Joonhee Lee[1], Honghee Lee[1], Sun Young Lee[1], Dongwon Seo[2], Jinbong Hwang[2], Byung-Man Kwak[3], Jongeun Won[3]

[1]*Center for Analytical Chemistry, Korea Research Institute of Standards and Science, Korea*
[2]*Food Analysis Center, Korea Food Research Institute, Korea*
[3]*Food Safety Center, Namyang Dairy Products Company, Korea*

KRISS, the National Metrology Institute (NMI) of Korea, launched a 5-year nutrient metrology program in 2014. The main scopes of the program are establishing national standards for the analysis of nutrients in food and developing certified reference materials (CRMs) for the dissemination of the established national standards. In this presentation, the overview of the program and analytical techniques developed through the program up to the date will be presented. As a part of establishing national standards, this laboratory has been developing isotope dilution mass spectrometry (IDMS) as higher-order reference methods for the accurate determination of nutrients in food and clinical samples.[1-4] IDMS methods have been used for assigning certified values of CRMs. IDMS methods ensure assigned values for CRMs to have metrological qualities (with traceability to SI unit and with associated uncertainties much smaller than those obtained by regular testing laboratories). The first CRM produced through this program was an infant formula CRM (KRISS CRM #108-02-003) with certified values for 14 vitamins and 8 essential fatty acids. CRMs for nutrients in grain (rice, wheat flour), vegetables (Kimchi cabbage, spinach), apple, beef, and tuna are under development. For nutrients which do not have existing IDMS methods, interlaboratory comparisons among KRISS, Namyang, and KFRI were carried out and results were provided as informative values after statistical evaluation. For proximates such as total protein, total fatty acid, total hydrocarbon, water contents, and ash contents, values are assigned based on interlaboratory studies in which 11 laboratories participated.

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Keynote Session-4

Accelerator mass spectrometry and its applications

Byung-Yong Yu, Joonkon Kim, JongHan Song

Accelerater Lab., Advanced analisys center, Korea Institute of Science and Technology, Seoul, 02792, Korea

Accelerator Mass Spectrometry, AMS (가속기질량분석법)는 동위원소를 질량수에 따라 분리하고 측정하는 질량분석법의 하나로, 가속기를 사용하여 질량수가 같을 수 있는 분자상태의 물질들을 모두 원자상태로 만들고 방사성동위원소와 안정동위원소를 분리하고 측정하여 그 비율($^{10}Be/^{9}Be$, $^{14}C/^{12}C$, $^{26}Al/^{27}Al$, $^{36}Cl/^{35}Cl$, $^{41}Ca/^{40}Ca$, $^{129}I/^{127}I$)을 결과 값으로 제시한다는 점에서 일반 질량분석법과 큰 차이를 보이고 있다. 탄소의 경우 자연계에 ^{12}C (99 %), ^{13}C (1 %), 그리고 ^{14}C (10^{-10} %)의 동위원소가 존재하며 AMS를 이용하여 방사성동위원소와 안정동위원소 비($^{14}C/^{12}C$)를 10^{-15}까지 측정가능하다. 이러한 초 극미량 ^{14}C의 측정이 가능해 짐으로서 AMS를 1970년대 부터 연대 측정(radiocarbon dating)에 주로 사용하고 있으며, 매우 낮은 농도의 방사성 동위원소를 측정할 수 있기 때문에 최근 환경과학, 지구과학, 생의학 분야에서 AMS를 적극적으로 활용하고 있다. 특히 생체 내에 포함된 방사성탄소(C-14) 량은 안정동위원소(C-12)의 10^{-10} % 정도로 매우 적어 AMS를 활용할 경우 극미량의 C-14 만으로도 충분한 신호를 얻을 수 있어 마이크로도즈, 나노트레이싱기법을 활용한 연구가 활발히 진행되고 있다. 생의학분야에서 AMS는 신약개발을 위한 후보 약물이나 기존 약물의 체내 거동을 살피기 위하여 극미량(~100 nCi)의 방사성 탄소를 표지한 약물을 다양한 방법 (PO, SC, IM, IV, IP)으로 체내에 투여하고 약물 또는 대사체의 거동 연구에 주로 사용하고 있다. 일반적으로 방사성동위원소를 추적자로 사용하여 신약개발에 사용할 경우 여러가지 법적 규제로 인하여 사용하기 쉽지 않지만, AMS를 사용 할 경우 규제를 받지 않을 정도인 수 100 nCi (흉부 X-선 촬영의 1/2000 정도) 정도의 방사성탄소만으로도 충분히 검출 가능하기 때문에 신약개발에서 혁신적인 분석기법중 하나로 자리잡고 있다. 특히 AMS는 신약개발에서 매우 중요한 개발 약물의 Absolute bioavailability, Mass balance, Metabolite profiling 연구에 강력한 분석기법이며, 분석 약물이 내인성 물질인 경우 체내에서 생성된 물질에 갑섭받지않고 분석할 수 있으며, 고 효력, 고 변동성 약물인 경우 위험성을 최소로 하여 연구가 가능하다. 본 발표에서 AMS의 소개 및 이를 사용한 생의학 분야에서의 활용연구에 대하여 소개하려고 한다.

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SPECIAL SESSION

Special Session-1

Microfluidic lipid extraction technology for mass spectrometry

Jeong Ah Kim[1,2,*]

[1]*Biomedical Omics Group, Korea Basic Science Institute, Chungbuk 28119, Republic of Korea*

[2]*Department of Bio-Analytical Science, University of Science & Technology, Daejeon 34134, Republic of Korea*

Pre-treatment of samples is the one of most important steps in analytical methods for efficient and accurate results. Generally, conventional lipid extraction demands multiple steps, including drying, incubation, partitioning, and centrifugation, which results in tedious labor and low performance. In this study, we suggest a microfluidic device that is capable of efficient lipid extraction from aqueous samples has been developed for mass spectrometry analysis. We employed super absorbent polymers (SAPs) in the lipid extraction process and this material removed the water-based liquid rapidly, while hydrophobic lipid components were efficiently eluted into the organic solvent without significant interruption with these polymer. The simplified process of lipid extraction and elimination of centrifugation steps enables the implementation of microfluidic chip-based lipid extraction device. The novel design of the microfluidic system using gravity flow greatly reduces the complexity of fully integrated lab-on-a chip system. The capability of the microfluidic device was demonstrated by several tests regarding the extraction efficiency and the recovery rate of lipids. This small-scale SAP method and its microfluidic platform will open up new possibilities in high-throughput lipidomic research for diagnosing diseases because this new technique saves time, labor, and cost.

Special Session-2

MALDI-TOF MS Characterization of the Reversed-phase Chromatographic Behavior of PEGylated Peptides

Dong Hee Na

College of Pharmacy, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul 06974, Korea

Modification of therapeutic biomolecules including peptides and proteins with polyethylene glycol (PEG), which is known as PEGylation, has become one of the most useful pharmaceutical techniques developed thus far. The separation mechanism of PEGylated peptides in reversed-phase high-performance liquid chromatography (RP-HPLC) is complex, because the PEGylated molecules exhibit physicochemical properties that are different from those of the parent molecules and have heterogeneous structure. Since most separation studies have focused on the hydrophobicity of the peptide relative to poly(ethylene glycol) (PEG), the role of PEG in the separation of PEGylated peptides on RP-HPLC is not clear. To elucidate the effect of the attached PEG on the retention of PEGylated peptides on RP-HPLC, the mono-PEGylated forms of collagen pentapeptide and octreotide were fractionated drop-by-drop from the outlet of the HPLC system and each drop was subjected to matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS). The MALDI-TOF MS analysis of drop fractions from RP-HPLC demonstrated that the dispersity of the attached PEG leads to the peak broadness of PEGylated peptides in RP-HPLC and the elution order inside the HPLC peak of PEGylated peptides was dependent on the attached PEG chain length. This presentation will overview the PEGylation technology and the chromatographic behavior of PEGylated peptides based on the PEG chain length dispersity will be discussed.

Special Session-3

Analytical Strategies for Exposomics Research with Deciduous Teeth

Sangwon Cha[1]*, Yujin Lee[1], Eunji Seo[1], Soobin Choi[1], and Tae-Min Park[1]

[1]Dept of Chemistry, Hankuk University of Foreign Studies, 81 Oedae-ro , Yongin, 17035, Korea

Recently, due to its specific structure and growth pattern, deciduous teeth have been proposed to be retrospective temporal biomarkers for exposomics researches which try to assess comprehensively environmental exposures from the fetal period onwards. However, sample preparation and analysis steps for teeth samples have not been explored extensively and need to be standardized. In this study, we investigated various sample preparation procedures and mass spectrometric methods for profiling organics and metals present in teeth samples. In order to evaluate sample preparation procedures including sampling, pulverization, incubation, and extraction, we employed ambient ionization MS, and MALDI MS. In addition, we tested various LC/MS methods for organic chemical analysis and laser ablation-based elemental mapping methods such as LA ICP MS and LIBS for spatially resolved metal analysis.

Special Session-4

Computational Method for Glycosylation Analysis by Tandem Mass Spectrometry

Gun Wook Park[1], Heeyoun Hwang[1,2], Ju Yeon Lee[1], Hyun Kyoung Lee[1,2], Eun Sun Ji[1], Kwang Hoe Kim[1,2], Ki Na Yun[1,3], Young-Mook Kang[1], Soo Youn Lee[1], Jong Shin Yoo[1,2] and Jin Young Kim[1]

[1]*Biomedical Omics Group, Korea Basic Science Institute, Ochang, Korea*

[2] *GRAST, Chungnam National Univ., Daejeon, Korea*

[3] *Sogang Univ.,Seoul, Korea*

Mass spectrometry has become a powerful tool for the identification and structural characterization of post translational modifications in proteins. The analysis of small post-translational modifications (PTMs) may be regarded as an extension of proteomics database searching, however, glycosylation requires specialized approaches. This is because glycosylation is heterogeneous by nature causing glycopeptides to exist as multiple glycosylated variants. Note that this complexity multiples when one considers additional modifications occurring in glycosylation such as O-acetylation and mannose phosphorylation. In recent, we have published a computational method called IQ-GPA for automatic identification and quantification of N-glycopeptides where the use of various tandem mass spectra including CID, HCD, and ETD was necessary for successful identification. In this study, we present the advanced computational method for more effective identification of glycosylation and glycan modification using feature fragment ions and fragmentation pattern in tandem mass spectra. It allows more identification and rapid analysis.

Special Session-5

In-depth analysis of plasma proteome for discovery of age-related macular degeneration biomarkers

Hye-Jung Kim[1,3,*], Se Joon Woo[2], and Cheolju Lee[1]

[1]Theragnosis Research Center, Korea Institute of Science and Technology, Seoul
[2]Department of Ophthalmology, Seoul National University College of Medicine, SeoulNational University Bundang Hospital, Seongnam
[3]New Drug Development Center, KBIO Osong Medical Innovation Foundation, Cheongju-si, Korea

Age-related macular degeneration (AMD) is a major cause of severe, progressive visual loss among the elderly. There are currently no established serological markers for the diagnosis of AMD. In this study, we carried out a large-scale quantitative proteomics analysis to identify plasma proteins that could serve as potential AMD biomarkers. We found that the plasma levels of phospholipid transfer protein (PLTP), mannan-binding lectin serine protease (MASP)-1 and vinculin were increased in AMD patients relative to controls. A proteogenomic combination model that incorporated PLTP, MASP-1 and vinculin along with two known risk genotypes of age-related maculopathy susceptibility 2 and complement factor H genes further enhanced discriminatory power. Additionally, mRNA and protein expression levels were upregulated in retinal pigment epithelial cells upon exposure to oxidative stress in vitro. These results indicate that PLTP, MASP-1 and vinculin can serve as plasma biomarkers for the early diagnosis and treatment of AMD, which is critical for preventing AMD-related blindness.

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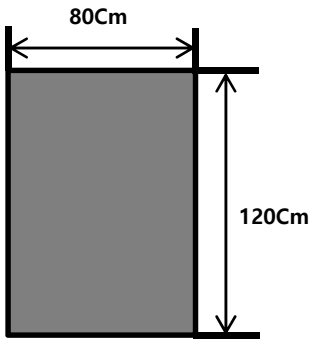
POSTER PRESENTATION

포스터 발표 및 우수포스터상 안내

■ **포스터 게시 및 발표**

- 게　　시 : **2018 년 2 월 2 일 (금) 10:00~**
- 발　　표 : **2018 년 2 월 2 일 (금) 12:10 ~ 14:00 /** 모든 발표자 시간에 맞추어 배석
- 발표 순서 : **홀수 (12:10 ~ 13:00) / 짝수 (13:00 ~ 13:50)**
- 철　　거 : **2018 년 2 월 2 일 (금) 18:00 ~**
- 포스터 발표자는 아래의 포스터 번호 및 배치도를 참고하여 포스터를 게시하고, 2일(금) 12:10 ~ 14:00까지 해당 번호 시간에 포스터 앞에 대기하여 질문에 응해야 합니다.
- 포스터 사이즈 안내 : 가로(80cm) x 세로(120cm)



■ **우수포스터 상**

- 포스터 발표 회원 중 심사를 거쳐 우수한 발표한 자를 선정하여 우수포스터상을 수여합니다.
- 시 상 : 2018 년 2 월 2 일, 폐회식
- 부 상 : 상장 및 상금 10 만원

■ **분야별 포스터 번호**

분야	포스터번호
Fundamental Instrumentation	01
Life & Informatics	02 ~ 10
Mass Spectrometry in Elemental Analysis	11 ~ 19
Medical/Pharmaceutical Science	20 ~ 27
Food Environment	28 ~ 33
General	34 ~ 53

Fundamental Instrumentation : PO1

P-01

MATLAB-based Statistical Analysis Software for Screening of Edible Oils and Establishing 3D Statistical Models

Minhee Son, Han Bin Oh*

Dept of Chemistry, Sogang University, Baekbum-ro 35, Seoul 04107, Korea

Life & Informatics : PO2 ~ P10

P-02

High-fat diet induced perturbations in the mouse brain lipids: cortex, hippocampus, hypothalamus, and olfactory bulb

Jong Cheol Lee, Se Mi Park and Myeong Hee Moon*

Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea

P-03

On-line proteolysis and glycopeptide enrichment with thermo-responsive porous polymer membrane reactors (TPPMR) and nLC-ESI-MS/MS

Joon Seon Yang[1], Juan Qiao[2], Jin Yong Kim[1], Liping Zhao[2], Li Qi[2,*] and Myeong Hee Moon[1,*]

[1]Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea

[2]Beijing National Laboratory for Molecular Sciences; Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Acedemy of Sciences, No. 2 Zhongguancun Beiyijie, Beijing, 100190, China

P-04

Profiling of plasma lipidome among five cancer types by nUPLC-ESI-MS/MS

Gwang Bin Lee, Jong Cheol Lee and Myeong Hee Moon*

Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea.

P-05

Bottom-up and Top-down proteomic and lipidomic analysis of lipoproteins from patients with coronary artery disease using flow field-flow fractionation and mass spectrometry

Jae Hyun Lee, Joon Seon Yang and Myeong Hee Moon*

Department of Chemistry, Yonsei University, Seoul, 03722, Korea.

P-06

Influence of high-fat diet on lipid profiles of mouse muscle tissues by nUPLC-ESI-MS/MS

Jung Yong Eum, Joon Seon Yang, Jong Cheol Lee, Gwang Bin Lee and Myeong Hee Moon*

Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea

P-07

Quantitative Profiling of Cervicovaginal Fluid Proteome Using a 2D-nLC-ESI-MS/MS for Early Detection of Preterm Birth

Kwonseong Kim[1,2], Young Eun Kim[2], Sun Young Lee[2], Han Bin Oh[1], Dukjin Kang[2]

[1]Department of Chemistry, Sogang University, Seoul 04107, Korea

[2]Center for Bioanalysis, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science, Daejeon, 34113, Korea

P-08

Discovery of plasma metabolite biomarker cluster for discriminating Graves' disease and its subtypes by using integrative GC-MS and LC-MS analysis.

Dong Yoon Ji[1], Soo Jin Park[1], Se Hee Park[2,3], Eun Jig Lee[2,4] and Do Yup Lee[1,*]

[1]The Department of Bio and Fermentation Convergence Technology, BK21 PLUS project, Kookmin University, Seoul, Republic of Korea

[2]Division of Endocrinology and Metabolism, Department of Internal Medicine, Yonsei University College of Medicine, Seoul, Republic of Korea

[3]Graduate School, Yonsei University College of Medicine, Seoul, Republic of Korea

[4]Institute of Endocrine Research, Yonsei University College of Medicine, Seoul, Republic of Korea

P-09

Korean whole saliva proteome, ethnically-different human saliva proteome

Ha Ra Cho[1], Han Sol Kim[1], Jun Seo Park[1], Seung Cheol Park[2], Kwang Pyo Kim[2], Troy D. Wood[3], Yong Seok Choi[1,*]

[1]College of Pharmacy, Dankook University, Cheonan, Chungnam, South Korea

[2]Department of Applied Chemistry, The Institute of National Science, College of Applied Science, Kyung Hee University, Yongin, Kyoungki, South Korea

[3]Department of Chemistry, The State University of New York at Buffalo, Buffalo, New York, The United States of America

P-10

High-throughput Cloud Computing System for Glycoproteomics with Mass Spectrometry

Young-Mook Kang[1], Gun Wook Park[1,2], Hyun Kyoung Lee[1,2], Ju Yeon Lee[1], Jin Young Kim[1,2] and Jong Shin Yoo[1,2]

[1]Department of Mass Spectrometry, Korea Basic Science Institute, Cheongju, 28119, Korea

[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, 34134, Korea

Mass Spectrometry in Elemental Analysis
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P-11

Chemical treatment of TIMS filaments for improvement of uranium sensitivity

Jong-Ho Park*

Nucelar Chemistry Research Division, Korea Atomic Energy Research Institute, 111 Daedeok-daero-989, Yuseong-gu, Daejeon 34057, Korea

P-12

Study of detection and analysis of arsenic species in marine samples using ion chromatography-inductively coupled plasma mass spectrometry

Sheng Cui, Yong-Hyeon Yim, Kyoung-seok Lee, Hyung Sik Min and Joung Hae Lee*

Korea Research Institute of Standards and Science, 267 Gajeong-ro, Yuseong-gu, Daejeon, 34114, Korea

P-13

Comparative analysis of heavy metal content of domestic commercial mushrooms

Sunghwa Choi[1], Jiyeon Kim[1], Minyoung Lee[1,2], Eun Mi Choi[1], Eunji Kim[1], Yuri Lee[1], Hyun-Jung Park[1], Kyungsu Park[1,*]

[1]Advanced Analysis Center, Korea Institute of Science and Technology,5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea,

[2]Department of Chemistry, Kyung Hee University, 1 Hoegi-dong, Dongdaemun-gu, Seoul 130-701, Republic of Korea

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Analysis of heavy metal contents in natto

Minyoung Lee[1,2,*], Jiyeon Kim[1], Sunghwa Choi[1], Eun Mi Choi[1], Eunji Kim[1], Yuri Lee[1], Hyun-Jung Park[1], Kyungsu Park[1,*]

[1]Advanced Analysis Center, Korea Institute of Science and Technology, 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul, 02792, Republic of Korea

[2]Department of Chemistry, Kyung Hee University, 1 Hoegi-dong, Dongdaemun-gu, Seoul, 130-701, Republic of Korea

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Efficient Enrichment of Phosphopeptides on Digital MicroFluidics(DMF) Chip Using TiO_2-Magnetic Bead by MALDI-TOF MS.

Jinwoo Kim, Hyunji Lee, Inae Jang and Han Bin Oh*

Dept of Chemistry, Sogang University , 35 Baekbeom-ro, Mapo-gu, Seoul, 04107, Korea

P-16

Analysis of total uranium and thorium in naturally occurring radioactive materials using standard addition method combined with inductively coupled plasma mass spectrometry

Hwijin Kim[1,2], Jong Wha Lee[2], Yeongran Lim[2], Sang Han Lee[3], Jung-Suk Oh[3], Yong-Hyeon Yim[2], Sung Woo Heo[2], Kyoung-Seok Lee[2,*]

[1]Department of Bio-Analytical Science, University of Science and Technology (UST), Daejeon, 34113, Korea

[2]Center for Analytical Chemistry, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea

[3]Center for Ionizing Radition, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea

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Determining collisional cross cections (CCS) of polycyclic aromatic hydrocabon (PAH) compounds in crude oil by using PAH compounds' mixture as calibrant

Dongwan Lim[1], Kimberly L. Davidson[2], Seungwoo Son[1], Arif Ahmed[1], Matthew F. Bush[2,*], and Sunghwan Kim[1,3,*]

[1]Kyungpook National University, Department of Chemistry, Daegu, 702-701, Republic of Korea

[2]Department of Chemistry, University of Washington, Seattle, Washington 98195, United States

[3]Green-Nano Materials Research Center, Daegu, 702-701 Republic of Korea

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Proteomic analysis of aqueous humor biomarkers associated with diabetic retinopathy and its complications using quantitative approach

Hye Min Kim[1], Jae Won Oh[1], Jae Hun Jung[1], Kwang Pyo Kim[1], Tae Wan Kim[2]

[1]Department of Applied Chemistry, College of Applied Sciences, Kyung Hee University, Yong-in 446-701, Republic of Korea.

[2]Department of Ophthalmology, Seoul Metropolitan Government, Seoul National University Boramae Medical Center, Seoul, Republic of Korea

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Study on the determination of boron in cathode active material of lithium ion battery by ICP-MS

In-Gi Kim, Jung-Ju. Lee and H. B. Lim*

Dept. of Chemistry, Dankook University, Anse-dong, Cheonan-si, Chungcheongnam-do, Korea

Medical/Pharmaceutical Science : P20 ~ P27

P-20

Global discovery Biomarker for Autism Spectrum Disorder (ASD) for early diagnose

Wooyoung (Eric) Jang, Kim Min Sik*

Department of Applied Chemistry College of Applied Sciences, Kyung Hee University Yong-in City, 446-701 Republic of Korea

P-21

Discovery of specific common fragments on trimethylsilylated PDE-5 inhibitors for their rapid screening and confirmation by GC-MS/MS combined with extracted common ion chromatogram

Na-Hyun Park, Myoung Eun Lee, Jisu Hur, Bum Hee Kim, Jongki Hong*

College of Pharmacy, Kyung Hee University, Seoul 02447, Korea

P-22

MS-based quantitation of a non human glycan in a therapeutic glycoprotein

Jaekyoung Ko[1,2], Nari Seo[1,2], MyungJin Oh[1,2] and Hyun Joo An[1,2,*]

[1]Graduate School of Analytical Science and Technology, Chungnam National University, Korea
[2]Asia-Pacific Glycomics Reference Site, Korea

P-23

An improved MALDI-TOF MS–based β-lactamase assay platform for clinically relevant cefotaxime resistant bacteria

Jiyeon Hong[1], Jae-Seok Kim[2] and Kyoung-Soon Jang[1,3,*]

[1]Biomedical Omics Group, Korea Basic Science Institute, Cheongju 28119, Korea
[2]Department of Laboratory Medicine, Hallym University College of Medicine, Kangdong Sacred Heart Hospital, Seoul 05355, Korea
[3]Department of Bio-Analytical Science, University of Science and Technology, Daejeon 34113, Korea

P-24

Metabolic changes in the bone tissue of aged mice with osteoporosis

Miso Nam[1,2], Geum-Sook Hwang[1,3]

[1]Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Seoul, 03759, Korea
[2]Department of Chemistry, Sungkyunkwan University, Suwon, 16419, Korea
[3]Department of Chemistry and Nano Science, Ewha Womans University, Seoul, 03760, Korea

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Lipid profiling of human Non-alcoholic fatty liver disease (NAFLD) based on liquid chromatography/mass spectrometry

Min Kyung Lee[1,2], Youngae Jung[1], Geum-Sook Hwang[1]

[1]Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Seoul 03759, Korea
[2]Dept of Pharmacy, Ewha Womans University, Seoul 03760, Korea

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Classification of serum glycoproteins based on pattern identification in Traditional Korean Medicine (TKM) from lung cancer patients

Jinwook Lee, Wonryeon Cho*

Department of Chemistry, Wonkwang University, Iksan,54538, Korea

P-27

Quantification of glycated hemoglobin in dried blood spot using isotope dilution HPLC-MS/MS

Thi Thanh Huong Tran[1,2], Ji-Seon Jeong[2,*]

[1]Department of Bio-Analytical science, University of Science and Technology (UST), Daejeon, Republic of Korea
[2]Center for Bioanalysis, Division of Metrology for Quality of Life, Korea Research Institute of Standards and Science (KRISS), Daejeon, Republic of Korea

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P-28

Interlaboratory validation of LC–Triple Quad MS/MS for the quantification of enrofloxacin in chicken meat

Joo Hee Chung[1], Kun Cho[2], Seongnyeon Kim[2], So Hyeon Jeon[3], Jueun Lee[3], Yun Gyong Ahn[3]

[1]Seoul Center, Korea Basic Science Institute, Seoul, 02855, South Korea
[2]Biomedical Omics Group, Korea Basic Science Institute, Ochang, 28119, South Korea
[3]Western Seoul Center, Korea Basic Science Institute, Seoul, 03759, South Korea

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Stable carbon isotope analysis of organic sediments. is it possible to analyze at the molecular level?

Seungwoo Son, Donghwi Kim, Sunghwan Kim*

Department of Chemistry, Kyungpook National University, Daegu, Republic of Korea

P-30

Qualitative determination of steviol and its glycosides in *Stevia rebaudiana* by liquid chromatography tandem mass spectrometry

Seongnyeon Kim[1], Moo Sung Kim[2], Heehoon Jung[2], Kun Cho[1]

[1]Biomedical Omics Group, Korea Basic Science Institute, Ochang, Chungbuk, 28119, Korea
[2]R&D center, Macrocare Tech Co., Ltd., 32, Gangni 1-gil, Ochang-eup, Cheongwon-gu, Cheongju-si, Chungcheongbuk-do, 28126, South Korea

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Determination of fumonisins in maize using isotope dilution-liquid chromatography tandem mass spectrometry

Yosi Aristiawan[1,2], Kihwan Choi[1,*], Byungjoo Kim[1,*]

[1]Center for Analytical Chemistry, Korea Research Institute of Standard and Science, Daejeon, 34113, Korea
[2]Department of Bio-Analytical Science, University of Science & Technology (UST), Daejeon, 34113, Korea

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Tracing Fragrance Chemicals in Cosmetics by GC-MS

Chae Won Lee[1], You Ri Choi[1], Ji Eun Kim[1], Min Seo Park[2], Sang Yun Han[1,*]

[1]Department of Nanochemistry, Gachon University, Seongnam, Gyeonggi (13120), Republic of Korea
[2]Department of Bionanotechnology, Gachon University, Seongnam, Gyeonggi (13120) Republic of Korea

P-33

Structural identification of an enzymatic oxidation product of a model lignin compound by tandem mass spectrometry

Woo-Young Song, Youri Yang, Sunil Ghatge, Hor-Gil Hur* and Tae-Young Kim*

School of Earth Science and Environmental Engineering, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju, 61005, Korea

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P-34

Enhancement of polypeptide ladder detection signal using derivatization method

Dabin Lee, Yeoseon Kim, Sol Han, and Jeongkwon Kim*

Department of Chemistry, Chungnam National University, Daejeon, 34134, Korea

P-35

Lipid profiling of lipoproteins from patients with mild cognitive impairment and Alzheimer's disease by asymmetrical flow field-flow fractionation and nUPLC-ESI-MS/MS

San Ha Kim, Joon Seon Yang, Jong Cheol Lee and Myeong Hee Moon*

Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul 03722, Korea

P-36

Effect of temperature on microwave-assisted tryptic digestion of protetins

Yeoseon Kim, Dabin Lee, Sol Han, and Jeongkwon Kim*

Department of Chemistry, Chungnum National University, Daejeon, 34134, Korea

P-37

Study of cross-interaction between amyloid β 1-42 and 1-40 in the early stage of fibrillation using ESI-MS

Chae-Eun Heo, Hugh I. Kim

Dept of Chemistry, Korea University, Seoul 02841, Republic of Korea

P-38

Discovery of metabolite candidates for elapsed time analysis of bloodstain

Ae Eun Seok[1], Jiyeoug Lee[2], You-Rim Lee[1], Arum Park[1], Sora Mun[1], Hyo-Jin Kim[2], Yoo-Jin Lee[2], Hee-Gyoo Kang[1,2]

[1]Laboratory of Signal Transduction and Disease Biomarker Discovery, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, 34824, Korea

[2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Gyeonggi-do, 13135, Korea

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Discovery of internal standard metabolite for accurate chemical analysis of bloodstain

You-Rim Lee[1], Jiyeong Lee[2], Ae Eun Seok[1], Arum Park[1], Sora Mun[1], Hyo-Jin Kim[1], Yoo-Jin Lee[1], Hee-Gyoo Kang[2]

[1]Laboratory of Signal Transduction and Disease Biomarker Discovery, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon 34824, Korea

[2]Department of Biomedical Laboratory Science, College of Health Science, Eulji University, Seongnam 13135, Korea

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Proteomics analysis of LNCaP reveals bicalutamide enhances cellular pathways associated with fodrin-mediate apoptosis through calpain

Sora Mun[1], Jiyeong Lee[2], Arum Park[2], Doojin Kim[2], Byung Heun Cha[2], AeEun Seok[2], You-Rim Lee[1], Hyo-Jin Kim[1], Yoo-Jin Lee[1], Hee-Gyoo Kang[1,2]

[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, Korea.

[2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Korea.

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Proteomics Analysis of Individual Serum Samples of Large Artery Atherosclerosis Stroke Patients and Healthy Subjects

Jiyeong Lee[1], Arum Park[1], Sora Mun[2], You-Rim Lee[2], AeEun Seok[1], Hyo-Jin Kim[2], Yoo-Jin Lee[2], Hee-Gyoo Kang[1,2]

[1]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Korea.

[2]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, Korea.

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Effective cleanup of trace diarrhetic shellfish poisoning toxins in high-lipid bivalves and their simultaneous determination by UPLC-ESI-MS/MS combined with time segment polarity switching

Myoung Eun Lee[1,+], Na-Hyun Park[1,+], Jeongmi Lee[2], Yong Seok Choi[3], Jongki Hong[1,*]

[1]College of Pharmacy, Kyung Hee University, Seoul 02447, Korea

[2]School of Pharmacy, Sungkyunkwan University, Suwon 16419, Korea

[3]College of Pharmacy, Dankuk University, Cheonan 31116, Korea

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Rapid lipid extraction using superabsorbent polymers for mass spectrometry

Geul Bang[1], Yeong Jun Yu[1,4], Jeong Ah Kim[1,2,*], Young Hwan Kim[1,2,3]

[1]Biomedical Omics Group, Korea Basic Science Institute, Chungbuk 28119, Republic of Korea.

[2]Department of Bio-Analytical Science, University of Science and Technology, Daejeon 34113, Republic of Korea.

[3]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon 34134, Republic of Korea.

[4]Program in Micro/Nano System, Korea University, Seoul 02841, Republic of Korea

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Selective screening of sulfonamides in supplements by UHPLC-Q/TOF-MS combined with high-resolution extracted common ion chromatogram and neutral loss scan

Nam-Yong Ki, Na-Hyun Park, Jisu Hur, Ina Choi, Jongki Hong*

College of Pharmacy, Kyung Hee University, 26 Kyunghee-daero, Dongdaemun-gu,

Seoul 02447, Korea

P-45

Absolute quantification of human growth hormone and brain natriuretic peptide-32 from human plasma using iCCM-based isotope dilution mass spectrometry

Sun Young Lee[1,2], Jongki Hong[2], Dukjin Kang[1]

[1]Center for Bioanalysis, Division of Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 305-340, Korea
[2]College of Pharmacy, Kyung Hee University, Seoul 130-701, Korea

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Glycomic Investigation of Human Saliva for Forensic Application

Jinyoung Park [1,2], Seunghyup Jeong[1,2], Bum Jin Kim[1,2] and Hyun Joo An[1,2,*]

[1]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon
[2]Asia-Pacific Glycomics Reference Site, Chungnam National University, Daejeon

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Construction of mouse brain glycome library using LC/MS and MS/MS

Jaekyung Yun[1,2], Jua Lee [1,2] and Hyun Joo An[1,2,*]

[1]Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea
[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea

P-48

LC/MS-based quantitative strategy to determine O-glycan expression in GALNT13 KO mouse brain

Sowon Mun[1,2], Jaekyung Yun[1,2], Jua Lee[1,2] and Hyun Joo An[1,2,*]

[1]Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea
[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea

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Proteomic Profiling of Tissue-based Map of the Canis (Beagle)

Na-Young Han[1,*], Jong-Moon Park[1], Jongho Jeon[1], Je-Yoel Cho[3], Hookeun Lee[1,2]

[1]Gachon Institute of Pharmaceutical Sciences, Gachon College of Pharmacy, Gachon University, 534-2 Yeonsu 3-dong, Yeonsu-gu, Incheon 406-799, Republic of Korea
[2]Gachon Medical Research Institute, Gil Medical Center, Incheon 405-760
[3]Department of Biochemistry, BK21 Plus and Research Institute for Veterinary Science, School of Veterinary Medicine, Seoul National University, Seoul, 151-742, Korea

P-50

Site-specific characterization of N- and O-glycoproteins in human and mouse plasma using LC-MS/MS and I-GPA search system

Hyun Kyoung Lee[1,2,*], Ju Yeon Lee[1], Gun Wook Park[1], Jin Young Kim[1] and Jong Shin Yoo[1,2]

[1]Korea Basic Science Institute, O-chang Cheongju, Korea
[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea

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Integrative multi-omic analysis of Th1 differentiation

Min Jung Kim, Kwang Pyo Kim and Min-Sik Kim*

Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea

P-52

Proteomics and phosphoproteomics studies of cell lines with CRISPR-Cas9 edited kinases for cancer disease.

Bitnara Han[1], Hyeong Min Lee[1], Jae Min Lim[1], Jin-Soo Kim[2,3], Kwang Pyo Kim[1]

[1]Department of Applied Chemistry, College of Applied Sciences, Kyung Hee University, Yongin 446-701, Republic of Korea
[2]National Creative Research Initiatives Center for Genome Engineering, Seoul National University, Seoul, South Korea
[3]Department of Chemistry, Seoul National University, Seoul, South Korea.

P-53

New pathological discovery of Preeclampsia through human placenta proteomics

Hyeong Min Lee, Jae Min Lim and Kwang Pyo Kim*

Dept of Applied Chemistry, College of Applied Science, Khung Hee University, Yongin, Gyeonggi-do,446-701, Republic of Korea

P-01

MATLAB-based Statistical Analysis Software for Screening of Edible Oils and Establishing 3D Statistical Models

Minhee Son, Han Bin Oh*

Dept of Chemistry, Sogang University, Baekbum-ro 35, Seoul 04107, Korea

In this study, we made a software that designed to be able to project and classify unknown edible oil mass spectra on 3D PCA / PLS-DA model by importing mass analysis data of unknown edible oil by using different amount and composition if lipids such diacylglycerols (DAGs) and triacylglycerols (TAGs) according to kinds of edible oil. For the statistical analysis model, 9 kinds of edible oil were used, such as sesame, perilla, olive, canola, grape-seed, sunflower-seed, corn, soybean, coconut oils, and the equipment was Tinkerbell MALDI-TOF (Asta, Korea). In addition to the existing statistical analysis models, we have built models directly based on user data and made the models available for classification or screening of samples.

P-02

High-fat diet induced perturbations in the mouse brain lipids: cortex, hippocampus, hypothalamus, and olfactory bulb

Jong Cheol Lee, Se Mi Park and Myeong Hee Moon*

Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea

High-fat diet (HFD), generally rich with saturated fats, induce obesity, cognitive impairment and neurodegenerative diseases. Lipids are known to be involved in variety of neuronal signals in brain, which is the most important and multifunctional organ. As chronic consumption of HFD causes celluar malfunctioning and insulin resistance in neurons of brain tissues, lipidomic analysis of HFD induced mouse brain tissues has attracted much attention.

In this study, nanoflow ultrahigh pressure LC-ESI-MS/MS was applied io investigate four different brain tissues from mice: cortex, hippocampus, hypothalamus, and olfactory bulb. Mice were fed with the various dietary schedules: 8 weeks - normal control (N), and weight gain (F), 16 weeks - normal control (NNN), weight maintenance (FNN), weight gain (NNF), and weight cycling (FNF). Lipids were extacted by modified Folch with MTBE/MeOH method and 359 lipids were identified from brain tissues. Quantitative analysis revealed that an HFD significantly pertubated the lipidome of all brain regions and diacylglycerols, known to be related with insulin resistance, increased. Furthermore, weight-cycling group (FNF) was proved to be more affected than weight gain group (NNF).

P-03

On-line proteolysis and glycopeptide enrichment with thermo-responsive porous polymer membrane reactors (TPPMR) and nLC-ESI-MS/MS

Joon Seon Yang[1], Juan Qiao[2], Jin Yong Kim[1], Liping Zhao[2], Li Qi[2,*] and Myeong Hee Moon[1,*]

[1]Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea
[2]Beijing National Laboratory for Molecular Sciences; Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Acedemy of Sciences, No. 2 Zhongguancun Beiyijie, Beijing, 100190, China

Protein N-glycosylation, one of post-translational momdifications (PTMs), is a process that glycans attach covalently to nitrogen atom in asparagine (asn, N) amino acid. Since several glycosylated proteins are known as biomarkers of disease such as cancers, it is important to analyze glycoproteins in biological samples. In this study, dual micro-scale thermo-sensitive porous polymer membrane reactor (TPPMR) was developed for on-line proteolysis and glycopeptide enrichment prior to nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS/MS).

PS-MAn-NIPAM (PNPAm) is thermo-sensitive porous polymer membrane which is synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization and is coated on nylon membrane by breath figure method. Trypsin and lectin mixtures (ConA and WGA) can be immobilized on the coated membrane for proteolysis and glycopeptide enrichment, respectively, and each of membrane is inserted in TPPMR module. Dual TPPMR modules are directly connected to nLC-ESI-MS/MS system and proteolysis efficiency in proteolysis and glycopeptides enrichment were evaluated by varying temperature. The developed method demonstrates that on-line proteolysis and glycopeptide enrichment can be performed with only about 1.5 μL human plasma sample with the successful identification of 155 glycoproteins.

P-04

Profiling of plasma lipidome among five cancer types by nUPLC-ESI-MS/MS

Gwang Bin Lee, Jong Cheol Lee and Myeong Hee Moon*

Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea.

As lipids are involved with various biological functions such as energy storage, cellular signaling, and cell to cell interaction, they play key roles in cellular survival, proliferation, and death. These cellular processes are associated with cancer genesis pathways, especially to transformation, progression, and metastasis, suggesting the bioactive lipids are mediators of a number of oncogenic processes. In a recent lipidomics research, lipid analysis about cancer gains much interests, because each type of cancer has different carcinogenesis pathways. In this study, lipids of patient's blood plasma sample from five different cancers (liver, stomach, lung, colorectal, and thyroid) were investigated in order to discover lipids that show significant difference among the groups and to find potential lipid biomarkers for each cancer. Blood plasma were extracted from each cancer patient using the modified Folch method with MTBE/methanol, and the extracted lipids were analyzed by nUPLC-ESI-MS/MS. A total of 243, 236, 239, 239, 239, and 225 plasma lipids from patients with liver, stomach, lung, colorectal, thyroid cancer, and controls, respectively, were characterized and statistically evaluated.

P-05

Bottom-up and Top-down proteomic and lipidomic analysis of lipoproteins from patients with coronary artery disease using flow field-flow fractionation and mass spectrometry

Jae Hyun Lee, Joon Seon Yang and Myeong Hee Moon*

Department of Chemistry, Yonsei University, Seoul, 03722, Korea.

Coronary artery diseases (CAD) refers to a condition in which coronary arteries become narrow by accumulation of cholesterols, fats, and other substances. Narrow coronary arteries restrict blood flow to heart and may even cause a partial or complete blockage of coronary arteries. In blood system, cholesterols are transported by lipoproteins. High density lipoprotein (HDL) is known to transport cholesterols from the cells to the liver, which helps removing excessive cholesterols out of cells.

Flow field-flow fractionation (FlFFF) is separation technique according to size in a range of nano to micrometer. In this study, FlFFF was utilized to separate HDL and LDL from human plasma samples with CAD and for the proteomic and lipidomic analysis using nUPLC-ESI-MS/MS. Miniaturized asymmetrical flow field-flow (AF4) channel was coupled on-line to electrospray ionization mass spectrometry (ESI-MS) for a high speed separation of lipoproteins and for simultaneous analysis of apolipoprotein A-1 (ApoA-1) which is one of HDL proteins and known to be related with the transport of cholesterol. .

P-06

Influence of high-fat diet on lipid profiles of mouse muscle tissues by nUPLC-ESI-MS/MS

Jung Yong Eum, Joon Seon Yang, Jong Cheol Lee, Gwang Bin Lee and Myeong Hee Moon*

Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea

Lipids play important roles in various cellular processes such as membrane structure, signaling, and apoptosis. High-fat diet is known to cause obesity which is induced by excess amount of lipid accumulation in skeletal muscles. Especially, high fat diet increases the accumulation of triacylglycerol (TAG) which is an energy source in skeletal, leading to a th dysfunction of mitochondria further to induce insulin-resistance diabetes.

In this study, effect of high-fat diet on the lipid profiles of the two types of skeletal muscle tissues, gastrocnemius (Gas) and soleus (Sol), from mice were investigated by nanoflow ultrahigh pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUPLC-ESI-MS/MS). Mice were grown with eight different diet programs including normal diet and high fat diet. Lipid from each muscle tissue were extracted by modified folch methods and a total of 269 lipid species were identifiedand quantified.

P-07

Quantitative Profiling of Cervicovaginal Fluid Proteome Using a 2D-nLC-ESI-MS/MS for Early Detection of Preterm Birth

Kwonseong Kim[1,2], Young Eun Kim[2], Sun Young Lee[2], Han Bin Oh[1], Dukjin Kang[2]

[1]*Department of Chemistry, Sogang University, Seoul 04107, Korea*
[2]*Center for Bioanalysis, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science, Daejeon, 34113, Korea*

Occurring preterm birth (PTB) before 37 weeks of pregnancy is one of major causes, resulting in perinatal mortality and neonatal morbidity. Nevertheless, the proteomic study on the development of biomarker(s) for early detection of PTB, unfortunately, has not been matured. In this study, we performed shotgun proteomic analysis of the cervicovaginal fluid (CVF) samples from PTB and its normal counterpart, so as to unveil the protein biomarkers using two dimension-nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (2D-nLC-ESI-MS/MS). The quantitative assessments of CVF proteome from both PTB and control were carried out through an isobaric labeling approach with iTRAQ. Out of 1044 proteins identified, 1009 proteins were able to be in common quantified in PTB/control CVF samples. From MS/MS-based isobarically quantitative determination, 30 proteins from PTB were twofold or more upregulated, compared to that of control ones, while 59 proteins were measured to be twofold decreased. Based on the bioinformatic analyses (*e.g.*, Gene Ontology and KEGG), we found that 18 proteins, having the different expression levels between PTB and control, were implicated in immune response in cell. Resultingly, both of up-/down-regulated proteins identified in this study might be applicable to the development of biomarker(s) having the potential in the clinical diagnosis of PTB.

P-08

Discovery of plasma metabolite biomarker cluster for discriminating Graves' disease and its subtypes by using integrative GC-MS and LC-MS analysis.

Dong Yoon Ji[1], Soo Jin Park[1], Se Hee Park[2,3], Eun Jig Lee[2,4] and Do Yup Lee[1,*]

[1]*The Department of Bio and Fermentation Convergence Technology, BK21 PLUS project, Kookmin University, Seoul, Republic of Korea*

[2]*Division of Endocrinology and Metabolism, Department of Internal Medicine, Yonsei University College of Medicine, Seoul, Republic of Korea*

[3]*Graduate School, Yonsei University College of Medicine, Seoul, Republic of Korea*

[4]*Institute of Endocrine Research, Yonsei University College of Medicine, Seoul, Republic of Korea*

Autoimmune disease is a condition that arises from abnormal immune responses to self-antigen, which leads to damage of tissues or dysfunction of biological system. Graves' disease (GD) is an autoimmune disorder that affects thyroid, and frequently results in hyperthyroidism. It often develops to an enlarged thyroid and eye bulging, Graves' ophthalmopathy (GO) with 25% frequency of GD. Since there is no specific molecular indicator for the disease, biomarker based on blood metabolite can be an effective and powerful tool for diagnosis, and suggest putative therapeutic target. In this study, a gas chromatography coupled time-of-flight mass spectrometry was employed to characterize primary metabolic profiles from plasma of GD (n=20), GO (n=27), and healthy control (n=32). Multivariate statistical analysis were applied to identify the metabolic phenotype of Graves' disease compared to health control. The most significant alteration was found in glycolysis and branched chain amino acids. The subsequent biomarker model consisting of 1,5-anhydroglucitol, proline, glucose and pyruvate showed excellent discrimination power. Area under the curve (AUC) values by receiver operating characteristic (ROC) analysis were 0.94 (control vs others), 0.87(GO vs others) and 0.86(GD vs others), respectively. In addition, lipid profiling revealed the dramatic alteration of sphingolipids and phospholipids in the disease, which included oleoyl-LPA and sphingosine 1-phosphate.

P-09

Korean whole saliva proteome, ethnically-different human saliva proteome

Ha Ra Cho[1], Han Sol Kim[1], Jun Seo Park[1], Seung Cheol Park[2], Kwang Pyo Kim[2], Troy D. Wood[3], Yong Seok Choi[1,*]

[1]College of Pharmacy, Dankook University, Cheonan, Chungnam, South Korea
[2]Department of Applied Chemistry, The Institute of National Science, College of Applied Science, Kyung Hee University, Yongin, Kyoungki, South Korea
[3]Department of Chemistry, The State University of New York at Buffalo, Buffalo, New York, The United States of America

While more than 3,000 salivary proteins have been identified since the early 2000s, there has not been any trial to build Korean saliva proteome. Additionally, ethnic differences in the human plasma proteome were recently reported, but there was not any report on this aspect in the human saliva proteome, yet. Thus, here, the Korean whole saliva (WS) proteome was constructed for the first time and it was characterized by the comparison with the integrated human saliva protein dataset for the determination of ethnic differences in the human saliva proteome. A total of 674 proteins were indexed in the catalogue by the nLC-Q-IMS-TOF analyses of WS samples collected from 11 healthy South Korean adult male volunteers and 11 healthy South Korean adult female volunteers. Among 674 proteins, 358 proteins were not found in the integrated human saliva protein dataset. Also, the significant uniqueness of the Korean WS proteome was observed in gene ontology. Since the inter-platform reproducibility of the nLC-Q-IMS-TOF system was confirmed, these observations are strong evidences to support ethnic differences in the human saliva proteome. Additionally, since 47 out of the 358 distinct Korean WS proteins were found to be associated with the top 10 deadliest diseases in South Korea, the potential of ethnicity-specific human saliva proteins as biomarkers for diseases highly prevalent in that ethnic group was confirmed. Finally, the present Korean WS protein catalogue is expected to be used as the first level reference for future Korean saliva proteome studies.

P-10

High-throughput Cloud Computing System for Glycoproteomics with Mass Spectrometry

Young-Mook Kang[1], Gun Wook Park[1,2], Hyun Kyoung Lee[1,2], Ju Yeon Lee[1], Jin Young Kim[1,2] and Jong Shin Yoo[1,2]

[1]*Department of Mass Spectrometry, Korea Basic Science Institute, Cheongju, 28119, Korea*
[2]*Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, 34134, Korea*

We have developed GlycoProteomeAnalyzer (GPA) for high throughput identification and quantification of N- and O-glycoproteins. GPA is a program for automatic identification of the glycan compositions and glycopeptide sequences by using four different scoring systems such as M-score for glycopeptide selection from oxonium-ions, S-score for theoretical isotope pattern match of molecular ion, Y-score for glycopeptide identification, and P-score for pinpointing O- and N-glycosylation sites from MS/MS fragmentation methods.

In this study, a glycoprotein mixture was digested by trypsin. Those site-specific N- and O-glycopeptides were enriched by hydrophobic interaction liquid chromatography and analyzed by nano-reversed-phase liquid chromatography coupled to tandem mass spectrometry with HCD, CID and EThcD-MS/MS fragmentation modes. The resultant LC/MS/MS data were automatically analyzed by IQ-GPA.

Here, we present the IQ-GPA Cloud which is a web based GPA application for automatic identification and quantification of site-specific N- and O-glycoproteins. IQ-GPA Cloud is a publicly accessible web application that enables users to quickly provide on-demand infrastructures for high-performance gylcoproteome analysis using cloud platforms. Users have instant access to a glycan database builder as well as N- and O-GPA modules. IQ-GPA Cloud has been designed to easily handle high-throughput glycoproteomic data with graphical user interfaces. Microsoft Azure Cloud provides more than thousands of CPU to increase throughput for data analysis. Therefore, users can use glycoproteome analysis easily through IQ-GPA Cloud without any high-powered computer.

The IQ-GPA Cloud is demonstrated on the website, https://www.igpa.kr/cloud/.

P-11

Chemical treatment of TIMS filaments for improvement of uranium sensitivity

Jong-Ho Park*

Nucelar Chemistry Research Division, Korea Atomic Energy Research Institute, 111 Daedeok-daero-989, Yuseong-gu, Daejeon 34057, Korea

Sensitivity improvement of thermal ionization mass spectrometry (TIMS) is essential to ensure the analytical reliability, especially for the nuclear safeguard purpose. A feasibility study on the carburization of uranium samples to enhance TIMS sensitivity. Graphite powder in a suspension form was deposited onto rhenium filaments at a high temperature was performed. The uranium ion ($^{238}U^{+}$) intensity of TIMS was monitored to investigate the effect of chemical treatment of TIMS filament, as well as the evaporation behaviour and ionization of uranium under newly development conditions, and the dependence of such behaviour on graphite deposition concentrations. Determination of isotopic uranium ratios (n(^{234}U)/n(^{238}U), n(^{235}U)/n(^{238}U), and n(^{236}U)/n(^{238}U)) was performed using simultaneous measurement and continuous heating methods to confirm the validity of our technique, given that our analysis agreed with certified values.

P-12

Study of detection and analysis of arsenic species in marine samples using ion chromatography-inductively coupled plasma mass spectrometry

Sheng Cui, Yong-Hyeon Yim, Kyoung-seok Lee, Hyung Sik Min and Joung Hae Lee*

Korea Research Institute of Standards and Science, 267 Gajeong-ro, Yuseong-gu, Daejeon, 34114, Korea

The chemical speciation of elements has been important because their bioactivity and toxicity rely on the particular chemical forms of elements. In all the arsenic species inorganic arsenic (As^{3+} and As^{5+}) has been reported to be more toxic than organic species. This study was focused on the analytical methods for arsenic species in seafood and marine sediment samples. Five main species (As^{3+}, As^{5+}, MMA, DMA and AsB) were investigated (inorganic species for sediment sample only). The extraction method for seafood was chosen with sonication in which a water : methanol mixture (1:1, v/v) was used as the extract solvent. And for marine sediment samples, the extraction of inorganic species was carried out by shaking using 0.5 M phosphoric acid as extract solvent. The species were separated by a Hamilton X100 analytical column, and detected by a mass spectrometry. Various certified reference materials (CRM) were used for the validation of the analytical methods. For seafood CRM sample about 90 % of AsB the main species in seafood was extracted by the method mentioned. And 85.7 % and 82.2 % recovery efficiencies for As^{3+} and As^{5+} spiked in marine sediment CRM sample were obtained using the extraction mentod.

P-13

Comparative analysis of heavy metal content of domestic commercial mushrooms

Sunghwa Choi[1], Jiyeon Kim[1], Minyoung Lee[1,2], Eun Mi Choi[1], Eunji Kim[1], Yuri Lee[1], Hyun-Jung Park[1], Kyungsu Park[1,*]

[1]Advanced Analysis Center, Korea Institute of Science and Technology,5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea,

[2]Department of Chemistry, Kyung Hee University, 1 Hoegi-dong, Dongdaemun-gu, Seoul 130-701, Republic of Korea

The purpose of this study was to evaluate heavy metal content of Mushrooms in Korea market. For the analysis, mushrooms are Neung-I (Sarcodon imbricatus), White Ferula Mushroom (Pleurotus nebrodensis), Song-go and Hen of the woods (Grifola frondosa). Samples were digested by microwave digestion system. This study analyzed for Pb, Cd, As and Hg by using ICP-MS (Inductively Coupled Plasma - Mass Spectrometer) and DMA (Direct Mercury Analyzer).

Linearity, LOD (limit of detection), LOQ (limit of quantitation), accuracy and precision for the analysis validation, through FAPAS (International Quality Control) was verified.

As a result, LOD was 0.00001 ~ 0.0033 mg/kg and LOQ was 0.00012 ~ 0.0109 mg/kg. Also, RSD was less than 5 %. Accuracy was 94.8 ~ 108.2% and precision was 0.14 ~ 4.30 %. FAPAS Satisfactory results were obtained below the Z-score 1.0, ensure high reliability of the analyses.

Analyzing heavy metals contents of Mushrooms, Pb, As, Hg was highest in Neung-I (Sarcodon imbricatus). Cd was highest in Hen of the woods (Grifola frondosa).

The standard of domestic heavy metals of mushrooms is 0.3 mg/kg for Pb and Cd in the case of Button (garicus bisporus (Lange) Imbach), Oyster (Pleurotus ostreatus (Jacq.) P. Kumm.), King oyster, Pyo-go (Lentinula edodes), Mok-i (Auricularia auricula-judae (Bull.) Quél.), Song-I (Tricholoma matsutake (S. Ito. & Imai.) Sing.).

As a result of the analysis, there was nothing exceeding the domestic standard specification.

P-14

Analysis of heavy metal contents in natto

Minyoung Lee[1,2,*], Jiyeon Kim[1], Sunghwa Choi[1], Eun Mi Choi[1], Eunji Kim[1], Yuri Lee[1], Hyun-Jung Park[1], Kyungsu Park[1,*]

[1]Advanced Analysis Center, Korea Institute of Science and Technology, 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul, 02792, Republic of Korea

[2]Department of Chemistry, Kyung Hee University, 1 Hoegi-dong, Dongdaemun-gu, Seoul, 130-701, Republic of Korea

The purpose of this study is to produce the monitoring data on contents of heavy metals in nattos. The samples which were purchased from Korean markets were analyzed for evaluating the contents of heavy metals (Pb, Cd, As and Hg). In this study, the analysis was conducted about heavy metal contents of natto which is a traditional Japanese food made from soybeans fermented with Bacillus subtilis var. natto.

The samples were digested by microwave digestion system. In this study, the analysis for Pb, Cd and As was performed by using Inductively Coupled Plasma Mass Spectrometer (ICP-MS) and contents of Hg was analyzed by Direct Mercury Analyzer (DMA).

Linearity, LOD (limit of detection), LOQ (limit of quantitation), accuracy and precision for the analysis validation, through FAPAS (International Quality Control) was verified.

As a result, LOD was 0.00001 ~ 0.0033 mg/kg and LOQ was 0.00012 ~ 0.0109 mg/kg. Also, RSD was less than 5 %. Accuracy was 94.8 ~ 108.2% and precision was 0.14 ~ 4.30 %. FAPAS Satisfactory results were obtained below the Z-score 1.0, ensure high reliability of the analyses.

The list of natto in the sequence of decreasing Hg, Cd, Pb, As (heavy metal concentration of natto is lower than soybeans except for Hg).

P-15

Efficient Enrichment of Phosphopeptides on Digital MicroFluidics(DMF) Chip Using TiO_2-Magnetic Bead by MALDI-TOF MS.

Jinwoo Kim, Hyunji Lee, Inae Jang and Han Bin Oh*

Dept of Chemistry, Sogang University , 35 Baekbeom-ro, Mapo-gu, Seoul, 04107, Korea

Phosphorylation is one of the most important post-translational modifications(PTMs) of proteins, which modulates a wide range of biological functions and activity of proteins. The analysis of phosphopeptides is still one of the most challenging tasks in proteomics research by mass spectrometry. In this study, phosphopeptide enrichment approach on a digital microfluidic(DMF) chip was demonstrated by analyzing phosphopeptides in the tryptic digested β-casein(bovine) and Ovalbumin(chicken). This approach was made using a magnetic beads(MB)-based titanium dioxide(TiO_2)-solid phase extraction(SPE) procedure. TiO_2-MB was employed to selectively isolate phosphopeptides from tryptic digests of β-casein and Ovalbumin. Droplet operation on a chip was made by the technique of mixing the magnetic bead and the liquid droplet, the technique of collecting the magnetic beads using a neodium magnet, and the technique of separating the magnetic beads and droplet. The enriched phosphopeptides were detected using matrix-assisted laser desorption ionization time-of-flight mass spectrometry(MALDI-TOF MS). This study shows that the phosphopeptide enrichment analysis can be automated and analyzed with a small sample volume.

P-16

Analysis of total uranium and thorium in naturally occurring radioactive materials using standard addition method combined with inductively coupled plasma mass spectrometry

Hwijin Kim[1,2], Jong Wha Lee[2], Yeongran Lim[2], Sang Han Lee[3], Jung-Suk Oh[3], Yong-Hyeon Yim[2], Sung Woo Heo[2], Kyoung-Seok Lee[2,*]

[1]*Department of Bio-Analytical Science, University of Science and Technology (UST), Daejeon, 34113, Korea*

[2]*Center for Analytical Chemistry, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea*

[3]*Center for Ionizing Radition, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea*

Radioactivity from naturally occurring radioactive materials (NORMs) are potentially harmful to human health. Regulation and quality control of NORMs are important to prevent hazards from these materials. Certified reference materials (CRMs) of NORMs are typically certified for radioactivity of the constituent elements using alpha spectrometry. However, the mass fractions of the radioactive elements are indirectly obtained by conversion of the radioactivity data using specific activities. In this study, we measured the mass fractions of radioactive elements uranium and thorium in environmental samples zircon, bauxite, and phosphogypsum and compared the results obtained using alpha spectrometry. As the unavailability of isotopically enriched materials prohibits the use of isotope dilution inductively coupled plasma mass spectrometry (ID-ICP-MS), standard addition was used to determine the mass fractions in the samples using ICP-MS. The samples were processed by alkali fusion employing lithium tetraborate/lithium bromide flux and recovered in dilute nitric acid. Standard uranium and thorium solutions were spiked into the sample solutions by appropriate amounts along with thalium as an internal standard, resulting in ten measurement solutions. The determined mass fractions of uranium and thorium were 0.9–300 mg kg^{-1}, and the expanded uncertainties (at a 95% level of confidence) were estimated to be less than 3.4%. Good agreement was observed between the values from ICP-MS and alpha spectrometry, supporting the validity of the measurement results. The analytical procedure developed in this study is expected to be a basis of future research for certification of radioactive elements in NORMs.

P-17

Determining collisional cross cections (CCS) of polycyclic aromatic hydrocabon (PAH) compounds in crude oil by using PAH compounds' mixture as calibrant

Dongwan Lim[1], Kimberly L. Davidson[2], Seungwoo Son[1], Arif Ahmed[1], Matthew F. Bush[2,*], and Sunghwan Kim[1,3,*]

[1]*Kyungpook National University, Department of Chemistry, Daegu, 702-701, Republic of Korea*

[2]*Department of Chemistry, University of Washington, Seattle, Washington 98195, United States*

[3]*Green-Nano Materials Research Center, Daegu, 702-701 Republic of Korea*

Identification of aromatic compounds existing in environmental, energy, and food samples are important for scientific and industrial researches and mass spectrometry (MS) is one of the most widely used analytical techniques to study. In this study, collisional cross section (CCS) values of a set of aromatic compounds were determined and the compounds were evaluated as calibration standards. The external calibration with poly-DL-alanine and internal and external calibration with the set of aromatic compounds were performed on the ion mobility mass spectrum obtained from crude oils. It was determined that external calibration method using the set of aromatic compounds is more accurate and easier method. The improved accuracy can be explained by structural similarity between the standards and the analytes compared to those of poly-DL-alanine.

P-18

Proteomic analysis of aqueous humor biomarkers associated with diabetic retinopathy and its complications using quantitative approach

Hye Min Kim[1], Jae Won Oh[1], Jae Hun Jung[1], Kwang Pyo Kim[1], Tae Wan Kim[2]

[1]Department of Applied Chemistry, College of Applied Sciences, Kyung Hee University, Yong-in 446-701, Republic of Korea.

[2]Department of Ophthalmology, Seoul Metropolitan Government, Seoul National University Boramae Medical Center, Seoul, Republic of Korea

Diabetic retinopathy is a microvascular complication caused by diabetes and the leading cause of blindness in adults. Diabetic retinopathy has initiative stages such as non-proliferative diabetic retinopathy (NPDR), vision-threatening stages such as proliferative diabetic retinopathy (PDR), neovascularization occurring stages such as neovascuar glaucoma (NVG). Chronic hyperglycemia is a major cause of all microvascular complications derived from diabetes. However, it is difficult to predict diabetic retinopathy and its progression as the diagnostic biomarkers are not yet fully understood. In this study, we used quantitative proteomics to analyze AH (Aqueous Humor) proteins from patients with NPDR, PDR, and NVG. The aim of this study was to obtain a panel of AH proteins that were differentially expressed between NPDR and PDR and between PDR and NVG for the investigation of biomarkers and pathogenesis of the 3 serious complications. Totally about 2000 proteins were identified using a high-resolution orbitrap mass spectrometer coupled online to a nanoflow-LC system. Using both label-free quantification and TMT-based quantification, 44 differentially expressed proteins were enriched. We also validated total 49 proteins from profiling experiments and references using a triple-quadrupole mass spectrometer for quantification of targeted proteins.

P-19

Study on the determination of boron in cathode active material of lithium ion battery by ICP-MS

In-Gi Kim, Jung-Ju. Lee and H. B. Lim*

Dept. of Chemistry, Dankook University, Anse-dong, Cheonan-si, Chungcheongnam-do, Korea

Recently lithium secondary battery has been a hot issue as a power source for not only portable electronic devices but also electric motors. Among various cathode active materials, $Li(Ni_xCo_yMn_z)O_2(x+y+z=1)$ (NCM) is one of the most prominent and representative materials for high capacity and efficiency. Since the analysis of trace elements is very important for developing efficient cathode materials of NCM, the determination of trace impurities, such as Na, Mg, etc., or additive elements, such as Al, B, etc., is often required for the improvement of quality. Among them, boron is an interesting element for high efficiency of NCM in lithium ion battery. However, boron is converted into a highly volatile complex compound, it can easily be lost during sample treatment, which makes the determination difficult.

In this work, we studied the analytical method to determine boron in NCM using ICP-MS. For higher accuracy and precision, external standard, internal standard, and the standard addition method were performed for calibration and the results were compared. The coefficients of determination (R^2) for calibration curves were assessed above 0.999 and the limits of detection were as low as 0.09946 ng/mL. In addition, the uncertainty of measurement was studied for standardization, which was based on identifying, quantifying and combining all the associated sources of uncertainty separately. The contents boron in NCM sample was 0.07605% (wt. %) and the expanded uncertainties values (±0.0000097%) were obtained in our primitive estimation.

P-20

Global discovery Biomarker for Autism Spectrum Disorder (ASD) for early diagnose

Wooyoung (Eric) Jang, Kim Min Sik*

Department of Applied Chemistry College of Applied Sciences, Kyung Hee University
Yong-in City, 446-701 Republic of Korea

Autism spectrum disorder (ASD) represents a disorder related to socio-psychological and neurodevelopmental problems. Fortunately, autistic behaviors if treated in early stages the patients can live their life with normal social functions and behaviors. [4] However, there is no molecular early diagnostic marker available. There is evidence that Cntnap2 protein is related to ASD. Using Cntnap2 KO mice and utilizing proteomics method, we aim to achieve in-depth profiling of tissue proteomes of the autistic animal model. The Cntnap2 KO mouse brain was dissected to isolate hippocampus, mPFC, and cerebellum. For quantification in discovery experiments, the isobaric TMT reagents (Tandem Mass Tag) were labeled with peptides prepared from the mouse brain tissues. Quantitative protein intensities were filtered using fold change greater than 1.5 and p-value less than 0.05. These proteins that were filtered were used to carry out bioinformatics Gene Ontology analysis to find affected biological pathways by the mutation. Using volcano plot, significant proteins were identified and these proteins were further studied. Among the significant proteins from 49 significant proteins, 16 of these proteins had been shown to be related to ASD. We identified that protein Tsc1 is down-regulated and this protein is part of the mTOR biological pathway which is related to Autism. Cacna1h is up-regulated and this protein is related to calcium channel biological pathway which is correlated with ASD. The other mice samples will be analyzed. By observing similarity pattern potential biomarker will be found. Using these biomarkers, MRM qualification experiment will be proceeded using Human plasma samples. The young children's blood samples are being collected by Seoul National University Hospital. The hope for the future is that by using the non-invasive method, clinicians will be able to diagnose young patients with ASD. Continual treatment of ASD in young patients' life will allow for the patience to live a quality life

P-21

Discovery of specific common fragments on trimethylsilylated PDE-5 inhibitors for their rapid screening and confirmation by GC-MS/MS combined with extracted common ion chromatogram

Na-Hyun Park, Myoung Eun Lee, Jisu Hur, Bum Hee Kim, Jongki Hong*

College of Pharmacy, Kyung Hee University, Seoul 02447, Korea

PDE-5 inhibitor counterfeit drugs have been increasingly adulterated in supplement diets and widely distributed through internet markets and underground routes. In this study, GC-MS/MS method was developed for the screening and confirmation of 63 erectile dysfunction drugs in supplements. The trimetylsilyl (TMS) derivatization of PDE-5 inhibitors produced the characteristic fragments within similar structural moiety for sildenafil, tadalafil, and vardenafil analogues. Specific common fragments enabling to reflect their structural characteristics were observed as m/z 383, 384, and 265 for sildenafil analogues, m/z 334 and 241 for tadalafil analogues, and m/z 476, 384, for vardenafil analogues. These ions were formed through the cleavage of piperazinosulfonamide or piperazine ring for sildenafil and vardenafil analogues, and the successive losses of benzodioxole and diketopiperazine for tadalafil analogues. For the rapid screening of multiple classes of the PDE-5 inhibitor adulterants, extracted common ion chromatograms (ECICs) based on specific fragments of similar molecular moieties were attempted. These ECICs of specific ions could effectively cover PDE-5 inhibitor adulterants and new emerging counterfeit drugs. Especially, selected reaction monitoring (SRM) mode in GC-MS/MS could offer high sensitivity and selectivity for erectile dysfunction drugs derivatives in complicate matrix samples. The established method was successfully applied for the monitoring of several types of dietary supplements to protection of public health and consumer safety.

Keywords: PDE-5 inhibitors; supplement diets; screening; trimethylsilylation; extracted common ion chromatogram; GC-MS/MS

P-22

MS-based quantitation of a non human glycan in a therapeutic glycoprotein

Jaekyoung Ko[1,2], Nari Seo[1,2], MyungJin Oh[1,2] and Hyun Joo An[1,2,*]

[1]*Graduate School of Analytical Science and Technology, Chungnam National University, Korea*

[2]*Asia-Pacific Glycomics Reference Site, Korea*

Sialic acid expressed as an outer terminal units on a therapeutic glycoprotein play immunological and physiological roles such as immunological processes, hormonal response, and signal transmission. In particular, sialic acid as a N-Glycolylneuraminic acid (Neu5Gc), which is not synthesized in human due to an inactivated CMAH gene, often observed in therapeutic glycoproteins produced from mammalian cell lines. Exogenous Neu5Gc can be metabolically incorporated into human cells and the Neu5Gc antibodies which lead immune response will be produced and circulated through blood. Therefore, the determination for a non-human sialic acid of biotherapeutics produced in mammalian cell is highly required for drug's safety i.e. immunogenicity. In this study, we developed an analytical tool using mass spectrometry to selectively identify and quantify Neu5Gc in biotherapeutics including Erythropoietin, Inflixmab, and Interferon-β with high sensitivity. Each therapeutic glycoprotein was enzymatically treated with PNGase F to release N-glycans, followed by chemical hydrolysis to liberate sialic acids (Neu5Ac and Neu5Gc). The Neu5Gc was chromatographically separated from Neu5Ac on PGC column. MRM transitions and instrument parameters of UHPLC/triple quadrupole (QqQ) MS were optimized with Neu5Gc standard. The limits of detection/ quantitation (LOD/ LOQ) for Neu5Gc and the linearity between Neu5Gc concentration and MS signal for quantitation were also examined. The concentration of a non-human glycan (Neu5Gc) from various therapeutic glycoprotein content was determined at low nano mole levels. This method will be a valuable platform for not only QbD processes of biotherapeutics but also QA/QC of products.

P-23

An improved MALDI-TOF MS–based β-lactamase assay platform for clinically relevant cefotaxime resistant bacteria

Jiyeon Hong[1], Jae-Seok Kim[2] and Kyoung-Soon Jang[1,3,*]

[1]*Biomedical Omics Group, Korea Basic Science Institute, Cheongju 28119, Korea*
[2]*Department of Laboratory Medicine, Hallym University College of Medicine, Kangdong Sacred Heart Hospital, Seoul 05355, Korea*
[3]*Department of Bio-Analytical Science, University of Science and Technology, Daejeon 34113, Korea*

We demonstrate an improved MALDI-TOF MS–based β-lactamase assay platform for cefotaxime, a representative third-generation cephalosporins, resistant bacteria. Cefotaxime that was incubated with the lysates of *E. coli* exhibiting extended-spectrum beta-lactamase (ESBL) activity was modified by Girard's reagent T to introduce permanent positive charge at the carboxyl functional groups of cefotaxime, resulting in dramatic advances on the ionization efficiency and quantitativeness during MS analysis. The method was validated with clinical isolates of a variety of ESBL-producing *E. coli*. In comparison with conventional UPLC system, it showed reliable data for distinguishing cefotaxime-resistant bacteria. This improved MS-based β-lactamase activity assay platform would be utilized to more rapidly and accurately detect clinically relevant antibiotic resistant bacteria in clinical settings.

P-24

Metabolic changes in the bone tissue of aged mice with osteoporosis

Miso Nam[1,2], Geum-Sook Hwang[1,3]

[1]*Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Seoul, 03759, Korea*

[2]*Department of Chemistry, Sungkyunkwan University, Suwon, 16419, Korea*

[3]*Department of Chemistry and Nano Science, Ewha Womans University, Seoul, 03760, Korea*

Age-related osteoporosis is characterized by reduced bone mineralization and reduced bone strength, which increases the risk of fractures. We examined metabolic changes associated with age-related bone loss by profiling lipids and polar metabolites in tibia and femur bone tissues from young (5 months old) and old (28 months old) male C57BL/6J mice using ultra-performance liquid chromatography quadrupole-time-of-flight mass spectrometry. Partial least-squares discriminant analysis showed clear differences in metabolite levels in bone tissues of young and old mice. We identified 93 lipid species, including free fatty acids, sphingolipids, phospholipids, and glycerolipids, that were significantly altered in bone tissues of old mice. In addition, the expression of 28 polar metabolites differed significantly in bone tissues of old mice and young mice. Specifically, uremic toxin metabolite levels (p-cresyl sulfate, hippuric acid, and indoxylsulfate) were higher in bone tissues of old mice than in young mice. The increase in p-cresyl sulfate, hippuric acid, and indoxylsulfate levels was determined using targeted analysis of plasma polar extracts to determine whether these metabolites could serve as potential osteoporosis biomarkers. This study demonstrates that LC-MS-based global profiling of lipid and polar metabolites can elucidate metabolic changes that occur during age-related bone loss and identify potential biomarkers of osteoporosis.

P-25

Lipid profiling of human Non-alcoholic fatty liver disease (NAFLD) based on liquid chromatography/mass spectrometry

Min Kyung Lee[1,2], Youngae Jung[1], Geum-Sook Hwang[1]

[1]*Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Seoul 03759, Korea*

[2]*Dept of Pharmacy, Ewha Womans University, Seoul 03760, Korea*

Non-alcoholic fatty liver disease (NAFLD) is the most common chronic liver disease that is closely linked to obesity, insulin resistance, hyperglycaemia and hyperlipidaemia. NAFLD progression encompasses simple steatosis, Non-alcoholic steatohepatitis (NASH), fibrosis and cirrhosis. The most common NAFLD study has focused on difference between healthy individual and NAFLD patient. However, metabolic difference following liver disease progression is still unclear and distinguishing NASH from simple steatosis currently requires a liver biopsy. So, we need to find disease occurrence at early stage of NAFLD and treat properly following liver histology by non-biopsy method.

We performed a lipid profiling to find metabolic difference between healthy individual (No NAFLD), simple steatosis, NASH and altered metabolites contribute to liver disease progression. This comprehensive lipid metabolic profiling performed on 350 serum samples from humans with 65 healthy individuals, 149 simple steatosis and 136 NASH patients. Serum metabolites were analyzed using ultra-performance liquid chromatography/quadrupole time-of flight mass spectrometry (UPLC/Q-TOF MS) coupled with statistical analysis. Principal Component Analysis (PCA) and Partial Least Squares for Discriminant Analysis (PLS-DA) were performed to visualize scatter score plots.

We found metabolic difference between healthy individuals (No NAFLD), simple steatosis and NASH. Specific lipid metabolites were altered depending on NAFLD progression such as Diacylglycerol (DAG), free fatty acid (FFA), lysophosphatidylcholine (LysoPC), phosphatidylinositol (PI) and triacylglycerol (TAG). This study can be a useful tool to distinguish NAFLD progression and we can suggest different approaches to diagnosis NAFLD at early stage by non-biopsy method.

P-26

Classification of serum glycoproteins based on pattern identification in Traditional Korean Medicine (TKM) from lung cancer patients

Jinwook Lee, Wonryeon Cho*

Department of Chemistry, Wonkwang University, Iksan,54538, Korea

Cancer patients have difficulties in seeking remedies for treating symptoms based on Traditional Korean Medicine (TKM) because of its lack of standardized diagnosis. This study is a preliminary research using a proteomics approach to pattern identification of lung cancer patients for patient-specific TKM. Glycoproteins are well-known to be associated with diseases and can be used as disease biomarkers. Six plasma groups (EX, ES, EN, RX, RS and RN) from Lung cancer patients are independently analyzed through glycoproteomics approach based on the pattern identification in TKM. Glycoproteins are separated from human plasma via Lycopersicon esculentum Lectin (LEL) affinity selection on HPLC system. The separated glycoproteins are first trypsin-digested and then deglycosylated with PNGase F. The resulting deglycosylated peptides are analyzed with nLC-MS/MS and the corresponding parent proteins from the each groups are categorized for protein classification. This leads to (1) establish the standardized proteomics methodology for the pattern identification in the lung cancers patients under the framework of TKM; (2) discover lung cancer biomarkers based on the patients' pattern identification in TKM and then develop in vitro diagnostic kits for lung cancers that optimize these biomarkers to establish patient-specific TKM for further treatment.

P-27

Quantification of glycated hemoglobin in dried blood spot using isotope dilution HPLC-MS/MS

Thi Thanh Huong Tran[1,2], Ji-Seon Jeong[2,*]

[1]*Department of Bio-Analytical science, University of Science and Technology (UST), Daejeon, Republic of Korea*

[2]*Center for Bioanalysis, Division of Metrology for Quality of Life, Korea Research Institute of Standards and Science (KRISS), Daejeon, Republic of Korea*

The collection of patient whole blood on paper, known as dried blood spot (DBS), was introduced in 1963 for the screening of inherited metabolic diseases in neonates. Compared with conventional venous blood sampling, DBS sampling is less invasive method, and easy to keep and transport samples. In this study, an isotope dilution-ultra performance liquid chromatography–tandem mass spectrometry (ID-LC-MS/MS) was investigated to quantify glycated hemoglobin (HbA_{1c}) in DBS. HbA1c has been widely used to assess glycemic control in diabetes mellitus. We used only one disc of 3.2-mm diameter for quantification of HbA1c, and that is about 3 μL of whole blood.

The bias factor caused by underestimation of area was strictly investigated and revised with area calculation software. The results were compared with areas by manual technique using ruler, or nominal value of puncher. The accuracy and precision of measurement showed sufficient results in the optimized sample treatment conditions. The variations of different position within a spot showed acceptable results (<3 %). As some unstable compounds in blood are easily susceptible to harsh environmental conditions, we examined the short-term effect of temperature (1-50 ºC) and humidity (<30% and 30- 70%) during a period of 10 days on the sample stability. The optimized analytical method was applied to real blood samples, and results showed excellent comparability with those of venous methods. This study provides reliability to constitute a practical procedure for a rapid measurement of HbA_{1c}.

P-28

Interlaboratory validation of LC–Triple Quad MS/MS for the quantification of enrofloxacin in chicken meat

Joo Hee Chung[1], Kun Cho[2], Seongnyeon Kim[2], So Hyeon Jeon[3], Jueun Lee[3], Yun Gyong Ahn[3]

[1]Seoul Center, Korea Basic Science Institute, Seoul, 02855, South Korea
[2]Biomedical Omics Group, Korea Basic Science Institute, Ochang, 28119, South Korea
[3]Western Seoul Center, Korea Basic Science Institute, Seoul, 03759, South Korea

Enrofloxacin is one of antibiotics as a class of fluoroquinolones and commonly used in intensive poultry farming to treat chronic respiratory disease, colibacillosis, and fowl cholera. However, the use of fluoroquinolones and other antibiotics for food-producing animals is now regulated and many countries have established maximum residue limits (MRLs) in their food products to safeguard human health from the risks of multi-resistant and aggressive bacteria. Accordingly, a validated analytical method as well as certified reference materials (CRM) for the evaluation of the method are required. Recently, CRM (KRISS CRM 108-03-003) have been developed by Korea Research Institute of Standards and Science. They have presented the concentration of enrofloxacin for CRM through the measurements of ten bottles in 10 g portions were taken randomly from the bulk meats ready-made in powders. The concentrations of the measurement results of ten bottles were calculated by one point calibration with isotope-ratio matching. The adoption of analytical method can be officially approved on the basis of a method's performance in the inter-laboratory collaborative studies and the comparison of these results is an external way of assuring quality control among laboratories concurrently. Thus, three laboratories were involved in an inter-laboratory collaborative study to test for the method evaluation using the CRM of enrofloxacin in chicken meat. The common method, a liquid–liquid extraction combined with clean-up procedure based on solid-phase extraction (SPE) followed by LC-MS/MS has been performed by three individual laboratories. Linearity, limit of detection (LOD) and limit of quantification (LOQ) were assessed and the laboratory variance of results for CRM was compared. The inter-laboratory comparison results showed approximately 95 % of z-scores have fallen within two standard deviations which is commonly designated as an acceptable range.

P-29

Stable carbon isotope analysis of organic sediments. is it possible to analyze at the molecular level?

Seungwoo Son, Donghwi Kim, Sunghwan Kim*

Department of Chemistry, Kyungpook National University, Daegu, Republic of Korea

Stable carbon isotope ratio ($^{13}C/^{12}C$) has been widely used in geochemistry, paleoclimatology and paleoceanography researches. It is well known that C_3 and C_4 plants have different isotope signatures. The reason for the difference can be attributed to difference in reaction rates differs caused by mass difference of ^{13}C and ^{12}C containing molecules. The stable carbon isotope ratios of organic sediments have been used to study geochemical origin and correlation between different area. Generally, stable isotope analysis of carbon is performed by burning an aliquot of material and analyzing the generated CO_2 gas by using specially designed sector mass spectrometry. Quantitative isotope ratio data can be obtained by using this method. However, the method is limited to obtain the ratio at the molecular level. Therefore, in this study, ultra-high resolution mass spectrometry has been evaluated for feasibility of molecular level ^{13}carbon isotope analysis. For the evaluation of crude oils, they were analyzed by (+) atmospheric pressure photo ionization Fourier transform ion cyclotron resonance mass spectrometry (APPI FT-ICR MS). And For the evaluation of humic acids, they were analyzed by (-) electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (ESI FT-ICR MS). In crude oils data, isotope ratio of sulfur class compounds were evaluated by using the equation, as well as humic acid data isotope ratio of oxygen compounds were evaluated by using same method. The obtained data were compared between organic sediments originated from different locations. The isotope ratio calculated from FT-ICR MS data were compared with the bulk ratio obtained with Elemental Analyzer–Isotope ratio mass spectrometry (EA-IRMS).

P-30

Qualitative determination of steviol and its glycosides in *Stevia rebaudiana* by liquid chromatography tandem mass spectrometry

Seongnyeon Kim[1], Moo Sung Kim[2], Heehoon Jung[2], Kun Cho[1]

[1]*Biomedical Omics Group, Korea Basic Science Institute, Ochang, Chungbuk, 28119, Korea*

[2]*R&D center, Macrocare Tech Co., Ltd., 32, Gangni 1-gil, Ochang-eup, Cheongwon-gu, Cheongju-si, Chungcheongbuk-do, 28126, South Korea*

Stevia rebaudiana leaves consist of non-cariogenic and non-caloric sweeteners (steviol-glycosides) whose consumption could utilize useful effects on human health. The object of this research was to develop and verify liquid chromatography methods with electrospray ionization mass spectrometry (LC-ESI/MS) to evaluate steviol-glycosides or steviol in Stevia leaves. Based on the specific fragmentation of these compounds, an LC–MS/MS method was developed with the aim of quantifying analytes in plant material. The possibility of applying this method was verified in the analysis of stevioside and rebaudioside A from Stevia plants. Finally, on the basis of this metabolomic targeted approach, the results acquired for the samples were handled by Principal Component Analysis, identifying specific genotypic differences based on the geographic origin of the plants.

P-31

Determination of fumonisins in maize using isotope dilution-liquid chromatography tandem mass spectrometry

Yosi Aristiawan[1,2], Kihwan Choi[1,*], Byungjoo Kim[1,*]

[1]*Center for Analytical Chemistry, Korea Research Institute of Standard and Science, Daejeon, 34113, Korea*

[2]*Department of Bio-Analytical Science, University of Science & Technology (UST), Daejeon, 34113, Korea*

Fumonisins are mycotoxins from a few species of fungi in the genus Fusarium causing a variety of diseases of both animals and humans. These fungi are commonly found in corn through systematic transfer from their roots. To detect fumonisin occurrence in corn or corn-based food, proper and decent analytical methods are required. In this study, we developed an analytical method for the determination of three types of fumonisins (FB_1, FB_2, and FB_3) in corn flour based on isotope dilution-liquid chromatography tandem mass spectrometric (ID-LC/MS/MS) method. Fumonisins were extracted from corn flour and the extracts were purified with immunoaffinity column before introduced to LC/MS/MS instrument. The experimental parameters, such as kind of extraction solvent, clean-up column, and solvent-to-sample ratio were studied. Solubility and extraction efficiency was better when phosphate buffered saline (PBS) was used as extractant compared to acetonitrile-water or methanol-water solutions. A post-column infusion system was used to investigate the clean-up efficiency of immunoaffinity columns. The amount of fumonisins bound to corn flour matrix could be extracted with PBS. Thus, hydrolysis was not necessary for fumonisin analysis in this study. Selected reaction monitoring (SRM) was employed in the mass spectrometer at m/z 706.5 ⟶ 334.4 (FB_1) and m/z 706.4 ⟶ 336.3 (FB_2 and FB_3). Through the gradient elution of 5 mM ammonium formate in water containing 0.1% formic acid and 5 mM ammonium formate in methanol containing 0.1% formic acid on C18 column, FB_1, FB_2, and FB_3 were successfully separated. The proposed method provided a detection limit range from 0.4 to 0.5 μg/kg and a limit of quantification range from 1.2 to 1.9 μg/kg. Following validation of the developed method, fumonisin level was investigated with additional corn-based products.

P-32

Tracing Fragrance Chemicals in Cosmetics by GC-MS

Chae Won Lee[1], You Ri Choi[1], Ji Eun Kim[1], Min Seo Park[2], Sang Yun Han[1,*]

[1]*Department of Nanochemistry, Gachon University, Seongnam, Gyeonggi (13120), Republic of Korea*

[2]*Department of Bionanotechnology, Gachon University, Seongnam, Gyeonggi (13120) Republic of Korea*

We, a group of undergraduate students, were interested in what and how much fragrance chemicals were involved in commercial cosmetic products such as shampoos and hand creams. For characterization and quantification of chemical compounds in the products, we employed GC-MS analysis. We first surveyed volatile chemicals arising from the products using the headspace sampling method. As a result, we could characterize various fragrances including limonene, linalool, and eucalyptol, which are contained in the commercial products. To quantify the detected fragrances, we did literature study and prepared our own protocols for the experiments. Using the protocols we prepared, we carried out extraction of fragrance chemicals and purified them using silica columns. The samples were then subject to quantification by GC-MS using the standard addition method, of which levels were determined to be about ~ nl/g. In this study, we could learn how to plan and peroform an experiment that would answer our research question as well.

P-33

Structural identification of an enzymatic oxidation product of a model lignin compound by tandem mass spectrometry

Woo-Young Song, Youri Yang, Sunil Ghatge, Hor-Gil Hur* and Tae-Young Kim*

School of Earth Science and Environmental Engineering, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju, 61005, Korea

Lignin, the second most abundant biopolymer on earth, is a promising source of industrial phenolic compounds. In spite of the increasing interest in structural analysis of lignin enzyme degradation product, there is hardly any method available for the full structural characterization of lignin oligomers higher than trimers, mainly due to the complicated nature of the lignin structure, possessing numerous linkage types. A tandem mass spectrometric method to identify the linkage type and structure of the lignin oxidation product has been developed and applied to the analysis of an enzyme oxidation product of a model lignin compound, guaiacylglycerol-β-guaiacyl ether (GGGE).

To investigate oxidative enzyme activity of a novel laccase on the model lignin compound, GGGE was treated with laccase and analyzed by UV high performance liquid chromatography quadrupole time-of-flight tandem mass spectrometry (UV-HPLC-Q-TOF MS/MS). The oxidation product was detected as a single UV absorption peak at 280 nm and subjected to untargeted MS/MS. From the linkage type-specific m/z differences of the fragment ions, β-aryl ether linkage was commonly identified in both GGGE and its oxidation product. By building up the structure from the β-aryl ether backbone based on the fragment ion information, biphenyl tetramer and/or biphenyl ether tetramer were suggested as the possible structures of the unknown oxidation product. The tandem mass spectrometric information and the UV absorption shift to a higher wavelength implied the biphenyl tetramer as the more reliable structure for the oxidation product. For the formation of biphenyl tetramer structure, a charge-driven fragmentation mechanism was proposed. As a result, MS/MS analysis of the GGGE oxidation product suggested that the novel laccase catalyzes radical coupling of GGGE to form a biphenyl tetramer.

P-34

Enhancement of polypeptide ladder detection signal using derivatization method

Dabin Lee, Yeoseon Kim, Sol Han, and Jeongkwon Kim*

Department of Chemistry, Chungnam National University, Daejeon, 34134, Korea

Protein De novo sequencing is a method to confirm peptide sequence without assistance of a sequence reference. Usually tandem mass spectrometry and Edman degradation are used to obtain protein sequence infromation. In tandem mass spectrometry, the sequence is determined using the mass difference between the two fragment ions to calculate the mass of the amino acid residue on the peptide backbone. The Edman degradation cleaves off the N-terminal amino acid of the protein. The sequence is determined by observing the separated amino acid.

Here we apply microwave-assisted weak acid hydrolysis to De novo sequencing. Proteins were made into polypeptide ladders using 1-hr microwave-assisted weak acid hydrolysis with a mixture of dilute HCl and 2% FA. C-terminals of aspartic acids are cleaved by 2 % FA and polypeptide ladders are generated by dilute HCl. Such as De novo sequencing using tandem mass spectrometry, the sequence information on both C-terminal and N-terminal can be identified using the mass difference between the two polypeptide ladders to calculate the mass of the amino acid residue on the peptide backbone.

In the case of polypeptide ladder, the signal is low because one peptide is split into several ladders. There is a limit to the sequencing. We try to improve the signal of polypeptide ladders through guanidination, which is known to enhance the signal of peptides. We are currently conducting an experiment to confirm the effect of signal enhancement by guanidination using O-methylisourea.

P-35

Lipid profiling of lipoproteins from patients with mild cognitive impairment and Alzheimer's disease by asymmetrical flow field-flow fractionation and nUPLC-ESI-MS/MS

San Ha Kim, Joon Seon Yang, Jong Cheol Lee and Myeong Hee Moon*

Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul 03722, Korea

Alzheimer's disease is known as a major cause of dementia and is known to be caused by the accumulation of amyloid-beta plaques in brain leading to dysfunction in cognitive abilities. Mild cognitive impairment (MCI) refers to a translational state between cognitive changes of normal aging and AD and it has been reported that up to 80% of MCI progressed to AD during 6 years. It is known that amyloid-beta, a major cause of Alzheimer's disease, is affected by plasma lipoproteins. Thus, studying lipid changes within the lipoproteins of patients with mild cognitive impairments and Alzheimer's disease is an important role in finding potential biomarker candidates.

In this study, lipids from human plasma samples of age-matched controls, patients with mild cognition impairment, and Alzheimer's disease patients were analyzed. Lipoproteins were size-sorted by using asymmetrical flow-field flow fractionation and lipids which were extracted from the collected fractions of high-density lipoprotein (HDL), low-density lipoprotein (LDL), and very-low density lipoprotein (VLDL) were quantitatively analyzed by using nanoflow ultrahigh-pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUPLC-ESI-MS/MS). A total of 363 lipid species were identified and quantitation.

P-36

Effect of temperature on microwave-assisted tryptic digestion of protetins

Yeoseon Kim, Dabin Lee, Sol Han, and Jeongkwon Kim*

Department of Chemistry, Chungnum National University, Daejeon, 34134, Korea

Protease is used in protein digestion. Trypsin, one of the most common proteases, cleaves exclusively at C-terminus of amino acid Lysine and Arginine in proteins. Moreover, organic solvents are often added for the trypsin digestion to modify native proteins to denatured proteins, and this tendency makes it effective to digest proteins. In this study, we investigate the digestion efficiency of trypsin for the digestion of bovine serum albumin and horse skeletal muscle myoglobin. Sample solutions were prepared with different amounts (0 %, 10 %, and 20 %) of acetonitrile and digested using trypsin with a help of microwave irradiation. Digested peptides were analyzed using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry and the sequence coverage and the intenstiy or the protein peak were used as indicators of trypsin activity.

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P-37

Study of cross-interaction between amyloid β 1-42 and 1-40 in the early stage of fibrillation using ESI-MS

Chae-Eun Heo, Hugh I. Kim

Dept of Chemistry, Korea University, Seoul 02841, Republic of Korea

Amyloid-β 1-42 (Aβ42) and 1-40 (Aβ40) peptides, whose self-assembly process has been linked with the formation of amyloid plaques in Alzheimer's disease, exist as a mixture in human fluids. For this reason, heteromeric self-assembly of Aβ42 and Aβ40 has been widely investigated to understand the influence of this mixture in Aβ fibrillation. However, understanding the role of heteromeric self-assembly in Aβ fibrillation is a challenge owing to the heterogeneous cross-interactions between Aβ42 and Aβ40. Herein, we demonstrated the influence of the cross-interaction of Aβ42 and Aβ40 in the early stage of fibrillation using electrospray ionization mass spectrometry (ESI-MS) and drift tube ion mobility spectrometry (DTIMS) along with solution small-angle X-ray scattering (SAXS) and molecular dynamics (MD) simulations. In the mixture of Aβ42 and Aβ40, Aβ42 has a slight preference for homo-oligomerization versus hetero-oligomerization with Aβ40 (1~2 fold) when forming small oligomers (from dimer to tetramer) in the early stage of the fibrillation. However, the cross-interaction is gradually attenuated as oligomerization proceeds because of the different conformations in Aβ42 and Aβ40 assemblies. Consequently, the competitive self-assembly of Aβ42 and Aβ40 can disturb homo-oligomerization of Aβ42 in the early stage of fibrillation, whereas Aβ42 and Aβ40 species prefer the independent self-assembly after the early stage.

P-38

Discovery of metabolite candidates for elapsed time analysis of bloodstain

Ae Eun Seok[1], Jiyeoug Lee[2], You-Rim Lee[1], Arum Park[1], Sora Mun[1], Hyo-Jin Kim[2], Yoo-Jin Lee[2], Hee-Gyoo Kang[1,2]

[1]Laboratory of Signal Transduction and Disease Biomarker Discovery, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, 34824, Korea
[2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Gyeonggi-do, 13135, Korea

Bloodstain is produced by the blood left at the crime scene, and it contains a lot of information. The elapsed time since the bloodstain was formed is called the age of a bloodstain, which is very important because it can identify the time of the attack. Although various methods have been reported to confirm the elapsed time of bloodstain, it has not yet been applied to the forensic analysis. Therefore, we used a mass spectrometer to analyze the metabolite of bloodstain to identify the new age of bloodstain markers. In this study, blood samples were collected from 6 healthy volunteers and bloodstain was prepared using filter paper. Metabolites were extracted from 0, 7, 14, and 21 days after collection and analyzed using HPLC Q-TOF. An average of 580 (range from 378 to 857) molecular features was identified in mass spectrometry (MS) data, and an average of 388 (range from 256 to 537) molecular features was identified in tandem mass spectrometry (MS/MS) data. In addition, it was confirmed that metabolites significantly increased or decreased at 7 days, 14 days, and 21 days were compared to day 0. Multivariate statistical data analysis (PCA, PLS-DA, and OPLS-DA) was performed to find candidates for the age of a bloodstain. The candidates selected through statistical analysis were identified by MSMS spectrum matching of METLIN database. We have found that changed metabolites according to elapsed time and the bloodstain as time passed can be classified with them. Therefore, it will be possible to estimate the elapsed time of the blood which is obtained at the scene of the incident.

Keyword: Metabolite, Elapsed time, Bloodstain, Forensic, HPLC Q-TOF

P-39

Discovery of internal standard metabolite for accurate chemical analysis of bloodstain

You-Rim Lee[1], Jiyeong Lee[2], Ae Eun Seok[1], Arum Park[1], Sora Mun[1], Hyo-Jin Kim[1], Yoo-Jin Lee[1], Hee-Gyoo Kang[2]

[1]Laboratory of Signal Transduction and Disease Biomarker Discovery, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon 34824, Korea
[2]Department of Biomedical Laboratory Science, College of Health Science, Eulji University, Seongnam 13135, Korea

Accurate analysis of a blood stains which found at the crime scene is extremely important in reconstructing the crime. Because the bloodstain is evidence that is closely related to the occurrence of the crime. Currently, chemical analysis of bloodstain has been actively studied from many perspectives. However, it has problems to apply the results of the research to the field. One of the problems is the unknown amount of initial blood volume of bloodstain. For example, index materials of bloodstain age change based on initial quantities. Because of unknown amount of initial blood volume, we couldn't apply the research results to the field. In order to solve these problems, we have found an internal standard metabolite that maintains a consistent amount of initial blood volume even after the passage of time. In this study, the sample for making bloodstain was collected from six healthy men and women in their 20s who did not take any medicine at least since a week ago. Using the HPLC-QTOF, metabolic profiling of bloodstain was performed according to the bloodstain age. We filtered metabolites that revealed on all samples. Among them, we selected metabolites with p-value <0.05. Then 36 metabolites were obtained by filtering which of selected metabolites had changed from the day 0 to the day 21 of less than 2-fold. The CV values were calculated from the abundance of all samples. Six metabolites with less than 5% CV was obtained. The candidate metabolites for internal standard found in this study will serve as a reference point for changes of the index materials and help prior study results of bloodstain analysis to be applied in the field. It can also be provided as a more objective clue.

P-40

Proteomics analysis of LNCaP reveals bicalutamide enhances cellular pathways associated with fodrin-mediate apoptosis through calpain

Sora Mun[1], Jiyeong Lee[2], Arum Park[2], Doojin Kim[2], Byung Heun Cha[2], AeEun Seok[2], You-Rim Lee[1], Hyo-Jin Kim[1], Yoo-Jin Lee[1], Hee-Gyoo Kang[1,2]

[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, Korea.

[2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Korea.

Prostate cancer is the most common cancer in men, and before it progresses and metastasizes, the anticancer drug bicalutamide is often administered to patients. It can develop into the androgen-independent form, which is a serious progressive and metastatic state. Many cases of androgen-dependent prostate cancer develop resistance during treatment with bicalutamide. Therefore, the effect of bicalutamide on androgen-dependent LNCaP prostate cancer cells is of clinical interest. The aim of this study was to demonstrate the effects of the anticancer drug bicalutamide on LNCaP prostate cancer cells by using a proteomics approach. Based on the results, we identified > 2-fold differentially expressed proteins, and 347 proteins were differentially expressed between the normal RWPE-1 prostate cells treated with androgen and LACaP cells treated with androgen. Furthermore, 314 proteins were differentially expressed between the LNCaP and LNCaP-Bic groups. The apoptosis pathway associated with differentially expressed proteins was shown in the Kyoto Encyclopedia of Gene and Genome (KEGG) pathway mapper. The KEGG pathway mapper results revealed that the fodrin-mediated apoptosis pathway is associated with the actions of bicalutamide and western blotting was performed to validate these results.

Keyword: Proteomics, Prostate, LNCaP, Bicalutamide, Apoptosis

P-41

Proteomics Analysis of Individual Serum Samples of Large Artery Atherosclerosis Stroke Patients and Healthy Subjects

Jiyeong Lee[1], Arum Park[1], Sora Mun[2], You-Rim Lee[2], AeEun Seok[1], Hyo-Jin Kim[2], Yoo-Jin Lee[2], Hee-Gyoo Kang[1,2]

[1]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Korea.

[2]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, Korea.

Ischemic stroke is classified into several subgroups based on causes. Large artery atherosclerosis is known as a major cause of ischemic stroke. Many studies have been reported that large artery atherosclerosis is closely associated with inflammation and several inflammation markers were also increased in patients with large artery atherosclerosis. However, there is no exact diagnostic marker for large artery atherosclerostic stroke. Most of studies have analyzed to identify novel biomarker in various disease using pooled serum samples. However, these studies can lead to biased results. Our aim is to analyze individual serum sample instead of pooled serum sample. 52 patients and 43 healthy subjects are used for biomarker of large artery atherosclerosis stroke. Quantification of identified 514 serum proteins were performed by SWATH-MS acquisition. As a result, differentially expressed proteins by more than 2 fold were 149. The result of functional analysis showed that the differentially expressed proteins are associated with alternative complement pathway-related immune response and positive regulation of tolerance induction to nonself antigen. The comparative analysis of serum proteins in patients with large artery atherosclerosis stroke and healthy subjects helps to understand pathophysiology of large artery atherosclerosis. We expect that inflammation-related proteins will distinguish subtype of stroke from healthy subjects.

P-42

Effective cleanup of trace diarrhetic shellfish poisoning toxins in high-lipid bivalves and their simultaneous determination by UPLC-ESI-MS/MS combined with time segment polarity switching

Myoung Eun Lee[1,+], Na-Hyun Park[1,+], Jeongmi Lee[2], Yong Seok Choi[3], Jongki Hong[1,*]

[1]*College of Pharmacy, Kyung Hee University, Seoul 02447, Korea*
[2]*School of Pharmacy, Sungkyunkwan University, Suwon 16419, Korea*
[3]*College of Pharmacy, Dankuk University, Cheonan 31116, Korea*

The development of a reliable analytical method for determining biotoxins levels in bivalves is important for the risk assessment of sea food. However, analysis of these toxins in high-lipid bivalves has several limitations due to the coexistence of lipid matrices, low biotoxin concentrations, and the different physiochemical properties of the various biotoxins. In this study, UHPLC-MS/MS method combined with an effective cleanup process (freezing-lipid filtration and solid-phase extraction) was developed for reliable quantification of six biotoxins in high-lipid bivalves. To eliminate lipid components after sample extraction, freezing-lipid filtration was applied to achieve lipid removal efficiency of approximately 91%. For further cleanup, a Strata-X solid-phase extraction cartridge was applied to separate the biotoxins from any remaining interfering compounds. Subsequently, trace biotoxins with acidic and neutral properties were determined simultaneously and sensitively by UHPLC-MS/MS using time segment polarity switching. Validation tests using a certified reference material and spiking experiments showed this method to be acceptable, with a relative standard deviation of < 14.44% and limits of quantitation of 0.63-3.08 ng/mL. The developed method was successfully applied to quantify biotoxins in 40 oyster and mussel samples collected from Korean fishery markets, ensuring sea food safety.

Keywords: bivalves, diarrhetic toxins, freezing-lipid filtration, time segment polarity switching mode, UHPLC-ESI-MS/MS

P-43

Rapid lipid extraction using superabsorbent polymers for mass spectrometry

Geul Bang[1], Yeong Jun Yu[1,4], Jeong Ah Kim[1,2,*], Young Hwan Kim[1,2,3]

[1]Biomedical Omics Group, Korea Basic Science Institute, Chungbuk 28119, Republic of Korea.

[2]Department of Bio-Analytical Science, University of Science and Technology, Daejeon 34113, Republic of Korea.

[3]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon 34134, Republic of Korea.

[4]Program in Micro/Nano System, Korea University, Seoul 02841, Republic of Korea.

In this study, a simple and rapid lipid extraction method is introduced. The effective lipid extraction from biological systems with a minimization of the matrix effect is important for the successful qualitative and quantitative analysis of lipids using mass spectrometry. We have devised the simple, rapid, and efficient lipid extraction method using super absorbent polymers (SAPs) for the purpose of isolating lipids from biological fluids. The SAPs method conducts similar or better recoveries of species of most all major lipid classes compared with the Folch method. The SAP method was applied to lipid extracts from complex biological samples, demonstrating that it can be powerfully utilized for fast (<3 min) preparation of lipids compared to the Folch method.

P-44

Selective screening of sulfonamides in supplements by UHPLC-Q/TOF-MS combined with high-resolution extracted common ion chromatogram and neutral loss scan

Nam-Yong Ki, Na-Hyun Park, Jisu Hur, Ina Choi, Jongki Hong*

College of Pharmacy, Kyung Hee University, 26 Kyunghee-daero, Dongdaemun-gu, Seoul 02447, Korea

Growing number of the sulfonamide adulteration in supplements has become a global problem due to their wide distribution and serious negative health effect. In this study, UHPLC-high resolution (HR) mass spectrometry method was developed for selective screening of 35 sulfonamides in supplements. Extraction of sulfonamides from dietary supplements was performed by simple pH control liquid-liquid extraction taking consideration into sulfonamide's unique properties. The separation of 35 sulfonamides was effectively achieved with solid inner core of shell particles C18 column within 7 min using 10 mM ammonium acetate in water (at pH 8) and acetonitrile. From the MS/MS spectra of sulfonamides, common ions (*m/z* 77.9655 $[SO_2N]^-$and *m/z* 79.9812 $[SO_2NH_2]^-$) and neutral loss fragments (HCl and SO_2) were found. HR-extracted common ion chromatograms (HR-ECICs) and neutral loss scan (NLS) could enable to selectively screen the sulfonamides in various types of supplements. Also, these characteristic HR fragments based on narrow mass window within mass tolerance ±5 ppm could cover targeted as well as new emerging sulfonamide class drugs and avoid false positive or negative results in dietary supplements. Overall calibration curves within dynamic range for all targets were shown to be linear correlation coefficient R^2>0.995 and limits of detection (LOD) ranged 0.04-11.18 ng/mL for all sulfonamides. The developed method will be helpful for the protection of the abuse of sulfonamide diuretics and anti-diabetics in dietary supplements, ensuring public health and consumer safety.

P-45

Absolute quantification of human growth hormone and brain natriuretic peptide-32 from human plasma using iCCM-based isotope dilution mass spectrometry

Sun Young Lee[1,2], Jongki Hong[2], Dukjin Kang[1]

[1]*Center for Bioanalysis, Division of Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 305-340, Korea*

[2]*College of Pharmacy, Kyung Hee University, Seoul 130-701, Korea*

Isotope dilution mass spectrometry (ID-MS) has been used as a primary method for the absolute quantitative determination. Although the conventional methods in quantitative proteomics, such as the absolute (e.g., synthetic proteins or peptides) or relative quantifications (e.g., ICAT, mTRAQ), have been considered as a reliable approach in shotgun proteomics, these methods have unfortunately several bottlenecks such as imperfect labeling, and time consumption of labeling for proteome samples. To improve above-mentioned problems, we applied the carbamidomethylation-based isotope labeling (iCCM) for absolute quantification of human growth hormone (hGH) and brain natriuretic peptide-32 (BNP-32) in human plasma in this study. In order to evaluate the iCCM labeling for absolute quantification, plasma sample was first labeled with iodoacetamide (IAA) as carbamidomethylation (CM), while both hGH and BNP-32 standards were isotopically alkylated with IAA isotope (IAA-13C2D2) as iCCM, followed by spiking those iCCM-labeled standards to plasma sample labeled with CM. The resulting plasma sample was directly performed tryptic digestion and subsequently applied to nLC-ESI-MS/MS analysis so as to obtain the absolute amounts of both hGH and BNP-32. In conclusion, iCCM-based ID-MS provides the simple, rapid, and high reproductive method for the assessment of the ratio of CM/iCCM, resulting in absolute quantification of hGH and BNP-32.

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Glycomic Investigation of Human Saliva for Forensic Application

Jinyoung Park [1,2], Seunghyup Jeong[1,2], Bum Jin Kim[1,2] and Hyun Joo An[1,2,*]

[1]Graduate School of Analytical Science and Technology,
Chungnam National University, Daejeon
[2]Asia-Pacific Glycomics Reference Site, Chungnam National University, Daejeon

Saliva often encountered at crime scenes is one of the most valuable resource for criminal identification or post-mortem interval estimation. However, the identification of saliva is quite challenging because most saliva has been found as a dry spot with very low concentration at crime scene. In addition, up to now, there is no any biosignature to differentiate human saliva from other human fluids and animal saliva. In previous study, we developed an analytical platform using glycomic approach to identify human saliva. We found that the presence of highly fucosylated N-glycans with significant abundances was saliva-specific feature to identify human saliva from other body fluids. Herein, we have developed and streamlined glycomics-based forensic platform using dried saliva spot (DSS) as a sampling technique for saliva samples. Briefly, dried saliva were prepared by spotting of human saliva on a protein saver card. N-glycans were released by PNGase F from saliva and enriched by PGC-SPE. Then, saliva N-glycans were characterized by nano LC/Q-TOF MS. In order to apply to forensic field, we compared N-glycans from liquid and dried saliva. Fifty N-glycan compositions were commonly identified and represent high correlation (R = 0.96). Additionally, highly fucosylated N-glycans, specific feature of human saliva, were equally observed from glycan profiles in DSS with similarity even in a trace amount. These studies can be useful to expand glycomic-based method to forensic science.
(1,496/1,500)

P-47

Construction of mouse brain glycome library using LC/MS and MS/MS

Jaekyung Yun[1,2], Jua Lee [1,2] and Hyun Joo An[1,2,*]

[1]Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea
[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea

Glycosylation on neuronal cell surface plays an important role in neuro-biological functions including synaptic plasticity and memory formation. Despite its biological importances, molecular-level investigation into brain glycome has remained in relative uncertainty due to the lack of effective analytical methods. In this study, a highly sensitive MS-compatible method for glycan/glycolipid extraction from brain tissue was combined with structure-specific nano-LC/MS and MS/MS to build up brain glycome library including N- and O-glycans and gangliosides. Briefly, N-glycans were enzymatically released by PNGaseF, while O-glycans were concentrated by beta-elimination method. Gangliosides were extracted based on modified Folch method. Purified and enriched glycans and gangliosides by SPE were identified and quantified by positive ion mode of nano-LC PGC Chip/Q-TOF MS and negative ion mode of nano-LC C18 Chip/Q-TOF, respectively. The biosynthetic library of mouse brain glycome was constructed using about one hundred glycans and 70 gangliosides with brain-specific glycans characterized by tandem MS using diagnostic fragment ions. The constructed library of mouse brain glycome was applied for monitoring glycome alteration in various neurobiological environments including different developmental stages and KO conditions (Maneal, Galnt13, St8sia3) with high speed and accuracy. This approach could be useful as the informative data for glycome study related the specific neurodiseases.

Keyword: Glycans, Ganglioside, LC/MS, Mouse brain

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LC/MS-based quantitative strategy to determine O-glycan expression in GALNT13 KO mouse brain

Sowon Mun[1,2], Jaekyung Yun[1,2], Jua Lee[1,2] and Hyun Joo An[1,2,*]

[1]*Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea*
[2]*Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea*

Although mammalian brain O-glycans account for only small amounts (~1%) of total brain glycans, it is closely related to neuro-biological processes such as synaptic plasticity and memory formation. Although GALNT (Polypeptide N-acetylgalactosaminyltransferase) is a major enzyme responsible for the synthesis of Tn antigen epitope in neurons, little is known about the association of GALNT expression with physiological and pathological brain functions. In this study, we compared brain O-glycan profiles obtained from GALNT13 KO mouse and wild type mouse (C57BL/6J), respectively in order to figure out specific biological functions of GALNT13 which is one of GALNT family. Briefly, brain tissues were grinded and sonicated for homogenization. Membrane was extracted using ultracentrifuge for O-glycan enrichment. O-glycans were chemically liberated by β-elimination from homogenized brain tissue., Purified and enriched O-glycans using PGC-SPE were chromatographically separated and identified by PGC(column) UPLC coupled with Q-TOF mass spectrometer. Structure information of O-glycans were obtained by tandem MS. This study would provide useful information on brain O-glycome which has languished in relative obscurity.

Keywords : Brain, GALNT13, LC-MS, O-glycan

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Proteomic Profiling of Tissue-based Map of the Canis (Beagle)

Na-Young Han[1,*], Jong-Moon Park[1], Jongho Jeon[1], Je-Yoel Cho[3], Hookeun Lee[1,2]

[1]*Gachon Institute of Pharmaceutical Sciences, Gachon College of Pharmacy, Gachon University, 534-2 Yeonsu 3-dong, Yeonsu-gu, Incheon 406-799, Republic of Korea*

[2]*Gachon Medical Research Institute, Gil Medical Center, Incheon 405-760*

[3]*Department of Biochemistry, BK21 Plus and Research Institute for Veterinary Science, School of Veterinary Medicine, Seoul National University, Seoul, 151-742, Korea*

Environment factors are significantly correlated with manifestations of pathogenesis. Profile of proteins of beagle organ tissue by mass spectrometry (MS) is necessary to early diagnosis of human disease by companion animal. Through proteomic analysis, we found 10,498 protein groups and 16,273 proteins in the database that has 28,946 proteins in Canis lupus familiaris of species. Based on this result, the identified protein information enables to utilize as beagle proteome library. In statistical analysis, the result was found 143 tissue enriched proteins in 12 organ tissue samples. We suggest that these tissue enriched proteins could be biomarkers of organ specific disease. Notably, for each organ tissue, number of identified protein groups was more than 3000 and the total proteins were covered in 56.22% of beagle protein database. In addition to the beagle protein library, major benefits are now being made in companion medicine spilling over into developments for human healthcare.

P-50

Site-specific characterization of N- and O-glycoproteins in human and mouse plasma using LC-MS/MS and I-GPA search system

Hyun Kyoung Lee[1,2,*], Ju Yeon Lee[1], Gun Wook Park[1], Jin Young Kim[1] and Jong Shin Yoo[1,2]

[1]Korea Basic Science Institute, O-chang Cheongju, Korea
[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea

Mouse has been used as an animal model for scientific research owing to its physiological similarity to human. However, their N- and O-glycosylation of glycoproteins showed many differences between mouse and human. Usually glycosylation is directly involved in various biological process and plays crucial role in human diseases due to their unusual biological sensitivity. Therefore, the site-specific characterization of glycosylation in model mouse is necessary in order to investigate progression of disease.

This study provided comparison of the site-specific N- and O-glycosylation between human and mouse plasma using LC-MS/MS with I-GPA (Integrated GlycoProteome Analyzer) search system[1]. The site-specific glycosylation between human and mouse has three differences in plasma. First, the sialic acid of N- and O-glycopeptides was almost entirely Neu5Gc in mouse plasma, while in human plasma was Neu5Ac. Second, O-acetylated NeuGc of N-glycopeptides was identified in mouse plasma only. Third, antennal HexNAc-NeuGc of N-glycopeptides was specifically identified from several glycoproteins in mouse plasma only. In conclusion, our study has provided a comprehensive overview of the site-specific N- and O-glycosylation of human and mouse in plasma.

Reference

1. Gun Wook Park and Jin Young Kim et al., *Scientific Reports*, 6:21175 (2016)

P-51

Integrative multi-omic analysis of Th1 differentiation

Min Jung Kim, Kwang Pyo Kim and Min-Sik Kim*

Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea

Naïve CD4+ T cells can be differentiated into T helper cells through several rounds of division, and these differentiated T helper cells are essential for human immune activities such as infection, allergic responses, macrophages and also mediate direct antiviral function. Here, we analyzed the proteins involved in signal transduction of early T cell differentiation by setting each time point divided into 6 time points. The samples were labeled by using TMT-reagent after digestion and the labeled peptides were subjected to LC-MS/MS analysis. After integrating RNA-seq, global and phosphorylated proteome profiling, we characterized the network of early signaling pathways for T cell differentiation. Through the analysis of transcriptomes based on RNA-seq, we classified networks of transcription factors of T cell differentiation. And we identified 847 differentially phosphorylated peptides from phosphoproteomic analysis and 755 differentially expressed proteins from global proteomics. All DEPs (fold changes>3) among each analysis were identified in the abundance of each time point to perform gene ontology and pathway analysis. In conclusion, our results and future experiment will be able to identify the modeling of drugs related to CD4 activation and T cell differentiation and also identify autoimmune diseases caused by T cell mutation.

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Proteomics and phosphoproteomics studies of cell lines with CRISPR-Cas9 edited kinases for cancer disease.

Bitnara Han[1], Hyeong Min Lee[1], Jae Min Lim[1], Jin-Soo Kim[2,3], Kwang Pyo Kim[1]

[1]*Department of Applied Chemistry, College of Applied Sciences, Kyung Hee University, Yongin 446-701, Republic of Korea*

[2]*National Creative Research Initiatives Center for Genome Engineering, Seoul National University, Seoul, South Korea*

[3]*Department of Chemistry, Seoul National University, Seoul, South Korea.*

As an important key to cancer treatment, signlaing pathways regulated by kinasses are the targets of most cancer drugs. However, targeted anticancer agents are facing limitations due to their resistance and low popularity and efficiencies. The kinase genes were edited using CRISPR-Cas9 technology and target deconvolution was performed by screening from various omics perspectives to find an aberrantly activated signaling pathway and an unintended target of kinase inhibitor.

Four kinases (ERK2, PIK3CA PLK1, and PAK4) of HCT116 cells, were knocked out using CRISPR-Cas9 to obtain cell lines. Proteins were extracted from these knockout cell lines and tryptic digestion followed by labeling using TMT reagent. We performed global profiling and phosphopeptides enrichment using IMAC method for the labeled proteins. As a result, a total of 7,500 proteins, 4200 phosphoproteins and 10877 phosphosites were identified by LC-MS / MS.

Results of GOBP enriched for DEPs (Differentially Expressed Proteins) and DPPs (Differentially Expressed Phosphoproteins) in each knockout cell line were obtained and a model of protein-protein interaction network was established.

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New pathological discovery of Preeclampsia through human placenta proteomics

Hyeong Min Lee, Jae Min Lim and Kwang Pyo Kim*

Dept of Applied Chemistry, College of Applied Science, Khung Hee University, Yongin, Gyeonggi-do,446-701, Republic of Korea

Preeclampsia(PE), one of the three most common causes of maternal death in the world, leads to serious social and emotional disorder characterized by phenomenon of an increase in the elderly pregnant women and a decrease of fertility rate. Until now, there is no cure other than delivery, so the importance of early prevention is increasing day by day. Regarding the study of PE, most of them were analyzed for genome and proteome in the maternal blood, but research on the placenta, especially the proteins directly involved in the mechanism, is insufficient. To identify specific markers of PE, we simultaneously analyzed global proteome in PE, other complications related to pregnancy, and the normal mother. Through global proteome analysis based on LC-MS/MS, about 7,800 proteins were identified from the placenta, and about 200 placenta - specific proteins were identified.

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