www.ksms.org

2017 한국질량분석학회

겨울심포지움

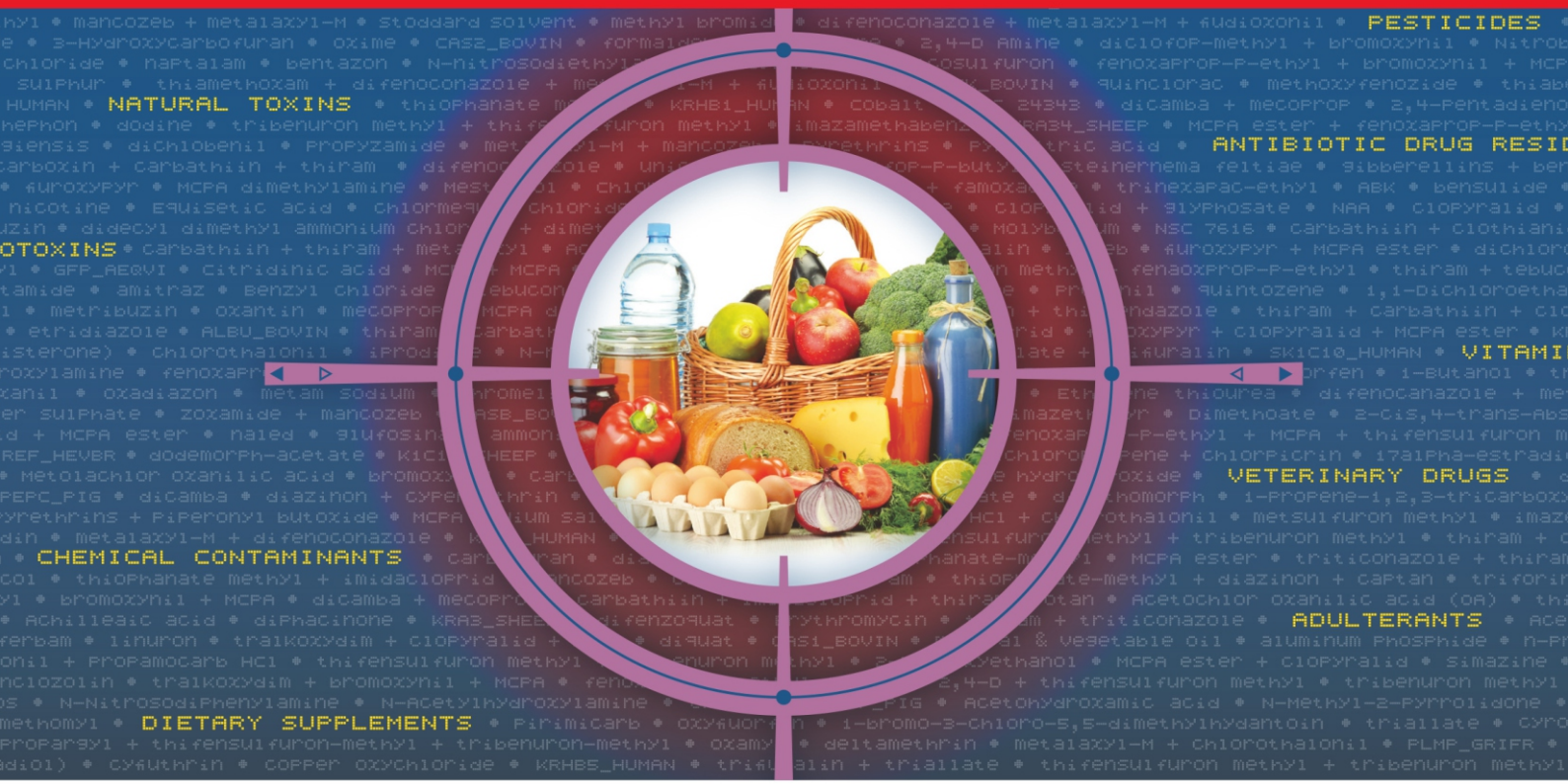
2017 13th KSMS Winter Symposium

2017. 2. 10. (금)

서울 KIST 국제협력관(1F) 컨벤션 홀

KSMS 한국질량분석학회
Korean Society for Mass Spectrometry

thermo scientific



More contaminants.
More accurately. Faster than ever.
Quantitation transformed.

Thermo Scientific™ TSQ Quantiva™ MS
Leading SRM sensitivity and speed in a triple quadrupole MS for targeted quantitation

Thermo Scientific™™ Q Exactive™ Focus MS
Proven performance of Orbitrap™ technology for screening, confirmation and quantitation

Thermo Scientific™ TraceFinder™ software
Designed to make routine quantitation and targeted analysis simple, fast and productive

Safeguarding the global food supply requires continuous, accurate and timely monitoring of harmful compounds. Quantify more chemical residues, at lower levels, while meeting global regulatory demands with our new portfolio of LC-MS instruments, sample prep solutions and software. Triple quadrupole MS delivers SRM sensitivity and speed to detect targeted compounds more quickly and HRAM solutions using Thermo Scientific™ Orbitrap™ MS enables screening with accurate quantitation of hundreds of contaminants. Meet today's challenges with us and together, we'll transform quantitative food safety analysis.

Find out more at **thermofisher.com/qefocus-ms**

ThermoFisher SCIENTIFIC

써모 피셔 사이언티픽 코리아 (주)
서울특별시 강남구 영동대로 302
국민 제1빌딩 6층

TEL : 02-3420-8600
FAX : 02-3420-8688
www.thermofisher.com

SHIMADZU
Excellence in Science

Shimadzu Liquid Chromatograph Mass Spectrometer

LCMS Series

Ultra Fast Triple Quadrupole LC/MS/MS
LCMS-8040

UFMS
ULTRA FAST MASS SPECTROMETRY

Liquid Chromatograph Mass Spectrometer
LCMS-8045

Ultra Fast Triple Quadrupole LC/MS/MS
LCMS-8050

Liquid Chromatograph Mass Spectrometer
LCMS-8060

Speed Beyond Comparison

Ultra-High Speed

- Ultra fast polarity switching speed .
- Enhanced ionization efficiency and ion transmission can 555 MRM / sec.
- Proprietary high-precision quadrupole machining capabilities, and unique high voltage power supply technology.

Ultra-High Reliability

- Minimum donwntime with Easy maintenance.
- Crosstalk minimization technique via UFsweeper.
- Maintain a stable measurement for a long time.
- Excellent linearity due to the wide dynamic range.

www.shimadzu.co.kr

동일시마즈주식회사

본 사 TEL.02)540-5541 FAX.02)541-2163 대전사무소 TEL.042)864-1161 FAX.042)864-1164 부산사무소 TEL.051)301-5400 FAX.051)301-5405 광주사무소 TEL.062)263-1293 FAX.062)263-1295
기술연구소 TEL.02)540-5960 FAX.02)540-5980 교 육 센 터 TEL.042)862-1734 FAX.042)864-1735 대구사무소 TEL.053)746-5541 FAX.053)746-5560 전주사무소 TEL.063)273-5540 FAX.063)273-5547

Perfect Balance to Elevate Your Lab's Performance

Made just for you, the X500R QTOF system is the first robust, high performance high resolution MS system designed for routine use.

Simple workflows that deliver reliable results, it's the solution that's ready to meet your challenges today and for the future, from the trusted LC-MS/MS industry leader.

Designed exclusively from user input with the perfect balance so it's easy to operate, easy to maintain, and easy to grow.

The X500R QTOF from SCIEX.

You designed it, we engineered it. In perfect balance to elevate your lab's performance.

sciex.com/X500R-INFO

SCIEX

AB Sciex is doing business as SCIEX.

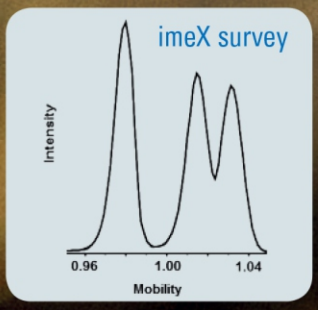
RUO-MKT-13-2990-A 11/2015

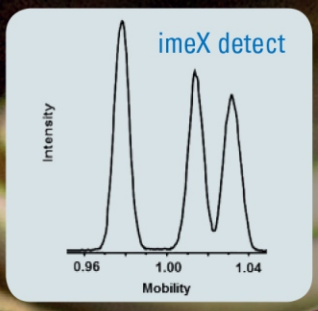
BRUKER

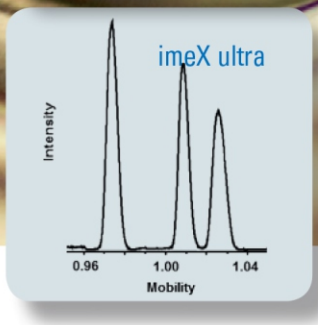
Bruker timsTOF™

Flexibility to Empower Your Ideas

The unique imeX™ technology provides high ion mobility resolution that is both adaptable and expandable. It allows you to resolve overlapping ions, focus on target peaks or accurately analyze collisional cross sections.







Ion mobility is a powerful separation extension to mass spectrometry based on the three-dimensional structure of an ion. It increases the peak capacity of the analytical system, as well as confidence in compound characterization.

With timsTOF, Bruker introduces the next generation of ion mobility-mass spectrometry.

Bruker engineered the timsTOF mass spectrometer as an open platform, so all you need to bring is your expertise and curiosity.

For more information, visit www.timstof.com

TIMS-QTOF MS

Innovation with Integrity

ANY ANALYTE
ANY METHOD
ONE PARTNER

ONLY AGILENT COVERS ALL YOUR MASS SPEC NEEDS

Whatever you need to analyze, we are here to help you implement the ideal method in your lab to achieve your goals. Agilent has decades of experience designing and building chromatography and mass spectrometry systems employed in longstanding partnerships and collaborations that span every field of application. This is what enables Agilent to provide you with the best solution for your analytical needs.

See how laboratories in your industry are using our solutions.
www.agilent.com/chem/mass-spec
고객지원센터 : **080-004-5090**

Agilent Technologies

Your gas generation partner

Why a gas generator?

Peak Scientific's laboratory gas generators set the benchmark for reliable, on-site and on-demand gas supply for GC and LC-MS instrument applications. Peak Scientific generator could improve the performance, productivity and workflow of your lab and give you more confidence in your analysis.

If you currently use nitrogen, zero air or hydrogen gas in your analytical process, contact us today to find out how a Peak generator can make a difference.

Genius NM32LA, 1050
Nitrogen generator
for **All LC/MS Applications**

Genius 1022
Nitrogen generator
for **Thermo Q Exactive LC/MS**

Genius 3013
Nitrogen generator
for **Agilent 6495,6550 LC/MS**

Genius 3051
N2 & Dry Air Gas Solution
for the **Shimadzu LCMS-8050, 8060**

Genius 3031
Nitrogen generator
for **SCIEX 6500 or other SCIEX LC/MS**

Precision Series
Nitrogen, Zero Air, Hydrogen Generator
for **CG applications**

goojung chromatech
서울시 구로구 디지털로 31길 20 (구로동, 에이스테크노타워 5차 1102호)
Tel. 02) 3281-2374 Fax. 02) 3281-3375 www.goojung.com
PEAK SCIENTIFIC

KRISS 한국표준과학연구원
Korea Research Institute of Standards and Science

조제분유 인증표준물질 (유기영양소분석용)
Infant formula CRM
KRISS 108-02-003 for organic nutrients

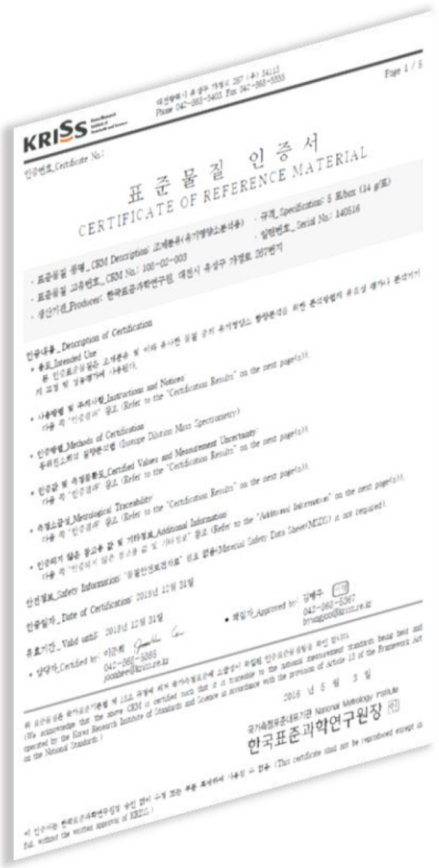
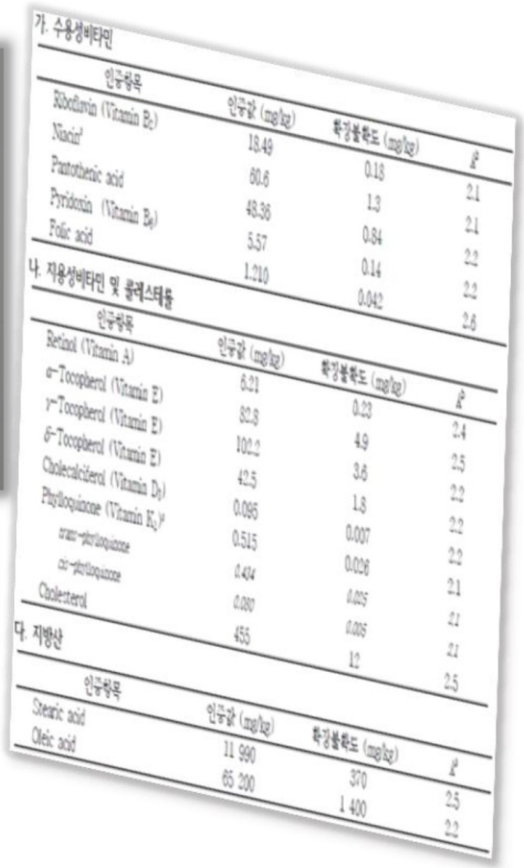


표 준 물 질 인 증 서
CERTIFICATE OF REFERENCE MATERIAL

추가정보 1. 일반성분의 시험소간 비교분석을 통한 합의값

항목	함량	확장불확도[a]	단위
조단백[b]	12.10	0.33	g/100 g
조지방[c]	24.2	1.2	g/100 g
수분[d]	23.3	2.5	g/kg
회분[e]	28.2	1.0	g/kg
탄수화물[f]	50.4	7.3	g/100 g


가. 수용성비타민
나. 지용성비타민 및 콜레스테롤
다. 지방산

세계 최고수준의 정확도와 측정불확도

- ISO 17025, ISO Guide 34와 35에 따라
- 최상위측정법(primary method)에 의해 결정된 인증결과
- 국가별 표준연구소 간 국제비교를 통해 검증된 측정능력

측정결과에 대한 국제적 동등성 제공

- CIPM-MRA에 의한 국제적 동등성 제공
- ISO 17025를 위한 분석법 유효성 검토에 활용

Water Soluble Vitamins	Fat Soluble Vitamins	Fatty acids	Amino acids
B1 Thiamin	A Retinol	Linoleic	Valine
B2 Riboflavin	E α-Tocopherol	Arachidonic	Leucine
B3 Niacin	γ-Tocopherol	α-Linolenic	Isoleucine
B5 Pantothenic acid	δ-Tocopherol	γ-Linolenic	Tyrosin
B6 Pyridoxine	D Cholecalciferol	Oleic	Threonine
B7 Biotin	K Phylloquinone	DHA	Lysine
B9 Folic	Cholesterol	EPA	Phenylalanine
B12 Cyanocobalamin		Stearic	Tryptophan
C Ascorbic acid			Histidine
			Alginine

측정표준 기술 서비스 쇼핑몰
표준과학한마당
교정 시험 CRM
http://eshop.kriss.re.kr
cal@kriss.re.kr
042-868-5555

KRISS 한국표준과학연구원
(34113)대전광역시 유성구 가정로 267
KRISS 한국표준과학연구원 Korea Research Institute of Standards and Science

KRISS 한국표준과학연구원
Korea Research Institute of Standards and Science

조제분유 인증표준물질 (원소분석용)
Infant formula CRM
KRISS 108-02-004 for elemental analysis

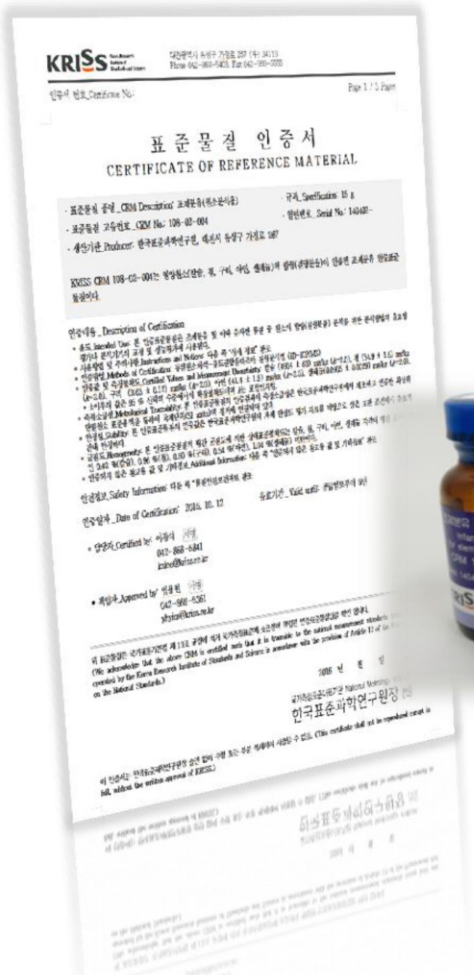
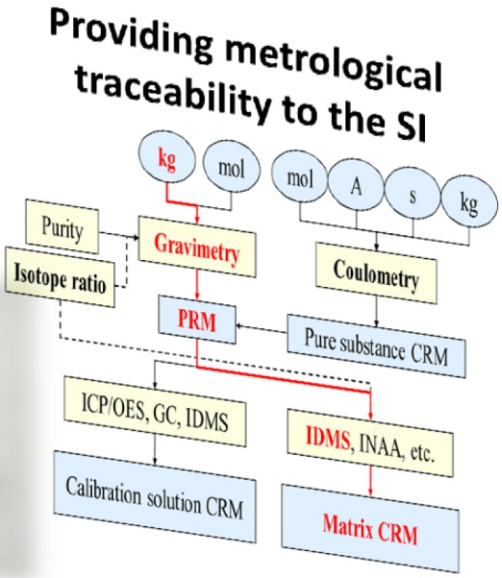


표 준 물 질 인 증 서
CERTIFICATE OF REFERENCE MATERIAL

Elements:
Ca, Cl, Cu, Fe, K, Mg, Se, Zn



세계 최고수준의 정확도와 측정불확도
- ISO 17025, ISO Guide 34와 35에 따라
- 최상위측정법(primary method)에 의해 결정된 인증결과
- 국가별 표준연구소 간 국제비교를 통해 검증된 측정능력

CCQM-K125 International comparison for elements in infant formula (www.bimp.org)

측정결과에 대한 국제적 동등성 제공
- CIPM-MRA에 의한 국제적 동등성 제공
- ISO 17025를 위한 분석법 유효성 검토에 활용

측정표준 기술 서비스 쇼핑몰
표준성과한마당
교정 시험 CRM

http://eshop.kriss.re.kr
cal@kriss.re.kr
042-868-5555

KSMS

2017 년 한국질량분석학회 겨울심포지움
일 시 : 2017 년 2 월 10 일 (금), 10:00 ~ 18:30
장 소 : 서울 KIST 국제협력관(1F) / 컨벤션 홀

목 차

안내사항

2017년 한국질량분석학회 겨울심포지움에 참가하신 회원 여러분 환영합니다

■ **현장 등록 시간 및 장소**

- 시 간 : 2017 년 2 월 10 일 (금) 10:00 ~ 18:30
- 장 소 : 서울 KIST 국제협력관(1F) 컨벤션 홀

■ **한국질량분석학회 2017 년 연회비 및 겨울심포지움 등록비 안내**

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

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

■ **포스터 게시 및 발표**

- 장소 및 게시 시간 : KIST 국제협력관 1F lobby / 2017 년 2 월 10 일 (금) 10:00~
  (포스터 부착 가능 시간: 2 월 10 일(금) 09:00~)
- 게 시 : 2017 년 2 월 10 일 (금) 10:00 ~ 18:00
- 발 표 : 2017 년 2 월 10 일 (금) 12:10 ~ 14:00 (홀수/짝수 발표 시간 참고, P.53)
- 철 거 : 2017 년 2 월 10 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 진동으로 바꾸시거나 전원을 꺼주십시오.
- 세션 중에는 개인적인 사진촬영이 금지되어 있습니다.

■ **겨울심포지움 현장 안내**

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

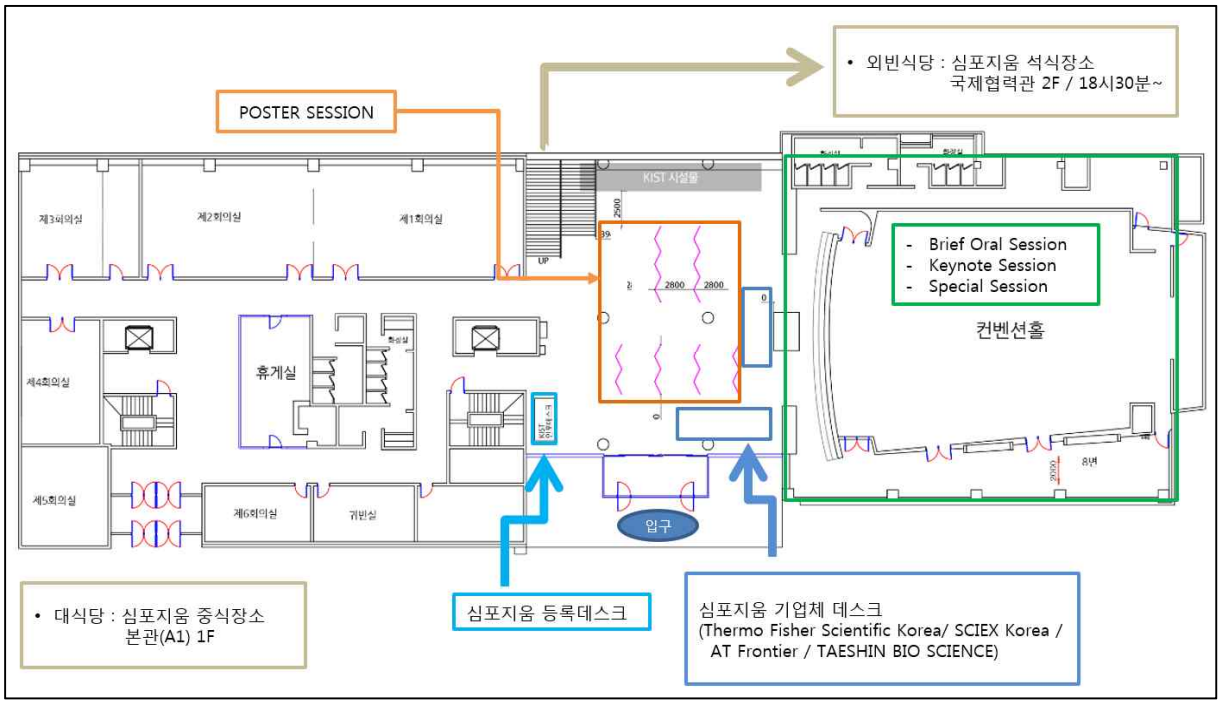
- KIST 출입 안내소
  - 22번: 북문 안내소
  - 21번: 준문 안내소

※ 지하철 6호선 이용자
: 22번 북문 안내소 이용가능

■ KIST(한국과학기술연구원)

- https://www.kist.re.kr
- 주 소 : 서울특별시 성북구 화랑로 14 길 5 우)02792 Tel. 02-958-5114
- 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 →
  한국과학기술연구원 (도보 5 분 소요)

■ **겨울심포지움 세션장소 안내**



■프로그램 안내

February 10 (Friday)

TIME	PROGRAM
10:00 ~	**등 록**
10:20 ~ 10:30	**개회사 (회장: 문명희)**
10:30 ~ 12:10	**Brief Oral Session** 조직책임자: 박종호(한국원자력연구원) / 차상원(한국외국어대학교) 좌장: 강덕진(한국표준과학연구원) / 차상원(한국외국어대학교) 20명 각 5분 발표 (대상자: 석·박사 학위과정 학생)
12:10 ~ 14:00	**중식 및 Poster Session** 조직책임자/좌장: 김정권(충남대학교) / 김태영(광주과학기술원)
14:00 ~ 16:00	**Keynote Session** 조직책임자: 서정주(한국기초과학지원연구원) / 황금숙(한국기초과학지원연구원) 좌장: 김영환(한국기초과학지원연구원) / 안현주(충남대학교 분석과학기술대학원)
14:00 ~ 14:30	Excited state dynamics using velocity map imaging technique 김상규 (한국과학기술원)
14:30 ~ 15:00	Developing Extensive Proteome-to-Genome Mapping Technologies for Effective Integration of Genomic and Proteomic Data: Proteogenomic Characterization of Early Onset Gastric Cancer 이상원 (고려대학교)
15:00 ~ 15:30	Application of Metabolomics to Discover Early Biomarkers and Novel Drug Target 박영자 (고려대학교)
15:30 ~ 16:00	TOF-SIMS imaging technique for drug screening 이태걸 (한국표준과학연구원)
16:00 ~ 16:10	**Coffee Break**
16:10 ~ 18:15	**Special Session** (MS for Public Interests) 조직책임자/좌장: 한상범(중앙대학교) / 최용석(단국대학교)
16:10 ~ 16:35	Introduction of Analytical Method of Pesticide Residues in Food Code 도정아 (식품의약품안전처 잔류물질과)
16:35 ~ 17:00	Forensic toxicological analysis in phytotoxin intoxication cases 최상길 (국립과학수사연구원 법독성학과)
17:00 ~ 17:25	Identification and quantification of flavonoids in agricultural and food material using UPLC-DAD-QTOF/MS 김정봉 (국립농업과학원 기능성식품과)
17:25 ~ 17:50	National birth cohort study(Ko-CHENS) and application of biological sample 김수진 (국립환경과학원 환경보건연구과)
17:50 ~ 18:15	Novel psychoactive substances: overview of trends, challenges and forensic identification 김희승 (대검찰청 과학수사 2과)
18:15 ~ 18:30	**우수 포스터 시상 및 폐회식**
18:30 ~	**만 찬**

KSMS

2017 한국질량분석학회 겨울심포지움

SYMPOSIUM

세부프로그램

FEBRUARY 10

BRIEF ORAL SESSION

10:30 – 12:10

컨벤션 홀

Organizer: 박종호 (한국원자력연구원) / 차상원 (한국외국어대학교)

Chairs: 강덕진 (한국표준과학연구원) / 차상원 (한국외국어대학교)

10:30–10:35	Do-It-Yourself (DIY) Manufacture of a Nano-LC MALDI Spotter Robot using a 3D Printing Technology 이재웅 (서강대학교)
10:35–10:40	Online non-contiguous fractionating and concatenating device coupled to two dimensional reverse phase/reverse phase liquid chromatography system for efficient and comprehensive proteomic analyses 이한겨레 (고려대학교)
10:40–10:45	A metabolomics-driven approach reveals metabolic responses and mechanisms in the rat heart following myocardial infarction 남미소 (한국기초과학지원연구원)
10:45–10:50	Size-dependent analysis of urinary exosomal lipids by flow field-flow fractionation and nanoflow ultrahigh-performance liquid chromatography tandem mass spectrometry (nUPLC-ESI-MS/MS) 양준선 (연세대학교)
10:50–10:55	Label free quantitative proteomics using peptide isotope peak intensities in mass spectrometry 윤기나 (한국기초과학지원연구원)
10:55–11:00	Evaluation of single particle ICP-MS for screening nanoparticles in environmental samples 이상준 (한국표준과학연구원/경희대학교)
11:00–11:05	Comprehensive profiling analysis of 20 urinary neurochemicals using in situ derivatization and liquid chromatography-tandem mass spectrometry 이원웅 (경희대학교)
11:05–11:10	Site-specific characterization of N-glycoproteins in human and mouse plasma samples by LC-MS/MS 이현경 (한국기초과학지원연구원)
11:10–11:15	Korean whole salivary proteome: a preliminary report 조하라 (단국대학교)
11:15–11:20	Comparative study on extraction method of fragrance allergens in water using GC-MS/MS 이인자 (서울물연구원)
11:20–11:25	Simultaneous determination of chlorogenic acid isomers and metabolites in rat plasma using LC-MS/MS 최원구 (가톨릭대학교)
11:25–11:30	UPLC-MS/MS based profiling of eicosanoids in RAW264.7 cells 최유리 (경희대학교)
11:30–11:35	Development of new chemical separation method for uranium age-dating of UO2 materials 최은주 (한국원자력연구원)

11:35–11:40 Steroidal CYP enzyme activities in human amniotic fluid by GC-MS
한소윤 (한국과학기술연구원)

11:40–11:45 Glycomic profiling of serum haptoglobin using nano LC/MS and LC/MS/MS
이성현 ((주)글라이칸)

11:45–11:50 Simultaneous analysis of thiamine and biotin in infant formula by isotope dilution-liquid chromatography mass spectrometry
주자연 (충남대학교)

11:50–11:55 Glycan signatures of human saliva
문한태 (충남대학교 분석과학기술대학원)

11:55–12:00 The effect of Sodium and Potassium ions for sucrose detection by comparing charcoal, DHB and CHCA matrices in MALDI-MS analysis
백지현 (충남대학교)

12:00–12:05 Reactive paper spray ionization mass spectrometry for the analysis of the conjugated ketones
최수빈 (한국외국어대학교)

12:05–12:10 Effect of Ca(II) on the conformation and aggregation process of alpha-synuclein
한종윤 (고려대학교)

KEYNOTE SESSION

14:00 – 16:00

컨벤션 홀

Organizer: 서정주 (한국기초과학지원연구원) / 황금숙 (한국기초과학지원연구원)

Chairs: 김영환 (한국기초과학지원연구원) / 안현주 (충남대학교 분석과학기술대학원)

14:00–14:30	Excited state dynamics using velocity map imaging technique 김상규 (한국과학기술원 화학과)
14:30–15:00	Developing Extensive Proteome-to-Genome Mapping Technologies for Effective Integration of Genomic and Proteomic Data: Proteogenomic Characterization of Early Onset Gastric Cancer 이상원 (고려대학교 화학과)
15:00–15:30	Application of Metabolomics to Discover Early Biomarkers and Novel Drug Target 박영자 (고려대학교 약학대학)
15:30–16:00	TOF-SIMS imaging technique for drug screening 이태걸 (한국표준과학연구원 나노바이오측정센터)

SPECIAL SESSION

16:10 – 18:15

컨벤션 홀

Organizer/ Chairs: 한상범 (중앙대학교) / 최용석(단국대학교)

16:10–16:35	Introduction of Analytical Method of Pesticide Residues in Food Code 도정아 (식품의약품안전처 식품의약품안전평가원 잔류물질과)
16:35–17:00	Forensic toxicological analysis in phytotoxin intoxication cases 최상길 (국립과학수사연구원 법독성학과)
17:00–17:25	Identification and quantification of flavonoids in agricultural and food material using UPLC-DAD-QTOF/MS 김정봉 (농촌진흥청 국립농업과학원 기능성식품과)
17:25–17:50	National birth cohort study(Ko-CHENS) and application of biological sample 김수진 (환경부 국립환경과학원 환경보건연구과)
17:50–18:15	Novel psychoactive substances: overview of trends, challenges and forensic identification 김희승 (대검찰청 과학수사 2과)

KSMS

2017 한국질량분석학회 겨울심포지움

BRIEF ORAL SESSION

Brief Oral Session-1

Do-It-Yourself (DIY) Manufacture of a Nano-LC MALDI Spotter Robot using a 3D Printing Technology

Jae-ung Lee, Han Bin Oh

Department of chemistry, Sogang University, Seoul 121-742, Korea

The 3D printing technology is growing very rapidly, and is bringing about significant advances in many research areas. On the 3d printing related website, the stories of making 3d printed parts and custom equipment have been posted. In this research, we made a DIY nano-LC MALDI spotter robot using 3D printed custom parts. Using this equipment, nano-LC and MALDI matrix loading can be conveniently coupled online and thus the separated eluents from nano-LC can be loaded automatically onto the MALDI plate. This DIY robot was made of only 3d printed parts and the parts on the online marketplace, so that anyone can make it and carry out maintenance easily and inexpensively. In this DIY robot, the loading speed can be readily controlled using a home-coded software. In addition, a camera is equipped so that the loading process can be monitored.

Brief Oral Session-2

Online non-contiguous fractionating and concatenating device coupled to two dimensional reverse phase/reverse phase liquid chromatography system for efficient and comprehensive proteomic analyses.

Hangyeore Lee, Jeong Eun So and Sang-Won Lee

Department of Chemistry, Korea University, Seoul 136-701

In this talk, a novel online two-dimensional reverse-phase/reverse-phase liquid chromatography (2D-RP/RPLC) separation platform, employing a newly developed online non-contiguous fractionating and concatenating device (NCFC fractionator), will be presented. In bottom-up proteomics analyses of a complex proteome, this system provided significantly improved exploitation of the separation space of the two RPs, considerably increasing the numbers of peptides identified compared to a conventional contiguous 2DRP/RPLC method. The fully automated online 2D-NCFC-RP/RPLC system bypassed many labor-intensive manual processes (i.e. offline fractionations, manual pooling, clean-up, drying/reconstitution, and autosampler fraction injection) required with the conventional offline 2D-NCFC RP/RPLC method, and thus, it offers minimal sample loss in a context of highly reproducible 2D-RP/RPLC experiments.

Brief Oral Session-3

A metabolomics-driven approach reveals metabolic responses and mechanisms in the rat heart following myocardial infarction

Miso Nam[1,2], Sunhee Jung[1,2], Do Hyun Ryu[2], Geum-Sook Hwang[1,3]

[1]*Intergated 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 Nono Science, Ewha Womans University, Seoul, 03760, Korea*

Myocardial infarction (MI) is caused by myocardial necrosis resulting from prolonged ischemia. However, the biological mechanisms underlying MI remain unclear. We evaluated metabolic and lipidomic changes in rat heart tissue from sham and MI at 1hr, 1day and 10day after coronary ligation, using global profiling based on metabolomics. A time-dependent increase or decrease in polar and lipid metabolite levels was measured. The S-adenosylmethionine (SAM) concentration and the SAM/S-adenosylhomocysteine (SAH) ratio gradually decreased in a time-dependent manner and were significantly downregulated 10 days after MI. Transcriptome analysis revealed that the levels of coenzyme Q (*Coq*)-*3* and *Coq5*, both of which are SAM-dependent methyltransferases, were decreased in the MI groups. These results suggested that dysregulation of SAM may be related to down regulated COQ biosynthetic pathway. In addition, short-chain (C3) and medium-chain (C4-C12) acylcarnitine levels gradually decreased, whereas long-chain acylcarnitine (C14-18) levels increased, owing to a defect in β-oxidation during ischemia. These changes are related to energy-dependent metabolic pathways, and a subsequent decrease in adenosine triphosphate concentration was observed. The comprehensive integration of various omics data provides a novel means of understanding the underlying pathophysiological mechanisms of MI.

Brief Oral Session-4

Size-dependent analysis of urinary exosomal lipids by flow field-flow fractionation and nanoflow ultrahigh-performance liquid chromatography tandem mass spectrometry (nUPLC-ESI-MS/MS)

Joon Seon Yang, Myeong Hee Moon*

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

Exosomes are small membrane vesicles (diameter of 20 to 100 nm) that are secreted by various kinds of cells. Exosomes contain biological molecules such as mRNA, proteins, and lipids that are originated from cells and they transport these molecules between cells. The cell-to-cell communication process, which is related to the immune system, affects transition of pathogens or growth of tumor cells and recent studies on exosomes have been focused on understanding its role and discovering biomarkers of diseases.

Exosomes are found in various kinds of body fluids, such as blood or urine, and urinary exosomes are usually originated from prostate or kidney cells. Closely related to prostate cancer (PCa), the size of PCa derived urinary exosomes is reported to be different from that of normal ones.

Flow field-flow fractionation (FlFFF) is an elution based analytical technique that separates sample components according to their sizes. In this study, urinary exosomes of controls and PCa patients were first retrieved by using ultracentrifugation and asymmetrical FlFFF (AF4) was adopted to sort out urinary exosomes according to their sizes. Exosomes in different sizes were collected and lipids within them were analyzed to discover any possible biomarker candidates. The overall lipid amounts were increased in PCa patient exosomes and lipids from small exosomes showed more changes than larger exosomes.

Brief Oral Session-5

Label free quantitative proteomics using peptide isotope peak intensities in mass spectrometry

Ki Na Yun[1,2], Gun Wook Park[1], Ju Yeon Lee[1], Eun Sun Ji[1], Mee-Jung Han[3], Han Bin Oh[2], Jong Shin Yoo[1], Jin Young Kim[1]

[1]Biomedical Omics Group, Korea Basic Science Institute, Ochang, Korea
[2]Department of Chemistry, Sogang University, Seoul, Korea
[3]Department of Biomolecular and Chemical Engineering, Dongyang University, Yeongju, Korea

We have developed an automated label-free protein quantification method that utilizes the combined intensity of top three isotope peaks at three highest MS spectral point. It was named three isotopes quantification (TIQ) that allows for a comparative protein analysis in a computational manner. The efficiency of TIQ was demonstrated by a benchmark dataset with two proteomes at known ratios. We accurately detected the mixing ratio over the entire protein expression range, with greater precision for abundant proteins. The performance of TIQ was also compared to that of SWATH-MS in terms of the number of quantified peptides and proteins and the specificity to detect differentially abundant proteins, where SWATH-MS is another approach for label free protein quantification utilizing the MS/MS intensity. There are a few advantages to TIQ. First, because it requires no peak area generation from the extracted ion chromatogram (XIC), it allows high-speed quantitation. Second, it is effective to remove signal interference from co-eluted ions with similar m/z values by evaluating the isotope pattern. And third, considering top three isotope peaks provides more sensitive results with better S/N ratios.

Brief Oral Session-6

Evaluation of Single Particle ICP-MS for Screening Nanoparticles in Environmental Samples

Sang-Jun Lee[1,2], Seok-Won Jang[1], Sung Ik Yang[1*], Yong-Hyeon Yim[2*]

[1]Department of Applied Chemistry, Kyung Hee University, Yongin, 17104 Republic of Korea

[2]Center for Inorganic Analytical Chemistry, Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 305-340 Republic of Korea

**E-mail: siyang@khu.ac.kr, yhyim@kriss.re.kr*

Increased use of engineered nanoparticles (NPs) in various fields of industry and consumer products has imposed potential risks to the environment and human health. Therefore, it is important to characterize NPs from the manufacturing to the final disposal in the environment for better understanding of the life-cycle of NPs and its impact. Recently, single particle (SP) ICP-MS has been attracted a lot of attentions to characterize the NPs, since it can simultaneously provide the information on elemental composition, particle size, and particle number concentration of a nanoparticle. It also allows detection of small numbers of NPs in a sample which is quite suitable for detection of low-abundant NPs in environmental samples. In a favorable condition, dissolved ion signals are distinguishable from NPs signals and provide additional information on dissolve ions. SP ICP-MS can be developed as a fast screening method for NPs in a real-world sample due to its decent analytical characteristics. For this purpose, we carried out preliminary investigation focused on technical limitations of SP ICP-MS. Relatively well-characterized Au and Ag NPs were used as the test samples. Element-dependent detection limits for NPs size, the influence of blank signal drift of easily dissoluble NPs, and separation of NPs pulses from electronic noises were investigated.

Brief Oral Session-7

Comprehensive profiling analysis of 20 urinary neurochemicals using *in situ* derivatization and liquid chromatography-tandem mass spectrometry

Wonwoong Lee, Hye Jung An, Youna Kim, Jongki Hong*

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

Dopamine, serotonin, GABA and their metabolites play a key role in multiple regulatory systems and the change of their physiological levels are closely associated with neurological disorders. Thus the development of a reliable analytical method of neurochemicals in biological fluids is important to discover potential biomarkers for the diagnosis, treatment and prognosis of neuronal disease. However, the analysis of neurochemicals in biological sample was challenging, because of highly different polarities between basic precursor and acidic metabolites, their low physiological amounts and high matrix interferences in biological samples. In this study, we developed a liquid chromatography-tandem mass spectrometry (LC-MS/MS) combined with Fischer esterification for comprehensive profiling of 20 neurochemicals in urine. *In situ* Fischer esterification could greatly improve the peak separation capacity and MS detection in a single run LC-ESI-MS/MS-positive ion mode due to reducing distinct physicochemical properties. After esterification, desalting process could significantly reduce the ion suppression of some analytes in MS detection. Esterified acidic neurochemicals were well retained on reversed-phase C18 column and separated with other basic neurochemicals within 6 min. Also, esterification analytes produced specific fragment ions to provide high sensitivity and selectivity in MRM mode. Established method was validated in terms of linearity, precision, accuracy, recovery, and matrix effect. Human urine samples collected from patients with Parkinson's disease and controls (patients; 21, controls; 10) were successfully analyzed to explore important biomarkers caused in metabolic disorder. In conclusion, this method may be helpful for comprehensive studying of neuropathological mechanism and discovering biomarkers for neurological disease.

Brief Oral Session-8

Site-specific characterization of N-glycoproteins in human and mouse plasma samples by LC-MS/MS

Hyun Kyoung Lee[1,2], Ju Yeon Lee[1], Gun Wook Park[1,2], 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-glycosylation of protein showed many differences between mouse and human. Usually N-glycosylation is directly involved in biological process and plays crucial role in human diseases due to their unusual biological sensitivity. Therefore, the specific characterization of N-glycosylation in model mouse is necessary in order to investigate progression of disease.

This study provided a method to characterize the site-specific N-glycosylation of human and mouse plasma. We compared site-specific N-glycosylation in human and mouse plasma samples using LC-MS/MS with GPA (GlycoProteome Analyzer) system[1]. As reported previously, we confirmed that the sialic acid of N-glycopeptides was almost entirely Neu5Gc in mouse plasma, while in human plasma was Neu5Ac. Especially, a unique trisialylated biantennary N-glycopeptide (peptide_$Hex_2HexNAc_2NeuGc_3$+$Man_3GlcNAc_2$) was specifically identified from several glycoproteins in mouse plasma. The trisialylated biantennary glycoform was recently reported in mouse serum, although it could not determine the binding position of the third Neu5Gc. We first report that it is directly linked to GlcNAc with evidence of specific oxonium ions and glycopeptide fragment ions in MS/MS spectra. This clearly proves that the new structure of trisialylated biantennary N-glycopeptide found only in mouse plasma.

Reference

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

Brief Oral Session-9

Korean whole salivary proteome: a preliminary report

Ha Ra Cho, Han Sol Kim, Yong Seok Choi*

College of Pharmacy, Dankook University, Cheonan-si, Chungnam 31116, South Korea

Saliva is considered as a good biological fluid for the purpose of monitoring biomarkers due to its suitable characteristics as a biological sample, for example, the non-invasive nature during its sampling and the easiness of collecting the relatively large volume of a sample. However, while proteomic studies on various types of saliva have been carried out in the United States and Europe over a decade, any proteomic research on saliva was never tried in Korea, yet. Thus, as the first step of Korean salivary proteomics, we are conducting a study to construct the first Korean reference salivary proteome, and its preliminary report is presented here. From the proteomic analyses of whole saliva (WS) samples from healthy Korean volunteers, many proteins in Korean WS have been being identified. While gene ontology distributions of Korean WS proteome are similar with those previous reported from other countries, a large portion of proteins in Korean WS is found to be unique by the comparisons with salivary proteome databases. Thus, the distinctiveness of Korean salivary proteome is strongly expected and the results from this on-going study could be widely used as the basement of future researches on the discovery/application of disease biomarkers from Korean WS.

Brief Oral Session-10

Comparative study on extraction method of fragrance allergens in water using GC-MS/MS

IN JA LEE*, Haksun Kwon, Chi-hwa An, Jae-Chan Ahn, Bogsoon Kim

Seoul Water Institute, Seoul Metropolitan Government, 04981, Korea

Products containing 26 of these compounds, which are fragrance allergens likely to cause contact allergies, are required under domestic cosmetic law to be labeled when their concentrations exceed 0.01% for rinse-off products (e.g. cleansers, shampoos), and 0.001% for leave-on products (e.g. lotions, deodorants) beginning in 2008. Fragrance allergens are continuously introduced into the environment via urban waste water effluents because they are important components of products used in daily life such as soaps, shampoos and lotions, so it is needed to develop the analysis to investigate those fragrance allergens.

Methods based on solid phase micro extraction(SPME) and liquid-liquid extraction(LLE) followed by GC-MS/MS have been studied for the analysis of 24 fragrance allergens excepting for 2 natural materials in water. Extraction conditions such as the kind of fiber, extraction temperature, type of solvent, amounts of sodium chloride were optimized using a multivariate approach.

In the case of using SPME, 15 of the 24 fragrance allergens were analyzed, and the correlation coefficient (r^2) of the calibration curve for quantification showed linearity of 0.9969 or more, and the method detection limits (MDL) and the limits of quantification (LOQ were 0.078 ~ 0.582 ug/L and 0.261 ~ 1.940 ug/L, respectively.

In the case of using LLE, 24 fragrance allergens were analyzed, and the correlation coefficient (r^2) of the calibration curve for quantification showed linearity of 0.9957 or more, MDL and LOQ were 0.020 ~ 0.138 ug/L and 0.065 ~ 0.440 ug/L, respectively.

It was concluded that the LLE pre-treatment method with low detection limit and more simultaneous analysis items was more effective to analyze fragrance allergens in water.

Brief Oral Session-11

Simultaneous determination of chlorogenic acid isomers and metabolites in rat plasma using LC-MS/MS

Won-Gu Choi, Ju-Hyun Kim, Ju-Yeon Moon, Tae Yeon Kong and Hye Suk Lee*

Drug Metabolism and Bioanalysis Laboratory, College of Pharmacy, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Buchen-si, Gyeonggi-do, 420-743,

A selective, sensitive and reliable liquid chromatography-tandem mass spectrometry method for the simultaneous determination of chlorogenic acid, neochlorogenic acid, cryptochlorogenic acid, caffeic acid, caffeic acid 3-O-glucuronide, caffeic acid 4-O-glucuronide, and ferulic acid in rat plasma was developed. After liquid-liquid extraction with ethyl acetate as sample preparation, seven analytes were seperated on Halo C18 column with gradient elution of 0.1% formic acid in water and methanol. The analytes were quantified by an electrospray ionization tandem mass spectrometry in the selected reaction monitoring mode. The standard curves were linear over the concentration range of 0.5-200 ng/mL for chlorogenic acid and neochlorogenic acid, 2.5-1000 ng/mL for cryptochlorogenic acid, caffeic acid, caffeic acid 3-O-glucuronide, and caffeic acid 4-O-glucuronide, and 12.5-5000 ng/mL for ferulic acid, respectively. The intra- and inter-day coefficient variations and relative errors were 4.1 to 18.1% and -8.8 to 16.0% at LLOQ and were 2.0 to 12.5% and -10.0 to 10.4% at three QC concentrations. This method was successfully applied to the pharmacokinetic study of chlorogenic acid, cryptochlorogenic acid, neochlorogenic acid, caffeic acid, caffeic acid 3-O-glucuronide, caffeic acid 4-O-glucuronide, and ferulic acid after an oral administration of the extract of *stauntonia hexaphylla* leaf at a dose of 100 mg/kg in male Sprague-Dawley rats.

Brief Oral Session-12

UPLC-MS/MS Based Profiling of Eicosanoids in RAW264.7 Cells

Yu-Ri Choi[1], Jae Won Lee[1], Hyuck Jun Mok[1], Seung Cheol Park[1], Hyung Don Kim[2], Kwang Pyo Kim[1*]

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

[2]*Department of Herbal Crop Research, National Institute of Horticultural and Herbal Science, RDA, Eumseong 369-873*

Although the pro-inflammatory and anti-inflammatory effects of various eicosanoids have been widely studied, changes in the levels of various eicosanoids during inflammation have not yet comprehensively studied. Thus, we designed two experiments in order to measure the levels of eicosanoids. We assessed the effect of lipopolysaccharide (LPS) treatment on the levels of eicosanoids in macrophage cells, and treated with LPS and 20(S)-ginsenoside-Rg3 (Rg3) for 12h, 24h. UPLC-MS/MS-based lipidomics analysis was used to profile various eicosanoids from macrophage cells treated with LPS and Rg3. The profiling data were statistically analyzed by principal component analysis, hierarchical clustering analysis, analysis of variance, and volcano plot. We have found that thirty-nine eicosanoids were upregulated, seven were down-regulated by LPS treatment in a concentration-dependent manner, and eighteen eicosanoids were recovered by Rg3 treatment.

Brief Oral Session-13

Development of new chemical separation method for uranium age-dating of UO_2 materials

Eun Ju Choi[1,2], Sang Ho Lim[1,2], Sun-Ho Han[1], Ranhee Park[1], Jinkyu Park[1], Chi-Gyu Lee[1]

[1]Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, Korea

[2]Radiochemistry & Nuclear Nonproliferation, University of Science & Technology, Korea

Age-determination of uranium samples is an important technique for nuclear forensics by analyzing a daughter-mother radionuclide pair such as $^{230}Th/^{234}U$, $^{231}Pa/^{235}U$, $^{232}Th/^{236}U$. $^{230}Th/^{234}U$ is one of the most commonly used isotope pair due to relatively rapid ingrowth of ^{230}Th in comparison with others and availability of high precision. For accurate and precise determination of $^{230}Th/^{234}U$ ratio, Th and U must be purified by removing interfering species from uranium samples prior to analysis as much as possible. Additionally, ^{232}Th impurities during chemical procedures should be minimized and well evaluated because standard ^{232}Th is used as a spike for isotope dilution technique.

In this study, we have developed new chemical separation method using UTEVA resin and optimized separation conditions. This new chemical separation method is expected to be more versatile than previous method using TEVA resin or ion exchange chromatograpy because it is possible to evaluate Pu age by analyzing $^{241}Am/^{241}Pu$ as well as $^{230}Th/^{234}U$ at the same time. For testing this method, we prepared simulated uranium samples. Elution curve and recovery yield were obtained from newly developed separation schemes. The optimal volumes of Th eluent (5 M HCl) was 6 mL and the recovery yield was 99.5 %. In addition we also verified this method with UO_2 reference materials and isotopic ratio measurements of $^{230}Th/^{234}U$ were performed using MC-ICP-MS equipped with desolvation system (Aridus-Ⅱ).

Brief Oral Session-14

Steroidal CYP enzyme activities in human amniotic fluid by GC-MS

Soyun Han[1,2], Ju-Yeon Moon[3], Jae-Hong Kim[2], Man Ho Choi[1]

[1]*Molecular Recognition Research Center, KIST*
[2]*College of Life Sciences and Biotechnology, Korea University*
[3]*Department of Pharmacy, The Catholic University of Korea*

Although the potential risk factors of preeclampsia are associated with placental oxidative stress and altered steroid metabolism, its pathogenesis has not fully been identified. To investigate whether human cytochrome P450 (CYP) enzymes are responsible to oxidative metabolism of endogenous steroids, gas chromatography–mass spectrometry in the selected-ion monitoring (GC–SIM/MS)-based steroid profiling was, firstly, developed for simultaneous quantification of CYP-mediated regioselective hydroxysteroids and their substrates, including 15 androgens, 7 estrogens, 4 progestins, 6 corticoids, and 8 sterols, with Oasis HLB™ solid-phase extraction. This CYP-mediated steroid signatures allows simultaneous assessment of CYP1A, CYP1B, CYP2C, CYP3A, CYP11B, CYP17A, CYP19A, and CYP21A. Then, the devised assay was applied to amniotic fluids obtained from patients with preeclampsia and normotensive controls. Due to its compositional changes of amniotic fluids along with gestational age according to the process of the fetal development, the assessment of steroidal CYP enzyme activities in amniotic fluids could serve as a useful tool for assessing the diagnostic biomarkers.

Brief Oral Session-15

Glycomic profiling of serum haptoglobin using nano LC/MS and LC/MS/MS

Sung Hyeon Lee

GLYCAN Co., Ltd., Healthcare Innovation Park, 172 Dolma-ro, Bundang-gu, Seongnam 13605, Korea

Glycosylation changes have been reported in a wide variety of human diseases, including immune disorders and cancers, and even is associated with malignant transformation. Recently, a targeted glycoproteomic approach has gained considerable attention as a novel method for biomarker discovery to improve the specificity and sensitivity for clinical use. Here, we comprehensively investigated the indirect and direct glycomic profile of a target glycoprotein, serum haptoglobin (Hp) by chip-based nano LC-QTOF MS and MS/MS analysis following antibody-assisted purification. From the results of significant N-glycan variations between GC patients and healthy controls, we conclusively suggest that aberrant glycans of serum Hp are associated with patients with gastric cancer and might be a promising marker for GC screening/monitoring.

Brief Oral Session-16

Simultaneous analysis of thiamine and biotin in infant formula by isotope dilution-liquid chromatography mass spectrometry

Jayeon Joo[1,2], Joonhee Lee[1*], Byungjoo Kim[1], Jeongkwon Kim[2]

[1]Center for Organic Analysis, Division of Metrology for Quality Life, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, South Korea

[2]Department of Chemistry, Chungnam National University, Daejeon, 34134 Korea

Thiamine and biotin are part of vitamin B complex and play a key role as a coenzyme in biochemical reaction in human body. A definite method for the analysis of water-soluble vitamins is necessary to produce reliable and SI traceable measurement data.

The aim of this study is to simultaneously determine thiamine and biotin in infant formula using isotope dilution-liquid chromatography mass spectrometry. Acid hydrolysis at room temperature was performed to extract thiamine and biotin in infant formula. Thiamine-[$^{13}C_3$] and biotin-[$^{2}H_2$] standard materials were spiked as internal standard. Waters X-bridge C18 column (4.6 x 150 mm, 3.5 μm) was selected for proper separation of thiamine and biotin, and 10 mmol/L ammonium formate in H_2O, pH 3.8 and methanol were decided as mobile phases. The post-column infusion method was used to study matrix effects originating from sample matrix in electrospray ionization mode.

For the quantification, selected reaction monitoring mode is applied to monitor the collisionally induced dissociation channels of m/z 265.1→122.0 and 245.1→227.1 for thiamine and biotin, respectively, and m/z 268.1→122.0 and 247.1→229.1 for corresponding isotope compounds. The repeatability and reproducibility test in infant formula showed less than 2 % of relative standard deviation.

An LC/MS/MS-based isotope dilution mass spectrometric method has been evaluated as a candidate reference method for the simultaneous determination of thiamine and biotin in infant formula.

Brief Oral Session-17

Glycan signatures of human saliva

Hantae Moon[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*

In recent years, saliva has received particular attention among researchers especially in the field of forensic sciences. Saliva encountered at crime scene is one of the most significant evidence and thus, the identification of saliva from other human fluids and non-human fluids is an essential prerequisite prior to further crime investigation. Conventional methods including enzymatic amylase and starch-iodine test to determine and distinguish saliva have low sensitivity in trace samples and lack of specificity due to cross-reaction with other fluids. In order to overcome these weaknesses in conventional methods, various studies have been attempted based on biochemical components. Glycosylated proteins, which are highly sensitive to the biochemical environment, are a major constituent in saliva and play an important and vital role in maintenance of oral health. Here, we have explored the possibility if glycan can be used as a bio-signature to identify and differentiate human saliva compared with other fluids. Briefly, N-glycans in human saliva (7 males and 11 females) were enzymatically released and enriched by solid phase extraction with a porous graphitized carbon cartridge. Human saliva N-glycans were carried out by nano LC-PGC chip/Q-TOF MS and –MS/MS. We could determine highly fucosylated N-glycans as a saliva-specific molecule.

Brief Oral Session-18

The effect of Sodium and Potassium ions for sucrose detection by comparing charcoal, DHB and CHCA matrices in MALDI-MS analysis

Jihyun Paek, Dabin Lee, Yeoseon Kim, Sooyeon Chae, Jeongkwon Kim*

Dept. of Chemistry, Chungnam National University, Deajeon, 34134, Korea

Matrix-assisted laser desorption/ionization (MALDI) is one of the most commonly used soft ionization method for the determination of large molecules such as proteins or peptides. MALDI conventionally uses organic matrices such as 2,5-dihydroxybenzonic acid (2,5-DHB) and α-cyano-4-hydroxycinnamic acid (α-CHCA). However, organic matrices usually break up under laser irradiation. Moreover, the product of the matrices have signal interferences with high intensity in the low molecular weight ranges (m/z<500). Many alternative matrices such as activated charcoal, carbon nanotubes, and porous silicon surface have been used to overcome the interferences of matrix-related ions. In this investigation, sucrose which has molar mass of 342.29, was analyzed using 2.5-DHB, CHCA, and charcoal. Among the three matrices, charcoal was found to be best since it provides the highest sucrose peak intensity and the lowest interferences. However, when using charcoal matrix and sodium ion addition, it was observed that sucrose was cleaved into glucose generating [glucose + Na]$^+$ peak. Therefore, it was necessary to explore new method for the detection of only intrinsic sucrose by MALDI. Lowering the laser intensity decreases the glucose peak intensity to only a certain extent and changing the additive cation from Na^+ to K^+ successfully removed the glucose peak. The addition of K^+ cation was found to be an efficient way for the determination of sucrose.

Brief Oral Session-19

Reactive paper spray ionization mass spectrometry for the analysis of the conjugated ketones

Soobin Choi, Sangwon Cha

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

Paper spray ionization (PSI) is an ambient ionization method which utilizes a triangular paper tip as a sampling base as well as an electrospray tip. In PSI, sample solution is usually deposited onto a paper tip and dried. Analytes in a sample spot are then extracted, transported to the end of the paper tip, and finally ionized by applying an electrospray solution and high voltage on a paper tip. In case an electrospray solution contains a reactant which can readily react with target analytes, *in situ* derivatization of target analytes can occur during PSI processes and this method is referred to as reactive PSI. In this presentation, we demonstrated reactive PSI mass spectrometric analysis of conjugated ketones including quinones and isothiazolones. The reactant for this application was cysteamine which readily reacts with a conjugated ketone *via* Michael addition reaction. Since the reaction product has an amine group which can be easily protonated, sensitivity was greatly enhanced by this approach. In addition, conjugated ketones could be selectively detected by monitoring the specific fragment ions of the reaction products.

Brief Oral Session-20

Effect of Ca(II) on the conformation and aggregation process of alpha-synuclein.

Jong Yoon Han, and Hugh I. Kim

Deptartment of Chemistry, Korea University, Seoul 02841, Korea

Parkinsons's disease (PD) is a neurodegenerative disease, characterized by aggregation of alpha-synuclein (αSyn). To understand factors affecting αSyn to form abnormal aggregates, chemical compounds and metal ions have been investigated *in vitro*. Among them, Ca(II), one of the most crucial metal ions in life, was shown to promote αSyn aggregation and it has been considered to have a relationship with PD. Ca(II) was observed to interact with C-terminal domain of αSyn and their binding affinity was measured (K_d ~ 1 mM). However, how the interaction affects the aggregation process of αSyn is not clearly understood. In this study, we investigated the effect of Ca(II) on the conformation and aggregation process of αSyn using mass spectrometry (MS), small-angle X-ray scattering (SAXS), and transmission electron microscopy (TEM). Our MS and SAXS results showed that interaction between Ca(II) and C-terminal of αSyn promotes conformational change of αSyn into extended structure. The conformation change is considered as a cause of increased rates of αSyn aggregation. Furthermore, we observed that Ca(II) can affect the aggregation process during nucleation and elongation steps, and even mature fibril. Our study will provide physicochemical understanding of interaction between αSyn and Ca(II) and the aggregation process of αSyn.

KSMS

2017 한국질량분석학회 겨울심포지움

KEYNOTE SESSION

Keynote Session-1

Excited state dynamics using velocity map imaging technique

Sang Kyu Kim

Dept of Chemistry, KAIST, Daejeon, Korea

Chemical reactions on the electronically excited states are complicated as the Born-Oppenheimer approximation quite often fails. Reactive flux does not stay on the adiabatic potential energy suface, and rather it switches to ride on nearby but different adiabatic potential energy surface by nonadiabatic transitions. As a bottleneck for this nonadiabatic transition, the so-called “conical intersection” plays an important role in controlling nonadiabaticity of reactions on the excited potential energy surfaces. Conical intersection is, however, a very difficult conceptual point which had only been theoretically predicted. We are keenly interested in unraveling the structure and dynamic role of conical intersections specialy in predissociation reactions. Specifically, photochemistry of hetero-aromatic molecular systems are investigated to reveal the multi-dimensional nature of the conical intersection seam developed along the surface crossings and encountered along the reaction coordinate. Experimentally, we have used velocity-map ion (or electron) imaging technique to determine the angular and kinetic distributions of fragments. Dynamic variables are measured in both frequency and time domains. In order to investigate the structure-reactivity relationship, we used the Stark deflector to spatically separate possible conformational isomers. Combined use of Stark and VMI gives unique opportunity to interrogate the conformer-specific reaction dynamics. We are going to discuss some recent findings from our laboratory regarding spectroscopic characterization of the conical intersection and possibly tracking of the reaction coordinate from the minimum energy structure to the transition-state.

Keynote Session-2

Developing Extensive Proteome-to-Genome Mapping Technologies for Effective Integration of Genomic and Proteomic Data: Proteogenomic Characterization of Early Onset Gastric Cancer

Sang-Won Lee

Dept of Chemistry, Korea University, 145 Anam-ro Seongbuk-gu Seoul, 02841, South Korea

Despite recent advances in genomics and proteomics technologies, and widespread interest in applying these technologies to achieve cancer biomarker discovery, the number of new FDA-approved protein cancer biomarkers reported over the past decade has declined. The reasons for this apparent disconnect between biomarker discovery efforts and FDA approval are many. Some issues are technological in nature: the need for proteome measurements that are sensitive, broad, quantitative, and at the same time with sufficient throughput to analyze enough samples for statistical confidence; the need to have standard metrics for quality assurance and quality control that enable cross comparison and validation of results. Some of the problems are based in cancer biology: the problems of human variability that require analysis of large numbers of samples; the problems of biological redundancy, that require a systematic computational analytical approach; the need to integrate multiple sources of information (e.g., genomics, transcriptomics, proteomics) and to link these data to clinical outcomes. We are developing and refining an advanced proteome mapping platform that integrates cutting-edge proteome technologies and provides unprecedented sensitivity, throughput, and robustness of proteome profiling. Here we discuss the proteome mapping core technologies and present the results of their application to proteogenomic characterization of human early onset gastric cancer.

Keynote Session-3

Application of Metabolomics to Discover Early Biomarkers and Novel Drug Target

Youngja H. Park

College of Pharmacy, Korea University, Sejong, 30019, Republic of Korea

Metabolomics is a powerful new technology involving the comprehensive characterization of metabolites and metabolism in biological systems to provide metabolic profiles related to the diseases. Recent advances in metabolomics and bioinformatics are emerging to the mainstream biomedical applications. In particular, metabolomics provides a powerful platform for discovering novel biomarkers and biochemical mechanisms as well as identifying novel drug targets.

In the current presentation, LC-MS based metabolomics was applied to extract the plasmodium specific potential biomarkers including multivariate statistical analyses. The number of significant metabolites associated with malaria infection was 1025 using false discovery rate at q=0.05. Two-way hierarchical cluster analysis showed that clear segregation of metabolic profile of parasite infected from non-infected supernatant. The pathway analysis was done using Kyoto encyclopedia Gene and Genomes.

The intensities of potential biomarkers were increased with culture time suggesting a positive association between the quantity of these molecules and level of parasitemia. These four molecules are: 1) 3-Methylindole, a mosquito attractant, 2) Succinylacetone, a heme biosynthesis inhibitor, 3) S-methyl-L-thiocitrulline, a nitric oxide synthase inhibitor,and 4) O-arachidonoyl glycidol, a fatty acid amide hydrolase inhibitor. In addition, we confirmed a previous finding which was the reduction of two important amino acids, arginine and isoleucine, under malaria infection.

In summary, metabolomics can be a potential tool in discovering parasite specific metabolites for future development of diagnosis assay for malaria infection and in suggesting the potential drug development.

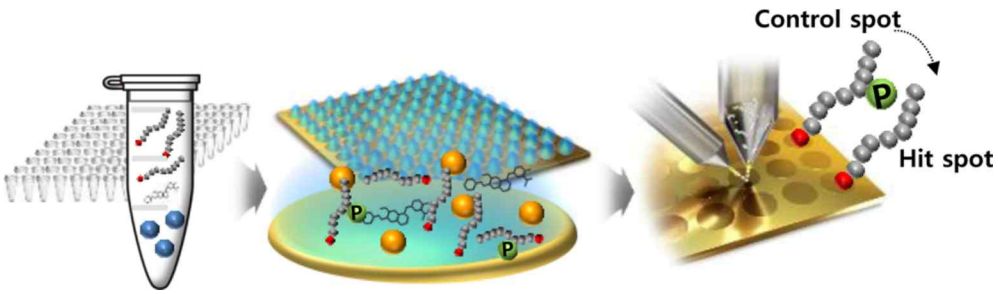
Keynote Session-4

TOF-SIMS imaging technique for drug screening

Tae Geol Lee*

Center for Nano-Bio Measurement, KRISS, Daejeon, 34113, Korea

Protein kinases are enzymes that are important targets for drug discovery because of their involvement in regulating the essential cellular processes. For this reason, the changes in protein kinase activity induced by each drug candidate (the inhibitor in this case) need to be accurately determined. Here, an on-chip secondary ion mass spectrometry (SIMS) imaging technique of the peptides was developed for determining protein kinase activity and inhibitor screening without a matrix. In our method, cysteine-tethered peptides adsorbed onto a gold surface produced changes in the relative peak intensities of the phosphorylated and unphosphorylated substrate peptides, which were quantitatively dependent on protein kinase activity. Using mass spectrometry imaging of multiple compartments on the gold surface in the presence of a peptide substrate, we screened 13,727 inhibitors, of which seven were initially found to have inhibitor efficiencies that surpassed 50%. Of these, we were able to identify a new breakpoint cluster region-abelson (BCR-ABL)^{T315I} kinase inhibitor, henceforth referred to as KR135861. KR135861 showed no cytotoxicity and was subsequently confirmed to be superior to imatinib, a commercial drug marketed as Gleevec. Moreover, KR135861 exhibited a greater inhibitory effect on the BCR-ABL^{T315I} tyrosine kinase, with an IC_{50} value as low as 1.3 μM. In *in vitro* experiments, KR135861 reduced the viability of both Ba/F3 cells expressing wild-type BCR-ABL and BCR-ABL^{T315I}, in contrast to imatinib's inhibitory effects only on Ba/F3 cells expressing wild-type BCR-ABL. Due to the surface sensitivity and selectivity of SIMS imaging, it is anticipated that our approach will make it easier to validate the small modifications of a substrate in relation to enzyme activity as well as for drug discovery. This mass spectrometry imaging analysis enables efficient screening for protein kinase inhibitors, thus permitting high-throughput drug screening with high accuracy, sensitivity, and specificity.[1]



[1] Cho *et. al.*, *Anal. Chem.* 2017, **89**, 799-806.

KSMS

2017 한국질량분석학회 겨울심포지움

SPECIAL SESSION

Special Session-1

Introduction of Analytical Method of Pesticide Residues in the Food Code

Jung-Ah Do

Pesticide and Veterinary Drug Resides Division, National Institute of Food and Drug Safety Evaluation, Ministry of Food and Drug Safety, Cheongju, Chungbuk, 28159, Korea

The Ministry of Food and Drug Safety (MFDS) has been setting pesticide MRLs(Maximum Residue Limits) as per Article 15 of the Food Sanitation Act (Article 5-2 of the Enforcement Decree of the Food Sanitation Act), and has been developing standard analytical methods, which are published in the Food Code. As of January 2017, the announcement of the "Notice No. 2016-154 of the Minitry of Food and Durg Safety" lists three categories of pesticide residue tests (i.e., single analytical method, analytical methods for pesticide multi-residues, and screening) for agricultural products, livestock products, and ginseng, with 236, 55, and 2 analytical methods, respectively. Recently, pesticide metabolites, in addition to major compound, were included in the definition of pesticide residue. Further, as per the introduction of the Positive List System in Korea in December 2016, pesticides without established MRLs are now uniformly noted as "not detected(0.01 mg/kg)," demanding remarkably more qualitified analytical techniques, such as techniques with limit of quantitation for even trace amounts and simultaneous analytical methods that detect metabolites. In response to the demands, simultaneous analytical methods using mass spectrometers are currently being developed. Morevoer, the NIFDS(National Institute of Food and Drug Safety Evaluation) of the MFDS published the "Guidelines for standard procedures for developing analytical methods for food." in April 2016 and is developing analytical methods accordingly. The MFDS will continue to contribute the safety of food for people by making every endeavor to develop standard methods for determining that pesticide residues in food.

Special Session-2

Forensic toxicological analysis in phytotoxin intoxication cases

Sanggil Choe*, Sucheun Kim, Sangwhan In

Drug and Forensic Toxicology Division, National Forensic Service, 10 Ipchoonro, Wonju, 26460, South Korea

A lot of plants producing natural toxic substances, called phytotoxin, grow whole through the world and *Aconitum camichaeli*, *Nerium indicum*, *Rhododendron schlippenbachii* are well-known representative toxic plants in South Korea. Phytotoxins have various chemical structures such as alkaloids, diterpenoids, and saponins, and also have different mechanisms of toxic action. Recently many foreign species were introduced for ornamental purpose and some of them were naturalized in our country. Phytotoxins can be very toxic to human with small amounts and the estimated letal dose of aconitine, for example, is known to be 1~2mg. Many intoxication cases by the administration of toxic plants or exposure to them have been reported in emergency room and the intoxication caused death in severe case. In this study, we reported intoxication cases caused by the plants of genus *Aconitum*, *Oleander*, *Rhododendron*, and *Delphinium*. Forensic exhibits from crime scenes and biological specimens from victims were collected and they were analyzed by GC-MS, LC-MS, and LC-QTOFMS. The target phytotoxins of *Aconitum* were aconitine, methaconitine and hypaconitine, oleandrin was of *Oleander*, grayanotoxins were of *Rhododendron*, and delphinine, delsoline and delcosine were of *Delphinium*, respectively. The developed analytical methods could be used for the identification of toxic substances in phytotoxin intoxication cases in forensic and clinical toxicological fields.

Special Session-3

Identification and quantification of flavonoids in agricultural and food material using UPLC-DAD-QTOF/MS

Jung-Bong Kim

Food Nutrition & Functionality Division National Institute of Agricultural Sciences(NIAS), RDA Wan-Ju, JeonBuk 55365, South Korea

Modern authorised physicians are increasing their use of pure flavonoids to treat many important common diseases, due to their proven ability to inhibit specific enzymes, to simulate some hormones, and to scavenge free radicals. The daily intake of flavonoids with normal food, especially fruit and vegetables.

Recently, the flavonoid DB, which was published in the book of 3 books by the RDA, contains analysis information such as 3205 flavonoids and related chromatograms, which were isolated from 268 kinds of agricultural products using UPLC-DAD-QTOF/MS (Ultra-performance liquid chromatography with diode array detection and quadrupole time of flight /mass spectrometry) system. Galangin was used as the internal standard for the determination of the content and all the samples were analyzed under the same conditions. In addition, this DB provides the mass spec., which is the actual identification information, by peak, and the chemical structure of each substance is expressed in the form of image, so that it can be easily seen by the general public.

It has been confirmed that mass is a useful for chemical DB creation, and it is planned to be used to make other DBs such as saponins. Last year, we successfully visualized these flavonoid analytical information in the PLS-DA format, and by the end of the year, the public will be able to service them on the web.

Special Session-4

Natioanl birth cohort study(Ko-CHENS) and application of biological sample

Suejin KIM*

Environmental Health Research Division, Environmental Health Research Department, National Institute of Environmental Research, Ministry of Environment, Incheon, 22689, Republic of Korea

Since May 2015, we have launched the Korean CHildren's ENvironmental health Study (Ko-CHENS), the national birth cohort study. The object of Ko-CHENS is to develop the list of environmental hazardous factors for each stage of growth from the fetus to adolescents. And another mission is to identify the scientific evidences between hazardous chemicals and health outcomes.

Ko-CHENS are consisted of the Main study and the Core study. For an efficient and systematic operation of this study, the organizational structure is developed. It consists of the headquarters, the 13 regional centers and the research support center. The total study period is 22 years, and the pregnant women will recruit for about 5 years from 2015. It will be recruited 65,000 pregnant women for the Main study and 5,000 pregnant women for the Core study. Biological samples such as blood, cord blood, DNA and urine are collected and hazardous chemicals and their metabolites are analyzed. Follow-up methods of the Core study include regular visit to regional center for physical and laboratory test and interview. On the other hand, in case of the Main study, the follow-up methods include mobile or on-line questionnaire and data link with National Registry data from National Health Insurance Service, Statistics Korea, etc.

Currently, 19 kinds of hazardous chemicals and metabolites including lead, mercury, cadmium, bisphenols and phthalates are analyzed. In addition, we have collected about 1.4 million bio-samples through this Study, and paln to utilize these samples for exposome study.

Special Session-5

Novel psychoactive substances: overview of trends, challenges and forensic identification

Hee Seung Kim*

Forensic Science Division II, Supreme Prosecutors' Office, 157 Banpo-daero, Seocho-gu, Seoul 06590, Korea

Novel Psychoactive Substances (NPSs) refer to synthetic substances designed to mimic the effects of known licit and illicit controlled substances. A large number of NPSs have appeared recently on the market. NPSs are being easily obtained via Internet websites. These compounds pose a great danger to the public because they are falsely perceived as “legal” alternatives to the illicit drugs they intend to mimic and because of their unpredictable health impacts. Synthetic cannabinoids and their products (K2 or Spice) continue to be a significant concern for public health and safety. These substances share biological activity with delta-9-tetrahydrocannabinol, the primary psychoactive constituent in marijuana and are sourced from chemical manufacturers and suppliers primarily in China. Synthetic cannabinoid substances are typically prepared for packaging in the United States, and marketed over the Internet. Synthetic cathinones, also commonly known as “bath salts,” can produce pharmacologic effects that are substantially similar to other controlled substances such as cathinone, methcathinone, methamphetamine, amphetamine, MDMA, and cocaine. In short, these substances are abused for their stimulant effects. These substances have been known to be marketed to consumers as “bath salts”. Synthetic cathinones are widely available and have been encountered as a replacement for MDMA. Unfortunately, when MFDS initiates temporary control of a synthetic designer drug, those who traffic them frequently alter the chemical composition of the drugs they produce. These new substances, like the original substance, have an unpredictable impact on the body and pose a potentially severe public health threat. The legislation to control these specific psychoactive substances continues to be enacted. Some of synthetic drugs such as synthetic cannabinoids and/or other synthetic designer drugs will remain prevalent for a while. The Narcotics Department at the Supreme Prosecutors’ Office will continue to see overdoses and crime stastistics as a result of synthetic drug use. The epidemic initiated by synthetic cannabinoids is showing no signs of cessation within the near future hence the development of methods for their detection and quantification is timely and urgently required.

KSMS

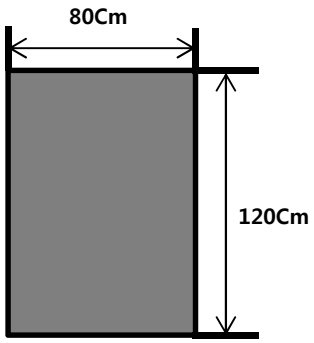
2017 한국질량분석학회 겨울심포지움

POSTER PRESENTATION

포스터 발표 및 우수포스터상 안내

■ **포스터 게시 및 발표**

- 게　　시 : **2017 년 2 월 10 일 (금) 10:00~**
- 발　　표 : **2017 년 2 월 10 일 (금) 12:10 ~ 14:00 /** 모든 발표자 배석
- 발표 순서 : **홀수 (12:10 ~ 13:05) / 짝수 (13:05 ~ 14:00)**
- 철　　거 : **2017 년 2 월 10 일 (금) 18:00 ~**
- 포스터 발표자는 아래의 포스터 번호 및 배치도를 참고하여 포스터를 게시하고, 10일(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 : 2017 년 2 월 10 일, 폐회식
- 부 상 : 상장 및 상금 10 만원

■ **분야별 포스터 번호**

분야	포스터번호
Fundamental Instrumentation	01 ~ 06
Life & Informatics	07 ~ 25
Mass Spectrometry in Elemental Analysis	26 ~ 40
Medical/Pharmaceutical Science	41 ~ 50
Food Environment	51 ~ 62
General	62 ~ 72

Fundamental Instrumentation : PO1 ~ PO6

P-01

Development of a MATLAB-based dissolved organic matters (DOMs) analysis program

Inae Jang[1], Ji-Hyung Park[2], and Han Bin Oh[1]*

[1]Dept of Chemistry, Sogang University, 35 Baekbeom-ro, Seoul, 04107, Korea
[2]Dept of Environmental Science & Engineering, Ewha Wamans University, 52, Ewhayeodae-gil, Seoul, 03760, Korea

P-02

Do-It-Yourself (DIY) Manufacture of a Nano-LC MALDI Spotter Robot using a 3D Printing Technology

Jae-ung Lee, Han Bin Oh

Department of chemistry, Sogang University, Seoul 121-742, Korea

P-03

Ionization and sensitivity of polycyclic aromatic hydrocarbons using GC-ESI/MS/MS, GC-APCI/HRMS and LC-ESI/MS/MS

Eunju Cha[1], Eun Sook Jeong[1], Hophil Min[1], Changmin Sung[1], Oh-Seung Kwon[1], Sangwon Cha[2], Jaeick Lee[1*]

[1]Doping Control Center, Korea Institute of Science and Technology, Hwarangno 14-gil 5, Seongbuk-gu, Seoul 136-791, Korea
[2]Department of Chemistry, Hankuk University of Foreign Studies, Oedae-ro, Mohyeon-myeon, Cheoin-gu, Yongin-si, Gyeongi-do 17035, Korea

P-04

Real-time ambient air monitoring using selected ion flow tube mass spectrometry (SIFT-MS)

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

P-05

Analysis of vehicle interior air quality in new cars using the syft technologies' VOICE 200 SIFT-MS instrument

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

P-06

Online non-contiguous fractionating and concatenating device coupled to two dimensional reverse phase/reverse phase liquid chromatography system for efficient and comprehensive proteomic analyses.

Hangyeore Lee, Jeong Eun So and Sang-Won Lee

Department of Chemistry, Korea University, Seoul 136-701

Life & Informatics : PO7 ~ P25

P-07

Profiles of hepatic lipids from rabbits using nanoflow UPLC-ESI-MS/MS

Seul Kee Byeon, Myeong Hee Moon*

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

P-08

Isotope-labeled methylation for quantitative analysis of phospholipids and enhancement in cardiolipin profiling by nUPLC-ESI-MS/MS

Jong Cheol Lee, Seul Kee Byeon, Myeong Hee Moon*

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

P-09

Lipidomic analysis of skeletal muscle tissues of p53 KO mice by Nanoflow LC-ESI-MS/MS

Se Mi Park, Seul Kee Byeon, Myeong Hee Moon*

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

P-10

Global changes in lipids of brain tissues from p53 KO mice: cortex, hippocampus and hypothalamus

Sang Tak Lee[1], Jong Cheol Lee[1], Je Kyung Seong[2], Myeong Hee Moon[1]*

[1]Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea
[2]College of Verterinary Medicine, Seoul National University, 1 Gwanak-ro, Seoul, 08826, Korea

P-11

Comprehensive profiling analysis of 20 urinary neurochemicals using *in situ* derivatization and liquid chromatography-tandem mass spectrometry

Wonwoong Lee, Hye Jung An, Youna Kim, Jongki Hong*

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

P-12

Korean whole salivary proteome: a preliminary report

Ha Ra Cho, Han Sol Kim, Yong Seok Choi*

College of Pharmacy, Dankook University, Cheonan-si, Chungnam 31116, South Korea

P-13

Metabolic profiling of human atherosclerotic aorta based on liquid chromatography/mass spectrometry.

Sunhee Jung[1,2], Miso Nam[1,2], Do Hyun Ryu[2], Geum-Sook Hwang[1,3]*

[1]Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institue, Book ah hyun-ro 150, Seoul, 120-140, Republic of Korea
[2]Dept of Chemistry, SungKyunKwan University, SeoBoo-to 2066, Suwon, 440-746, Republic of Korea
[3]Department of Life Science, Ewha Womans University, Seoul 120-750, Republic of Korea

P-14

Targeted and global metabolic analysis of rat urine from high tryptophan availability models

Yu Ri Cho[1], Mi Jung Ji[1], Mi Yeon Lee[1], Suk Youn Son[1], Ki Soo Lee[1], Soo Hyun Lee[2], and Hyun-Mee Park[1]

[1]Advanced Analysis Center, Korea Institute of Science and Technology, Korea
[2]Department of Medical Record and Health Information Management, Kongju National University

P-15

Intact glycopeptide analysis of targeted serum haptoglobin

Seunghyup Jeong[1, 2], Unyong Kim[1, 2], and Hyun Joo An[1, 2*]

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

P-16

Evaluation of Single Particle ICP-MS for Screening Nanoparticles in Environmental Samples

Sang-Jun Lee[1,2], Seok-Won Jang[1], Sung Ik Yang[1*], Yong-Hyeon Yim[2*]

[1]Department of Applied Chemistry, Kyung Hee University, Yongin, 17104 Republic of Korea
[2]Center for Inorganic Analytical Chemistry, Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 305-340 Republic of Korea
**E-mail: siyang@khu.ac.kr, yhyim@kriss.re.kr*

P-17

Proteomic Analysis to Identify Interactomes of Human N-alpha-acetyltransferases 40 (hNAA40) using LC-MS/MS

Yeirin Lee[1], Dowoon Nam[1], Hyun Seok Kim[2*] and Sang-Won Lee[1*]

[1]Department of Chemistry, Korea University, Seoul, 02841, South Korea
[2]Department Bioinspired Science, Ewha Womans University, Seoul, 03760, South Korea

P-18

Proteomic analysis to reveal the mechanism of E-cadherin loss in a gastric cancer mouse model

Seung-Ik Ko[1], Min-Sik Kim[2] and Sang-Won Lee[1*]

[1]Department of Chemistry, Korea University, Seoul, 136-701, Republic of Korea
[2]Department of Applied Chemistry, Kyunghee University, Gyeonggi-do, 446-701, Republic of Korea

P-19

Quantitative mouse retinal proteome analysis of Vascular Endothelial Growth Factor (VEGF)-induced vascular hyperpermeability by LC-MS/MS

Jingi Bae, and Sang-Won Lee*

Department of Chemistry, Korea University, Seoul, 136-701, South Korea

P-20

Increasing Sensitivity and Accuracy in Co-fragmented Peptide Identifications from Tandem Mass Spectra using Multiplexed Post-Experimental Monoisotopic Mass Refinement (*m*PE-MMR)

Inamul Hasan Madar, Seung-Ik Ko, Hokeun Kim and Sang-Won Lee*

Laboratory of Gaseous Ion Chemistry, Department of Chemistry, Research Institute for Natural Sciences, Korea University, Seoul 136-701, South Korea

P-21

Relative metabolite ratio of di(2-ethylhexyl) phthalate in obese children.

Jiwon On[1,2], Sang Won Lee[2], Mi jung Park[3], Jeongae Lee[1], Heesoo Pyo[1*]

[1]Molecular Recognition Research Cent'er, Korea Institute of Science and Technology
[2]Department of Chemistry, Korea University
[3]Department of Pediatrics, Sanggye Paik Hospital, Inje University College of Medicine

P-22

Label free quantitative proteomics using peptide isotope peak intensities in mass spectrometry

Ki Na Yun[1,2], Gun Wook Park[1], Ju Yeon Lee[1], Eun Sun Ji[1], Mee-Jung Han[3], Han Bin Oh[2], Jong Shin Yoo[1], Jin Young Kim[1]

[1]Biomedical Omics Group, Korea Basic Science Institute, Ochang, Korea
[2]Department of Chemistry, Sogang University, Seoul, Korea
[3] Department of Biomolecular and Chemical Engineering, Dongyang University, Yeongju, Korea

P-23

A metabolomics-driven approach reveals metabolic responses and mechanisms in the rat heart following myocardial infarction

Miso Nam[1,2], Sunhee Jung[1,2], Do Hyun Ryu[2], Geum-Sook Hwang[1,3]

[1]Intergated 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 Nono Science, Ewha Womans University, Seoul, 03760, Korea

P-24

Site-specific characterization of N-glycoproteins in human and mouse plasma samples by LC-MS/MS

Hyun Kyoung Lee[1,2], Ju Yeon Lee[1], Gun Wook Park[1,2], 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

P-25

Size-dependent analysis of urinary exosomal lipids by flow field-flow fractionation and nanoflow ultrahigh-performance liquid chromatography tandem mass spectrometry (nUPLC-ESI-MS/MS)

Joon Seon Yang, Myeong Hee Moon*

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

Mass Spectrometry in Elemental Analysis
: P26 ~ P40

P-26

Comparative study on extraction method of fragrance allergens in water using GC-MS/MS

IN JA LEE*, Haksun Kwon, Chi-hwa An, Jae-Chan Ahn, Bogsoon Kim

Seoul Water Institute, Seoul Metropolitan Government, 04981, Korea

P-27

Isotopic analysis of uranium particles for NUSIMEP-7 using SEM-TIMS combined with simultaneous measurement

Jong-Ho Park[1,2] *, Kahee Jeong[3]

[1]Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, 111 Daedoek-daero-989, Yuseong-gu, Daejeon, 34057, Korea
[2]Department of Radiochemistry & Nuclear Nonproliferation, University of Science and Technology, 217 Gajeong-ro, Yuseong-gu, Daejeon 34113, Korea
[3]Chemistry & Environment Group, Central Research Insitute, Korea Hydro & Nuclear Power, 70 Yuseong-daero-1312, Yuseong-gu, Daejeon 34101, Korea

P-28

Targeted lipidomics approach applied to characterize the lipid metabolism of autophagic liver cells

Seung Cheol Park[1], Jae Won Lee[1], Ah Young Lee[2], Myung-Haing Cho[2], Kwang Pyo Kim[1*]

[1]Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea
[2]Laboratory of Toxicology, Research Institute for Veterinary Science and College of Veterinary Medicine, Seoul National University, Seoul, Republic of Korea.

P-29

Comparative analysis of human milk oligosaccharides by pasteurization and lyophilization

Ye Rin Jin[1,2], Nari Seo[1,2], Tuyen Nguyen[3], Nam Mi Kang[4], Jae Han Kim[3], and Hyun Joo An[1,2*]

[1]Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea
[2]Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea
[3]Department of Food and Nutrition, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea
[4] College of Nursing Konkuk University,268 Chungwondae-ro, Chungju, 27478, Korea
**E-mail: sugar@cnu.ac.kr Tel: 82-42-821-8547, Fax: 82-42-821-8541*

P-30

Alteration of diacyl and ether phosphatidylcholines and phosphatidylethanolamines in the plasma and tissues of HBV mouse model

Sue Ah Noh[1], Jae Won Lee[1], Hyuck Jun Mok[1], Hong Seok Kang[2], Kyun-Hwan Kim[2], Kwang Pyo Kim[1*]

[1]Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea
[2]Department of Pharmacology, School of medicine, Konkuk University, Seoul 143-701, Republic of Korea

P-31

UPLC-MS/MS Based Profiling of Eicosanoids in RAW264.7 Cells

Yu-Ri Choi[1], Jae Won Lee[1], Hyuck Jun Mok[1], Seung Cheol Park[1], Hyung Don Kim[2], Kwang Pyo Kim[1*]

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

[2]Department of Herbal Crop Research, National Institute of Horticultural and Herbal Science, RDA, Eumseong 369-873,

P-32

Steroidal CYP enzyme activities in human amniotic fluid by GC-MS

Soyun Han[1,2], Ju-Yeon Moon[3], Jae-Hong Kim[2], Man Ho Choi[1]

[1]Molecular Recognition Research Center, KIST

[2]College of Life Sciences and Biotechnology, Korea University

[3]Department of Pharmacy, The Catholic University of Korea

P-33

Characterization of site-specific N-glycoproteins in Dried Blood Spot by LC-MS/MS and customized database

Na Young Choi[1,2*], Eun Sun Ji[1], Gun Wook Park[1], Heeyoun Hwang[1], Ju Yeon Lee[1], Hyun Kyoung Lee[1,2], Jin Young Kim[1] and Jong Shin Yoo[1,2]

[1]Biomedical Omics Group, Division of Bioconvergence Analysis, KBSI, Ochang, Korea

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

P-34

Platinum analysis in the kidney of mouse treated with the newly developed anticancer drugs

Sunghwa Choi[1], Eunji Song[1], Eunmi Choi[1], Jiyeon Kim[1], Youngmi Yang[1], Narae Keum[1,2], Minyoung Lee[1,3], Heh-In Im[4], Sang joon Lee[4], Youn Soo Sohn[5], Kyungsu Park[1*]

[1]Advaced Analysis Center, Korea Institute of Science and Technology,

[2]Department of chemistry, Yonsei University,

[3]Department of Chemistry, Graduate school, Kyung Hee University

[4]Center for Neuroscience, Brain Science Institute. Korea korea Institute of Science and Technology,

[5]C&Pharm, Rm 211 Science Building B, Ewha Womans University,

P-35

Analysis of inorganic element content compared to foreign fruits

Sunghwa Choi[1], Eunmi Choi[1], Jiyeon Kim[1], Youngmi Yang[1], Eunji Song[1], Narae Keum[1,2], Minyoung Lee[1,3], Kyungsu Park[1*]

[1]Advaced Analysis Center, Korea Institute of Science and Technology

[2]Department of chemistry,Yonsei University

[3]Department of Chemistry,Graduate school, Kyung Hee University

P-36

Chromium Speciation in Wooden Containers and Packing Materials Using HPLC-ICP-MS

Na-rae Keum[1,2*], Eun-mi Choi[1], Ji-yeon Kim[1], Young-mi Yang[1], Eun-ji Song[1], Sung-hwa Choi[1], Min-young Lee[1,3], Kyung-su Park[1*], Ki-Jung Paeng[2*]

[1]Advanced Analysis Center, Korea Institute of Science and Technology

[2]Department of Chemistry, Graduate school, Yonsei University

[3]Department of Chemistry, Graduate school, Kyung Hee University

P-37

Observations on human milk oligosaccharides affected by pasteurization or lyophilization

Ye Rin Jin[1,2], Nari Seo[1,2], Tuyen Nguyen[3], Nam Mi Kang[4], Jae Han Kim[3], and Hyun Joo An[1,2*]

[1]Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea

[2]Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea

[3]Department of Food and Nutrition, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea

[4]College of Nursing Konkuk University, 268 Chungwondae-ro, Chungju, 27478, Korea

**E-mail: sugar@cnu.ac.kr, Tel: 82-42-821-8547, Fax: 82-42-821-8541*

P-38

Development of LC-MS/MS method for quantitation of alpha-Galactosyceramide.

Soo Hyun Lee[1], Ki Young Choi[2] and Taegwon Oh[2]

[1]Department of Medical Record and Health Information Management, Kongju National University, 56 Gonju Daehak-ro Gongju-si Chungcheongnam-do, Korea

[2]Cellid, Inc., 1 Gwanak-ro, Gwanak-gu, Seoul, Korea

P-39

Development of new chemical separation method for uranium age-dating of UO_2 materials

Eun Ju Choi[1,2], Sang Ho Lim[1,2], Sun-Ho Han[1], Ranhee Park[1], Jinkyu Park[1], Chi-Gyu Lee[1]

[1]Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, Korea

[2]Radiochemistry & Nuclear Nonproliferation, University of Science & Technology, Korea

P-40

Simultaneous determination of chlorogenic acid isomers and metabolites in rat plasma using LC-MS/MS

Won-Gu Choi, Ju-Hyun Kim, Ju-Yeon Moon, Tae Yeon Kong and Hye Suk Lee*

Drug Metabolism and Bioanalysis Laboratory, College of Pharmacy, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Buchen-si, Gyeonggi-do, 420-743,

Medical/Pharmaceutical Science : P41 ~ P5O

P-41

High Throughput Platform to Enirch Native Glycans on Therapeutic Glycoproteins using Liquid Handling System

Gyeong Mi Park[1,2], Youngsuk Seo[1,2], and Hyun Joo An[1,2*]

[1]Graduate School of Analytical Science and Technology, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea
[2]Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea

P-42

Analytical method development and validation of for the quantification of 24S-, 25- and 27-hydroxycholesterols in the cerebrospinal fluid using LC-ESI/MS/MS with picolinic derivatization

Eunju Cha, Kang Mi Lee, Eun Sook Jeong, Ho Jun Kim, Oh-Seung Kwon, Jaeick Lee*

Doping Control Center, Korea Institute of Science and Technology, Hwarangno 14-gil 5, Seongbuk-gu, Seoul 136-791, Korea

P-43

Development of a screening method for multi-class prohibited substances by hybrid sample preparation and liquid Chromatography - Mass spectrometry in doping control

Yongseok Kim, Jaeick Lee, Junghyun Son, Ho Jun Kim, Kang Mi Lee, Ju-Hyung Park, Hophil Min, Changmin Sung, Oh-Seung Kwon, Ki Hun Kim*

Doping Control Center, Korea Institute of Science and Technology, Hwarang-ro 14-gil 5, Seongbuk-gu, Seoul 02792, Republic of Korea

P-44

Metabolomic approach to the effect of co-administration of fenofibrate with atorvastatin in hyperlipidemic patients

Ji Soo Han[1,2], Sang-Hak Lee[3], Sang Yoon Choi[2], Geum-Sook Hwang[1,4*]

[1]Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Book ah hyun-ro 150, Seoul, 120-140, Republic of Korea
[2]Dept of Life Sciences, Korea University, Seoul, 02841, Republic of Korea
[3]Division of Cardiology, Department of Internal Medicine, Severance Hospital, Yonsei University College of Medicine, 50-1 Yonsei-ro, Seodaemun-gu, Seoul 03722, Korea
[4]Department of Life Science, Ewha Womans University, Seoul 120-750, Republic of Korea

P-45

Streamlined Analytical Platform for Primary structure characterization of Therapeutic Interfeon-beta-1a using LC-MS

Nayoung Yun[1, 2,] Nari Seo[1,2,] Unyong Kim[1,2,] Hyun Joo An[1,2*]

[1]Graduate School of Analytical Science Technology, Chungnam National University, Daejeon 305-764, Korea
[2]Asia-Pacific Glycomics Reference Site, Daejeon 305-764, Korea
**E-mail: sugar@cnu.ac.kr, Tel: 82-42-821-8547, Fax: 82-42-821-8541*

P-46

Structural Analysis of Fucosylated N-glycan in Gastric Cancer using LC-QTOF MS/MS

Su Hee Kim*, Sung Hyeon Lee

GLYCAN Co., Ltd., Healthcare Innovation Park, 172 Dolma-ro, Bundang-gu, Seongnam 13605, Korea

P-47

Integrated omics for development of Nm23 activator, NMAC1

Jae-Jin Lee, Jin-Hwan Cho, and Kong-Joo Lee

Graduate School of Pharmaceutical Sciences, College of Pharmacy, Ewha Womans University, Seoul, Korea 120-750

P-48

Degradation of redox-sensitive proteins is promoted by oxidation-induced conformational changes and ubiquitination

In-Kang Song, Jae-Jin Lee, Jin-Hwan Cho, and Kong-Joo Lee

College of Pharmacy and Graduate School of Pharmaceutical Sciences, Ewha Womans University, Seoul 120-750, South Korea.

P-49

The Plasma lipidomic profiling from patients with atrial fibrillation

Youngae Jung[1,2], Geum-Sook Hwang[1,3*]

[1]Western Seoul Center, Korea Basic Science Institute, 150 Bugahyeon-ro, Seodaemun-gu, Seoul 03759, Korea
[2]Department of Life Science, Ewha Womans University, 52 Ewhayeodae-gil, Seodaemun-gu, Seoul, 03760, Korea
[3]Department of Chemistry and Nano Science, Ewha Womans University, 52 Ewhayeodae-gil, Seodaemun-gu, Seoul, 03760, Korea

P-50

Glycomic profiling of serum haptoglobin using nano LC/MS and LC/MS/MS

Sung Hyeon Lee

GLYCAN Co., Ltd., Healthcare Innovation Park, 172 Dolma-ro, Bundang-gu, Seongnam 13605, Korea

Food Environment : P51 ~ P62

P-51

Analysis of perfluorinated compounds, brominated flame retardants, and insecticides in river water samples using LC-MS/MS

Hyeri Lee*, Bo-Mi Lee, Sohui Kim, Jong Beom Khan, Junbae Lee, and Se Uk Cheon

Geum River Environmental Research Center, National Institute of Environmental Research, Okcheon gun, 29027, Republic of Korea

P-52

Simultaneous analysis of thiamine and biotin in infant formula by isotope dilution-liquid chromatography mass spectrometry

Jayeon Joo[1,2], Joonhee Lee[1*], Byungjoo Kim[1], Jeongkwon Kim[2]

[1]Center for Organic Analysis, Division of Metrology for Quality Life, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, South Korea
[2]Department of Chemistry, Chungnam National University, Daejeon, 34134 Korea

P-53

Simple, Instant Determination of Fish and Seafood Freshness

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

P-54

Simple, Instant Evaluation of Beef Freshness

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

P-55

Heavy Metal Content Comparison of Dried Fruit Chips in Korea Market Selling

Young-Mi Yang[1], Eun-mi Choi[1], Ji-yeon Kim[1], Eun-ji Song[1], Sung-hwa Choi[1], Na-rae Keum[1,2], Min-young Lee[1,3], Kyung-su Park[1*]

[1]Advanced Analysis Center, Korea Institute of Science and Technology
[2]Department of Chemistry, Graduate School, Yonsei University
[3]Department of Chemistry, Graduate School, Kyung Hee University

P-56

A Comparative Study of Heavy Metal Concentration in Nut products.

Eun Ji Song[1], Young Mi Yang[1], Sung Hwa Choi[1], Ji Yeon Kim[1], Eun Mi Choi[1], Narae Keum[1,2], Min young Lee[1,3], Kyung Su Park[1*]

[1]Advanced Analysis Center, Korea Institute of Science and Technology
[2]Department of Chemistry, Yonsei University Graduate School
[3]Department of Chemistry, Graduate School, Kyung Hee University

P-57

Changes of the flavonoid glycosides during different stage of tea-processing in green and black tea (*Camelia sinensis*)

Min-Ki Lee[1], Heon-Woong Kim[1], Seon-Hye Lee[1], Young Jin Kim[1], Hyun-Ah Jung[2], Jeong-Sook Choe[1], Jung-Bong Kim[1*]

[1]National Academy of Agricultural Science, Rural Development Administration, 166, Nongsaengmyeong-ro, Iseo-myeon, Wanju-gun, Jeollabuk-do, Republic of Korea
[2]Department of Food Science and Human Nutrition, Chonbuk National University, 567 Baekje-daero, deokjin-gu, Jeonju-si, Jeollabuk-do, Republic of Korea

P-58

Analysis of isoflavone patterns by food processing conditions in Korean soybean (*Glycine max* L.) varieties using UPLC-DAD-QTOF/MS

Heon Woong Kim, Min Ki Lee, Seon Hye Lee, Young-Jin Kim, Hwan Hee Jang, Sung Hyen Lee, Jeong-Sook Choe, Jung Bong Kim*

National Institute of Agricultural Sciences, RDA, 166, Nongsaengmyeong-ro, Iseo-myeon, Wanju

P-59

Characterization of flavonoid glycosides from Korean common sage (*Salvia plebeia* R. Br.) by UPLC-DAD-QTOF/MS

Seon-Hye Lee[1], Heon-Woong Kim[1], Min-Ki Lee[1], Young Jin Kim[1], Youn-Soo Cha[2], Jeong-Sook Choe[1], and Jung-Bong Kim[1*]

[1]National Academy of Agricultural Science, Rural Development Administration, 166, Nongsaengmyeong-ro, Iseo-myeon, Wanju-gun, Jeollabuk-do, Republic of Korea
[2]Department of Food Science and Human Nutrition, Chonbuk National University, 567 Baekje-daero, deokjin-gu, Jeonju-si, Jeollabuk-do, Republic of Korea

P-60

Comparison of flavonoid characteristics between blueberry (*Vaccinium* spp.) and raspberry (*Rubus* spp.) in South Korea using UPLC-DAD-QTOF/MS

Young Jin Kim[1], Heon-Woong Kim[1], Min-Ki Lee[1], Seon-Hye Lee[1], Hwan-Hee Jang[1], Yu-Jin Hwang[1], Jeong-Sook Choe[1], Youn-Soo Cha[2] and Jung-Bong Kim[1*]

[1]Department of Agro-food Resources, National Institute of Agricultural Sciences, Wanju, 55365, Korea
[2]Department of Food Science and Human Nutrition, College of Human Ecology, Chonbuk National University, Jeonju, 561756, Korea

P-61

Rapid screening of 29 sulfonamide diuretics in dietaty supplements based on extracted common ion chromatogram and neutral loss scan by UHPLC-Q/TOF MS

Nam-Yong Ki, Wonwoong Lee, Jisu Hur, Keon-Hee Ko, Jongki Hong*

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

P-62

Simultaneous analysis of the 3 PFASs in rat plasma and tissues using UPLC-MS/MS: Application to pharmacokinetics and tissue distribution

Sook-Jin Kim, Dong-Seok Lee, Hea-Young Cho*

College of Pharmacy, CHA University, 335 Pangyo-ro, Seongnam-si, 13488, Korea

General
: P63 ~ P72

P-63

MS/MS fragmentations of biotoxins and simultaneous determination of diarrhetic shellfish toxins in bivalves by UPLC-ESI-MS/MS combined with time segment polarity switching mode

Myoung Eun Lee, Wonwoong Lee, Jongki Hong*

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

P-64

Glycan signatures of human saliva

Hantae Moon[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

P-65

The importance for van der Waals potential for accurate collision cross section calculations

Jong Wha Lee[1,2], Hugh I. Kim[2*]

[1]Dept of Chemistry, Pohan University of Science and Technology, 77 Cheongam-Ro, Pohang 37673, Republic of Korea
[2]Dept of Chemistry, Korea University, 145 Anam-ro, Seoul 02841, Republic of Korea

P-66

The effect of Sodium and Potassium ions for sucrose detection by comparing charcoal, DHB and CHCA matrices in MALDI-MS analysis

Jihyun Paek, Dabin Lee, Yeoseon Kim, Sooyeon Chae, Jeongkwon Kim*

Dept. of Chemistry, Chungnam National University, Deajeon, 34134, Korea

P-67

Metabolic profiling of *Cirsium* species during floral budding and full flowering

Min-Sun Kim[1], Geum-Sook Hwang[1,2*]

[1]Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Seoul 120-140, Republic of Korea
[2]Department of Life Science, Ewha Womans University, Seoul 120-750, Republic of Korea

P-68

Reactive paper spray ionization mass spectrometry for the analysis of the conjugated ketones

Soobin Choi, Sangwon Cha

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

P-69

Real-time Resolution of Analytes, without Chromatographic Separation

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

P-70

Serial lectin affinity chromatography for comparative serum glycoproteomics on colon cancer biomarker discovery

Jinwook Lee, Wonryeon Cho*

Department of Bionanochemistry, Wonkwang University, Iksandearo 460, Iksan, 54538, South Korea

P-71

Study of variations in human saliva N-glycans

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

P-72

Effect of Ca(II) on the conformation and aggregation process of alpha-synuclein

Jong Yoon Han, and Hugh I. Kim

Deptartment of Chemistry, Korea University, Seoul 02841, Korea

P-01

Development of a MATLAB-based dissolved organic matters (DOMs) analysis program

Inae Jang[1], Ji-Hyung Park[2], and Han Bin Oh[1]*

[1]*Dept of Chemistry, Sogang University, 35 Baekbeom-ro, Seoul, 04107, Korea*

[2]*Dept of Environmental Science & Engineering, Ewha Wamans University, 52 Ewhayeodae-gil, Seoul, 03760, Korea*

Dissolved organic matters (DOMs) is a complex mixture of degradation products from plants and animals and it plays a key role in the global carbon cycle. The ultra-high resolution mass spectrometer, such as Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS), is required to analyze DOMs in a river or ocean. Because the number of DOMs that exist in the mass spectrum is at least over 2000 peaks, an automatic analysis software is needed for the analysis of the numerous peaks of DOMs. Thus, we developed a software for the analysis of DOMs using a MATLAB language. In this study, we collected water samples of the Han River at Amsa located in the main stem and Jungnang located in the tributary. The collected water samples divided into two microtubes, and then one was treated C18 solid phase extraction (SPE) and the other was subjected to C18 SPE after microbal incubation for 5 days. Mass spectra were obtained by 15 T FT-ICR MS (SolariX XR, Bruker Daltonics, Germany) and various Van Krevelen diagrams were plotted using a home-coded MATLAB program. To conclude, the Han River of Amsa and Jungnang water samples were analyzed by a semi-automatic home-coded program, and a graphic user interface (GUI) will be added in the near future.

P-02

Do-It-Yourself (DIY) Manufacture of a Nano-LC MALDI Spotter Robot using a 3D Printing Technology

Jae-ung Lee, Han Bin Oh

Department of chemistry, Sogang University, Seoul 121-742, Korea

The 3D printing technology is growing very rapidly, and is bringing about significant advances in many research areas. On the 3d printing related website, the stories of making 3d printed parts and custom equipment have been posted. In this research, we made a DIY nano-LC MALDI spotter robot using 3D printed custom parts. Using this equipment, nano-LC and MALDI matrix loading can be conveniently coupled online and thus the separated eluents from nano-LC can be loaded automatically onto the MALDI plate. This DIY robot was made of only 3d printed parts and the parts on the online marketplace, so that anyone can make it and carry out maintenance easily and inexpensively. In this DIY robot, the loading speed can be readily controlled using a home-coded software. In addition, a camera is equipped so that the loading process can be monitored.

P-03

Ionization and sensitivity of polycyclic aromatic hydrocarbons using GC-ESI/MS/MS, GC-APCI/HRMS and LC-ESI/MS/MS

Eunju Cha[1], Eun Sook Jeong[1], Hophil Min[1], Changmin Sung[1], Oh-Seung Kwon[1], Sangwon Cha[2], Jaeick Lee[1*]

[1]Doping Control Center, Korea Institute of Science and Technology, Hwarangno 14-gil 5, Seongbuk-gu, Seoul 136-791, Korea

[2]Department of Chemistry, Hankuk University of Foreign Studies, Oedae-ro, Mohyeon-myeon, Cheoin-gu, Yongin-si, Gyeongi-do 17035, Korea

Polycyclic aromatic hydrocarbons (PAHs) as nonpolar compound are composed of a number of fused aromatic rings, and this structural characteristics can cause poor ionization. In this study, we investigated ionization profiles according to analyt phase or ionization source for analysis of PAHs using various ionization methods such as GC-ESI/MS/MS, GC-APCI/HRMS and LC-ESI/MS/MS. Despite the difficulty of ionization under ESI, gas-phase PAHs were easily protonated and were predominantly ionized to $[M+H]^+$ using GC-ESI/MS/MS. In contrast, liquid-phase PAHs using LC-ESI/MS/MS were generated both radical cation ($[M]^{+\bullet}$) and $[M+H]^+$ under ESI, and gas-phase PAHs using GC-APCI/HRMS were also showed competitive ionization profile. In addition, the limit of detection (LOD) was performed to evaluate the sensitivity using GC-ESI/MS/MS, and this result was compared with LC-ESI/MS/MS and GC-APCI/HRMS. Moreover, relationship between sensitivity and proton affinity (PA) was investigated based on structural characteristics. The sensitivity was enhanced as the PA increased and benzene rings were continuously arranged. The developed GC-ESI/MS/MS method provided good sensitivity and selectivity with narrow peak shape. Therefore, we presented the potential of GC-ESI/MS/MS method as new ionization tool for PAH analysis, in this study.

This work was supported by an intramural grant from Korea Institute of Science and Technology.

P-04

Real-time ambient air monitoring using selected ion flow tube mass spectrometry (SIFT-MS)

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) is a real-time analytical technique that detects volatile organic compounds and certain inorganic gases down to part-per-trillion levels usually with no sample preparation. These characteristics mean that SIFT-MS can easily be applied to real-time detection of volatile organic air pollutants.

This paper presents the results of a field evaluation of real-time air analysis using SIFT-MS undertaken at Shu-Lin Primary School in Taoyuan County, near Taipei, Taiwan R.O.C. from 19 to 21 July 2011. Full scan SIFT-MS data were acquired and subsequently processed using Syft's proprietary software package to give analyte

P-05

Analysis of vehicle interior air quality in new cars using the syft technologies' VOICE 200 SIFT-MS instrument

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

On 1 March 2012, the Chinese government issued a standard to regulate the Vehicle Interior Air Quality (VIAQ) of new vehicles (Table 1). The Japanese standard adds additional VOCs: tetradecane, p-dichlorobenzene, dibutylphthalates and dihexylphthalates. The standards are based around two traditional laboratory-based analytical methods (GC/MS and HPLC) that are expensive, have slow sample turnaround, and are incompatible with rapid testing on the production line or in the parking lot.

P-06

Online non-contiguous fractionating and concatenating device coupled to two dimensional reverse phase/reverse phase liquid chromatography system for efficient and comprehensive proteomic analyses.

Hangyeore Lee, Jeong Eun So and Sang-Won Lee

Department of Chemistry, Korea University, Seoul 136-701

In this study, a novel online two-dimensional reverse-phase/reverse-phase liquid chromatography (2D-RP/RPLC) separation platform, employing a newly developed online non-contiguous fractionating and concatenating device (NCFC fractionator), will be presented. In bottom-up proteomics analyses of a complex proteome, this system provided significantly improved exploitation of the separation space of the two RPs, considerably increasing the numbers of peptides identified compared to a conventional contiguous 2DRP/RPLC method. The fully automated online 2D-NCFC-RP/RPLC system bypassed many labor-intensive manual processes (i.e. offline fractionations, manual pooling, clean-up, drying/reconstitution, and autosampler fraction injection) required with the conventional offline 2D-NCFC RP/RPLC method, and thus, it offers minimal sample loss in a context of highly reproducible 2D-RP/RPLC experiments.

P-07

Profiles of hepatic lipids from rabbits using nanoflow UPLC-ESI-MS/MS

Seul Kee Byeon, Myeong Hee Moon*

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

Deposit of fat in the liver due to causes other than alcohol consumption leads to non-alcoholic fatty liver disease (NAFLD), in which the liver becomes damaged. As lipid play central roles in various cellular functions, any change in hepatic lipid homeostasis is directly related with pathogenesis of liver disease such as NAFLD. In this study, ultrahigh-pressure liquid chromatography-electrospray ionization tandem mass spectrometry (nUPLC-ESI-MS/MS) was utilized in order to profile any change in lipidome of rabbits that were grown under highly probable conditions that would induced NAFLD, such as inflammation, high cholesterol diet, and high cholesterol diet with inflammation.

More than 300 phospholipids (PLs), sphingolipids (SLs), and glycerolipids (GLs) were structurally determined and rapidly quantified within merely 20 minutes in selective reaction monitoring (SRM) mode. When compared with healthy control rabbits, significant and dramatic changes were observed in various classes of lipids from groups that were treated with high cholesterol diet and high cholesterol diet with inflammation, indicating that intake of high cholesterol directly affects hepatic lipidome.

P-08

Isotope-labeled methylation for quantitative analysis of phospholipids and enhancement in cardiolipin profiling by nUPLC-ESI-MS/MS

Jong Cheol Lee, Seul Kee Byeon, Myeong Hee Moon*

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

Quantitative analysis of phospholipids using liquid chromatography-electrospray ionization-mass spectrometry (LC-ESI-MS) is generally achieved using various types of internal standards. However, the stability of the ESI fluctuates at times and as a number of internal standards avaialable are very limited, not to mention that they tend to be very expensive. In this study, an isotope-labeled methylation (ILM) method for the relative quantification of phospholipids (PLs) with nanoflow LC-ESI-MS/MS and its applicability for cardiolipins (CLs) were investigated. The ILM method is based on methylation (CH_3 or CHD_2) of the phosphate or carboxyl group of PL using (trimethylsilyl)diazomethane, which is a methylation reagent. For light labeled methylation, methanol with HCl were used while deuterated methanol with DCl were used for heavy labeled methylation. The methylation efficiency values were higher than 96% for most PL class under acidic condition. For evaluation of ILM method, nLC-ESI-MS/MS analysis of PLs in SRM mode was carried out by varying the mixing ratio of H-/D-methylated PL standards and good linear relationship was observed with error values less than 6.6% in average.

As a result, ILM method was applied to lipid extracts from DU145 cell line with and without D-allose treatment, resulting in quantification of 83 PLs. This method revealed that identification/quantification of lipids, especially PAs and CLs, were highly enhanced relative to quantification without ILM.

P-09

Lipidomic analysis of skeletal muscle tissues of p53 KO mice by Nanoflow LC-ESI-MS/MS

Se Mi Park, Seul Kee Byeon, Myeong Hee Moon*

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

Lipids play crucial roles in storing energy, maintaining cell structure, and mediating cell signaling in various biological systems. The tumor-suppressor gene p53 is a key player in regulating the cell cycle and apoptosis when cell is damaged either in their DNA, telomere erosion, or hypoxia. In addition, it is known to play a balancing role between glycolytic pathways and mitochondrial respiration for energy generation. In this study, a total of 329 lipid species from skeletal muscle tissues (gastrocnemius (Gas) and soleus (Sol)) in p53 KO mice were structurally identified and quantitatively analyzed using nanoflow ultrahigh-performance liquid chromatography-electrospray ionization tandem mass spectrometry (nUPLC-ESI-MS/MS). Lipids from Sol tissues were affected by p53 KO more significantly than those from Gas in all lipid profile, overall. In p53 KO mice, the total level of 5 lipid classes (lysophosphatidylcholine (LPC), lysophosphatidylserine (LPS), phosphatidic acid (PA), triacylglycerol (TAG), and sphingomyelin (SM)) were significantly increased ($p < 0.05$) by about 2-fold in Sol tissue while monohexosylceramide (MHC) was significantly increased by greater than 2-fold in Gas tissue. Among 65 TAGs that were identified, 6 TAGs (44:2-, 46:0-, 58:5-, 58:8-, 58:9-, and 50:0-) were significantly increased ($p < 0.05$) by 2~3-fold in Sol tissue. Overall MHC including 3 MHC (d18:0/24:0-, d18:1/22:0-, and d18:1/24:0-) were significantly increased ($p < 0.05$) by 2~4-fold in Gas tissue.

P-10

Global changes in lipids of brain tissues from p53 KO mice: cortex, hippocampus and hypothalamus

Sang Tak Lee[1], Jong Cheol Lee[1], Je Kyung Seong[2], Myeong Hee Moon[1]*

[1]*Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea*
[2]*College of Verterinary Medicine, Seoul National University, 1 Gwanak-ro, Seoul, 08826, Korea*

Lipidomics has attracted great attention due to their significiant roles in formation of cell membrane, energy storage, and as signaling messengers in central nervous system. Among various roles, lipids in central nervous system are often perturbed in myelin sheath and other tissues after certain pathologic event, such as cancer and neurodegenerative diseases. A p53 gene is a well-known tumour suppressor that prevents genome mutations that can cause cancers and related to metabolism involved in cancer development.

In this study, a comprehensive lipidomic profiling from three different brain tissues (cortex, hippocampus, and hypothalamus) of mice with and without p53 deficiency was carried out by nanoflow liquid chromatography tandem mass spectrometry (nLC-MS/MS). Non-targeted global profiling of lipids was performed and total 455 lipids including phospholipids (PLs), sphingolipids (SLs), and triacylglycerols (TAGs) were identified based on spectra from collision-induced dissociation (CID). A targeted quantification of lipids was accomplished by selective reaction monitoring (SRM) method. As a result, changes of PLs containing acyl chains (docosahexaenoic acid and arachidonic acid) were expressed in relation to cell apoptosis on p53 KO mice. Furthremore, sphingomyelines (SMs) and Ceramides (Cers) showed that accumulation of SMs is likely to occur due to the inhibition of apoptosis in the p53 KO condition.

P-11

Comprehensive profiling analysis of 20 urinary neurochemicals using *in situ* derivatization and liquid chromatography-tandem mass spectrometry

Wonwoong Lee, Hye Jung An, Youna Kim, Jongki Hong*

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

Dopamine, serotonin, GABA and their metabolites play a key role in multiple regulatory systems and the change of their physiological levels are closely associated with neurological disorders. Thus the development of a reliable analytical method of neurochemicals in biological fluids is important to discover potential biomarkers for the diagnosis, treatment and prognosis of neuronal disease. However, the analysis of neurochemicals in biological sample was challenging, because of highly different polarities between basic precursor and acidic metabolites, their low physiological amounts and high matrix interferences in biological samples. In this study, we developed a liquid chromatography-tandem mass spectrometry (LC-MS/MS) combined with Fischer esterification for comprehensive profiling of 20 neurochemicals in urine. *In situ* Fischer esterification could greatly improve the peak separation capacity and MS detection in a single run LC-ESI-MS/MS-positive ion mode due to reducing distinct physicochemical properties. After esterification, desalting process could significantly reduce the ion suppression of some analytes in MS detection. Esterified acidic neurochemicals were well retained on reversed-phase C18 column and separated with other basic neurochemicals within 6 min. Also, esterification analytes produced specific fragment ions to provide high sensitivity and selectivity in MRM mode. Established method was validated in terms of linearity, precision, accuracy, recovery, and matrix effect. Human urine samples collected from patients with Parkinson's disease and controls (patients; 21, controls; 10) were successfully analyzed to explore important biomarkers caused in metabolic disorder. In conclusion, this method may be helpful for comprehensive studying of neuropathological mechanism and discovering biomarkers for neurological disease.

P-12

Korean whole salivary proteome: a preliminary report

Ha Ra Cho, Han Sol Kim, Yong Seok Choi*

College of Pharmacy, Dankook University, Cheonan-si, Chungnam 31116, South Korea

Saliva is considered as a good biological fluid for the purpose of monitoring biomarkers due to its suitable characteristics as a biological sample, for example, the non-invasive nature during its sampling and the easiness of collecting the relatively large volume of a sample. However, while proteomic studies on various types of saliva have been carried out in the United States and Europe over a decade, any proteomic research on saliva was never tried in Korea, yet. Thus, as the first step of Korean salivary proteomics, we are conducting a study to construct the first Korean reference salivary proteome, and its preliminary report is presented here. From the proteomic analyses of whole saliva (WS) samples from healthy Korean volunteers, many proteins in Korean WS have been being identified. While gene ontology distributions of Korean WS proteome are similar with those previous reported from other countries, a large portion of proteins in Korean WS is found to be unique by the comparisons with salivary proteome databases. Thus, the distinctiveness of Korean salivary proteome is strongly expected and the results from this on-going study could be widely used as the basement of future researches on the discovery/application of disease biomarkers from Korean WS.

P-13

Metabolic profiling of human atherosclerotic aorta based on liquid chromatography/mass spectrometry.

Sunhee Jung[1,2], Miso Nam[1,2], Do Hyun Ryu[2], Geum-Sook Hwang[1,3]*

[1]*Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institue, Book ah hyun-ro 150, Seoul, 120-140, Republic of Korea*

[2]*Dept of Chemistry, SungKyunKwan University, SeoBoo-to 2066, Suwon, 440-746, Republic of Korea*

[3]*Department of Life Science, Ewha Womans University, Seoul 120-750, Republic of Korea*

Atherosclerosis is the main cause of mortality in industrialized countries. However, only a limited number of studies on atherosclerosis was proceeded in metabolic profiling of human tissue. In the present study, we performed a global and targeted metabolic profile of plaque-containing aortic tissue from patients undergoing aortic surgery using liquid chromatography/mass spectrometry (LC/MS). Partial least squares-discriminant analysis (PLS-DA) plots obtained from ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/Q-TOF MS) analysis showed a clear differentiation between plaque-containing and control plaque-free aortic tissue. Significantly altered metabolite species were amino acids, purines, pyrimidines, cholines, ceramides, and lysophosphocholines. We confirmed the increase of tryptophan, kynurenine, and kynurenine/tryptophan ratio in plaques by targeted metabolic profiling using ultra-performance liquid chromatography/triple quadrupole mass spectrometry (UPLC/QqQ MS). In addition, the down-regulated glutathione (GSH), oxidized glutathione (GSSG), and GSH/GSSG were observed. The change of metabolites in the purine and glutathione pathways showed dysregulation of oxidative stress in plaques, whereas altered level of ceramide, tryptophan, and kynurenine results from inflammation in plaques. This study demonstrated that LC/MS based metabolite profiling can be a useful tool to understand metabolic distribution of human atherosclerotic aorta and may provide the insight for pharmacotherapeutic intervention.

P-14

Targeted and global metabolic analysis of rat urine from high tryptophan availability models

Yu Ri Cho[1], Mi Jung Ji[1], Mi Yeon Lee[1], Suk Youn Son[1], Ki Soo Lee[1], Soo Hyun Lee[2], and Hyun-Mee Park[1]

[1]*Advanced Analysis Center, Korea Institute of Science and Technology, Korea*
[2]*Department of Medical Record and Health Information Management, Kongju National University*

Tryptophan, an essential amino acid, is related to various physiological activities such as mood and inflammation. The primary metabolic functions are protein, serotonin, and kynurenine synthesis, which are affected by tryptophan availability in the circulatory system. In this study, we investigated how high tryptophan availability influences endogenous metabolism including serotonin and kynurenine synthesis. Two types of animal model for high tryptophan availability were established by oral administration at excess dose of 125mg/kg tryptophan (Type1), and at dose of 100mg/kg caffeic acid with 125mg/kg of tryptophan (Type2) for 7 days (Caffeic acid is known to inhibit tryptophan breakdown in physiological condition). Analytical urine samples were collected two times at 6 and 24 hours after final administration. The effects on serotonin and kynurenine synthesis were evaluated through targeted metabolic analysis by LC-MS/MS and those on entire metabolism were with global metabolomics by UPLC-QTOF-MS. In targeted analysis, serotonin level in 6 hour urine sample from Type2 was higher than that form Control and Type1. In global metabolomic analysis, significant changes were recognized at the levels of taurine, norepinephrine, and cysteine, which are involved in various metabolism such as the methionine, tryptophan, phenylalanine, B6, folate metabolism and TCA cycle. To assure chronic effect of high tryptophan availability on endogenous metabolism, long term studies are needed.

P-15

Intact glycopeptide analysis of targeted serum haptoglobin

Seunghyup Jeong[1, 2], Unyong Kim[1, 2] and Hyun Joo An[1, 2*]

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

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

Glycosylation is one of the most common post-translational modification. Glycans in blood are secreted from cells and these glycans are changed depending on health condition and a variety of diseased including immune disorders and cancers. Generally, glycosylation analysis has to be performed on three different approach: released glycans, glycopeptides, and intact glycoproteins. Released glycan analysis can provide detailed compositional and isomer information of each glycans. Intact glycoprotein analysis yield intuitive information of the overall glycoforms of protein population and has additional advantages such as simple, easy handling of sample preparation and time saving for analysis. However, these two types of analysis cannot provides information on the actual site of glycosylation. In this study, we have applied intact glycopeptide analysis method to haptoglobin, a positive acute-phase protein with immunomodulatory properties, without purification step. First, haptoglobin is denatured and alkylated by DTT and IAA. Afterward, haptoglobin is treated by trypsin for digestion. Finally, digested haptoglobin is analyzed by UHPLC Q-TOF MS. Haptoglobin have 4 glycosylation sites and 3 tryptic glycopeptides GP1 [MVSHH**N**LTTGATLINEQWLLTTAK], GP2 [NLFL**N**HSE**N**ATAK], and GP3 [VVLHP**N**YSQVDIGLIK] (peptide sequence order). We successfully separate 3 tryptic glycopeptides and profile the glycoform of each glycosylation sites. In further study, we will apply this method to clinical sample for gastric cancer biomarker discovery.

P-16

Evaluation of Single Particle ICP-MS for Screening Nanoparticles in Environmental Samples

Sang-Jun Lee[1,2], Seok-Won Jang[1], Sung Ik Yang[1*], Yong-Hyeon Yim[2*]

[1]*Department of Applied Chemistry, Kyung Hee University, Yongin, 17104 Republic of Korea*

[2]*Center for Inorganic Analytical Chemistry, Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 305-340 Republic of Korea*

**E-mail: siyang@khu.ac.kr, yhyim@kriss.re.kr*

Increased use of engineered nanoparticles (NPs) in various fields of industry and consumer products has imposed potential risks to the environment and human health. Therefore, it is important to characterize NPs from the manufacturing to the final disposal in the environment for better understanding of the life-cycle of NPs and its impact. Recently, single particle (SP) ICP-MS has been attracted a lot of attentions to characterize the NPs, since it can simultaneously provide the information on elemental composition, particle size, and particle number concentration of a nanoparticle. It also allows detection of small numbers of NPs in a sample which is quite suitable for detection of low-abundant NPs in environmental samples. In a favorable condition, dissolved ion signals are distinguishable from NPs signals and provide additional information on dissolve ions. SP ICP-MS can be developed as a fast screening method for NPs in a real-world sample due to its decent analytical characteristics. For this purpose, we carried out preliminary investigation focused on technical limitations of SP ICP-MS. Relatively well-characterized Au and Ag NPs were used as the test samples. Element-dependent detection limits for NPs size, the influence of blank signal drift of easily dissoluble NPs, and separation of NPs pulses from electronic noises were investigated.

P-17

Proteomic Analysis to Identify Interactomes of Human N-alpha-acetyltransferases 40 (hNAA40) using LC-MS/MS

Yeirin Lee[1], Dowoon Nam[1], Hyun Seok Kim[2*] and Sang-Won Lee[1*]

[1]Department of Chemistry, Korea University, Seoul, 02841, South Korea
[2]Department Bioinspired Science, Ewha Womans University, Seoul, 03760, South Korea

Protein N-alpha-terminal acetylation is one of the most abundant modifications of eukaryotic proteins, where an acetyl moiety is transferred from acetyl-coenzyme A to protein N-terminal amino group and is catalyzed by N-terminal acetyltransferases (NATs). There are six enzymes in eukaryotic NAT family (NatA through NatF) and they differ in both subunit composition and substrate specificity. Unlike other NATs, NatD consists of one catalytic subunit, named Naa40p, which determines its catalytic activity and specificity, and only two substrates of NatD have been found in both yeast and humans: histones H2A and H4.

In this work, I have investigated proteins existing in immunoprecipitates with FLAG-tagged human Naa40p (hNaa40) to identify interactomes of hNaa40 using bottom-up proteomics. The immunoprecipitates of hNaa40 were digested into peptides and tryptic digests were analyzed via liquid chromatography-tandem mass spectrometer (LC-MS/MS). From results of data analysis, total 667 of representative proteins were identified. DNA-PK, Ku80, PARP1 and Ku70 were identified with high confidences suggesting that hNaa40 play important roles in response to DNA damage.

P-18

Proteomic analysis to reveal the mechanism of E-cadherin loss in a gastric cancer mouse model

Seung-Ik Ko[1], Min-Sik Kim[2] and Sang-Won Lee[1*]

[1]Department of Chemistry, Korea University, Seoul, 136-701, Republic of Korea
[2]Department of Applied Chemistry, Kyunghee University, Gyeonggi-do, 446-701, Republic of Korea

Despite a decrease in the number of reported cases of intestinal type of gastric cancer, which is influenced by environmental factors and responds well to treatment, diffuse type of gastric cancer is increasing, which is influenced by genetic impacts and responds poorly to treatment. The loss of E-cadherin is well known to develop gastric cancer, but the mechanism is not explained in previous researches. In this study, we performed proteomic analysis for diffuse-type gastric cancer in a mouse model which was conditional knockout of Smad4, p53 and E-cadherin (*i.e. Pdx-1-Cre; Smad4$^{F/F}$;Trp53$^{F/F}$;Cdh1$^{F/+}$*). From NCC (National Cancer Center), we received three types of tissues of spontaneous gastric cancer mouse model using the conditional knockout system as follows: gastric normal, gastric tumor and duodenal tumor. One allele of *Cdh1* in gastric cancer resulted in down regulating of E-cadherin expression for transcriptional repression to the other allele, whereas a mouse of duodenal cancer had no loss of E-cadherin at the same condition. Here, our study revealed a new mechanism by which loss of E-cadherin in the gastric cancer with one allele of *Cdh1* was proceeded. In summary, by performing extensive quantitative proteome profiling experiments, we identified 8,897 protein groups of 142,226 non-redundant peptides and 2,115 differentially expressed proteins (DEPs, >2.0 fold & p-value < 0.1). A transcriptional factor *Zeb2* repressed expression of *Cdh1*, and *Pkp2*, which is one of the target genes of *Zeb2*, was also down-regulated as *Cdh1*.

P-19

Quantitative mouse retinal proteome analysis of Vascular Endothelial Growth Factor (VEGF)-induced vascular hyperpermeability by LC-MS/MS

Jingi Bae, and Sang-Won Lee*

Department of Chemistry, Korea University, Seoul, 136-701, South Korea

Vascular endothelial growth factor (VEGF) is known as vascular permeability factor which causes dysregulation of junction integrity between endothelial cells and resultant vascular leakage. Also, retinal vascular hyperpermeability causes macular edema which leads to visual deterioration and various retinal disease such as diabetic retinopathy. Accordingly, anti-VEGF agents have been used to treat retinal vascular hyperpermeability. However, VEGF not only promotes vascular permeability, but also plays an important role in the survival of normal endothelial and neuronal cells in the retina. Also, because anti-VEGF has potential toxicity, the goal of this study is to identify novel therapeutic targets for retinal vascular hyperpermeability.

In this study, we performed quantitative proteome profiling analysis on mice under three conditions (Control, VEGF, VEGF plus Anti-VEGF group). We used the iTRAQ (Isobaric tag for relative and absolute quantitation) for labeling on the peptide after modified FASP (Filter Aided Sample Preparation) for digestion. The labeled peptide samples were divided into 24 fractions by using a mid pH reverse phase liquid chromatography and each fraction was individually analyzed by LC-MS/MS.

As a result, we identified a total 205,730 non redundant peptides, 8,685 proteins with 479 DEPs. Among them, β2 integrin was up-regulated by VEGF treatment, but the alteration was inhibited by co-treatment of VEGF and anti-VEGF antibody which also confirmed by western blotting analysis. Finally, we experimentally demonstrated that inhibition of the β2 integrin pathway salvaged VEGF-induced retinal vascular hyperpermeability, thus β2 integrin can serve as an effective therapeutic target for retinal vascular hyperpermeability.

P-20

Increasing Sensitivity and Accuracy in Co-fragmented Peptide Identifications from Tandem Mass Spectra using Multiplexed Post-Experimental Monoisotopic Mass Refinement (*m*PE-MMR)

Inamul Hasan Madar, Seung-Ik Ko, Hokeun Kim and Sang-Won Lee*

Laboratory of Gaseous Ion Chemistry, Department of Chemistry, Research Institute for Natural Sciences, Korea University, Seoul 136-701, South Korea

Mass spectrometry (MS)-based proteomics, which uses high-resolution hybrid mass spectrometers such as the quadrupole-orbitrap mass spectrometer, can yield tens of thousands of tandem mass (MS/MS) spectra of high resolution during a routine shotgun proteomics experiment. Despite being a fundamental step in MS-based proteomics, the accurate determination and assignment of precursor monoisotopic masses to the MS/MS spectra remains difficult. The difficulties stem from imperfect isotopic envelopes of precursor ions, inaccurate charge states for precursor ions, and cofragmentation of MS/MS spectra. Here, we describe a composite method of utilizing MS data to efficiently assign accurate monoisotopic masses to MS/MS spectra, including those subject to cofragmentation and unassigned charge state. The method, "multiplexed post-experiment monoisotopic mass refinement" (*m*PE-MMR), consists of the following: multiplexing of precursor masses to assign multiple monoisotopic masses of cofragmented peptides to the corresponding multiplexed MS/MS spectra, multiplexing of charge states to assign correct charges to the precursor ions of MS/MS spectra with no charge information, and mass correction for inaccurate monoisotopic peak picking. When combined with MS-GF+, a database search algorithm based on fragment mass difference, *m*PE-MMR effectively increases both sensitivity and accuracy in PSMs and peptide identification from complex high-throughput proteomics data compared to conventional methods.

P-21

Relative metabolite ratio of di(2-ethylhexyl) phthalate in obese children.

Jiwon On[1,2], Sang Won Lee[2], Mi jung Park[3], Jeongae Lee[1], Heesoo Pyo[1*]

[1]*Molecular Recognition Research Cent'er, Korea Institute of Science and Technology*

[2]*Department of Chemistry, Korea University*

[3]*Department of Pediatrics, Sanggye Paik Hospital, Inje University College of Medicine*

Di(2-ethylhexyl) phthalate (DEHP) is endocrine disrupting chemicals that are commonly used in plastic products as plasticizers. It is known that DEHP causes adverse effects on endocrine functions and reproductive organs of humans. DEHP is primarily metabolized to mono(2-ethylhexyl)phthalate (MEHP), further oxidized to secondary metabolites(MEOHP, MEHHP, MECPP). Relative metabolite ratio (RMR) were calculated to examine the difference in DEHP exposure levels to the primary and secondary metabolites. In this study, we examined the association between DEHP exposure by relative metabolite ratio (RMR) and obesity.

We used a spot urine sample from 5 to 16 years. We used to classify participants as overweight (BMI>85th pecentile) or obese (BMI>95th percentile). We analysed concentration of DEHP metabolites with trimethylsilylation (TMS) using isotope dilution gas chromatography–tandem mass spectrometry.

Major metabolites of DEHP are mono(2-ethyl-5-carboxypentyl)phthalate≫ mono(2-ethyl-5-hydroxyhexyl)phthalate≥mono(2-ethyl-5-oxo-hexyl)phthalate〉MEHP. There were no statistically significant differences between concentration of DEHP metabolites and obesity status. On the other hand, RMR were statistically some significant.

P-22

Label free quantitative proteomics using peptide isotope peak intensities in mass spectrometry

Ki Na Yun[1,2], Gun Wook Park[1], Ju Yeon Lee[1], Eun Sun Ji[1], Mee-Jung Han[3], Han Bin Oh[2], Jong Shin Yoo[1], Jin Young Kim[1]

[1]Biomedical Omics Group, Korea Basic Science Institute, Ochang, Korea
[2]Department of Chemistry, Sogang University, Seoul, Korea
[3]Department of Biomolecular and Chemical Engineering, Dongyang University, Yeongju, Korea

We have developed an automated label-free protein quantification method that utilizes the combined intensity of top three isotope peaks at three highest MS spectral point. It was named three isotopes quantification (TIQ) that allows for a comparative protein analysis in a computational manner. The efficiency of TIQ was demonstrated by a benchmark dataset with two proteomes at known ratios. We accurately detected the mixing ratio over the entire protein expression range, with greater precision for abundant proteins. The performance of TIQ was also compared to that of SWATH-MS in terms of the number of quantified peptides and proteins and the specificity to detect differentially abundant proteins, where SWATH-MS is another approach for label free protein quantification utilizing the MS/MS intensity. There are a few advantages to TIQ. First, because it requires no peak area generation from the extracted ion chromatogram (XIC), it allows high-speed quantitation. Second, it is effective to remove signal interference from co-eluted ions with similar m/z values by evaluating the isotope pattern. And third, considering top three isotope peaks provides more sensitive results with better S/N ratios.

P-23

A metabolomics-driven approach reveals metabolic responses and mechanisms in the rat heart following myocardial infarction

Miso Nam[1,2], Sunhee Jung[1,2], Do Hyun Ryu[2], Geum-Sook Hwang[1,3]

[1]*Intergated 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 Nono Science, Ewha Womans University, Seoul, 03760, Korea*

Myocardial infarction (MI) is caused by myocardial necrosis resulting from prolonged ischemia. However, the biological mechanisms underlying MI remain unclear. We evaluated metabolic and lipidomic changes in rat heart tissue from sham and MI at 1hr, 1day and 10day after coronary ligation, using global profiling based on metabolomics. A time-dependent increase or decrease in polar and lipid metabolite levels was measured. The S-adenosylmethionine (SAM) concentration and the SAM/S-adenosylhomocysteine (SAH) ratio gradually decreased in a time-dependent manner and were significantly downregulated 10 days after MI. Transcriptome analysis revealed that the levels of coenzyme Q (*Coq*)-*3* and *Coq5*, both of which are SAM-dependent methyltransferases, were decreased in the MI groups. These results suggested that dysregulation of SAM may be related to down regulated COQ biosynthetic pathway. In addition, short-chain (C3) and medium-chain (C4-C12) acylcarnitine levels gradually decreased, whereas long-chain acylcarnitine (C14-18) levels increased, owing to a defect in β-oxidation during ischemia. These changes are related to energy-dependent metabolic pathways, and a subsequent decrease in adenosine triphosphate concentration was observed. The comprehensive integration of various omics data provides a novel means of understanding the underlying pathophysiological mechanisms of MI.

P-24

Site-specific characterization of N-glycoproteins in human and mouse plasma samples by LC-MS/MS

Hyun Kyoung Lee[1,2], Ju Yeon Lee[1], Gun Wook Park[1,2], 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-glycosylation of protein showed many differences between mouse and human. Usually N-glycosylation is directly involved in biological process and plays crucial role in human diseases due to their unusual biological sensitivity. Therefore, the specific characterization of N-glycosylation in model mouse is necessary in order to investigate progression of disease.

This study provided a method to characterize the site-specific N-glycosylation of human and mouse plasma. We compared site-specific N-glycosylation in human and mouse plasma samples using LC-MS/MS with GPA (GlycoProteome Analyzer) system[1]. As reported previously, we confirmed that the sialic acid of N-glycopeptides was almost entirely Neu5Gc in mouse plasma, while in human plasma was Neu5Ac. Especially, a unique trisialylated biantennary N-glycopeptide (peptide_$Hex_2HexNAc_2NeuGc_3$+$Man_3GlcNAc_2$) was specifically identified from several glycoproteins in mouse plasma. The trisialylated biantennary glycoform was recently reported in mouse serum, although it could not determine the binding position of the third Neu5Gc. We first report that it is directly linked to GlcNAc with evidence of specific oxonium ions and glycopeptide fragment ions in MS/MS spectra. This clearly proves that the new structure of trisialylated biantennary N-glycopeptide found only in mouse plasma.

Reference

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

P-25

Size-dependent analysis of urinary exosomal lipids by flow field-flow fractionation and nanoflow ultrahigh-performance liquid chromatography tandem mass spectrometry (nUPLC-ESI-MS/MS)

Joon Seon Yang, Myeong Hee Moon*

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

Exosomes are small membrane vesicles (diameter of 20 to 100 nm) that are secreted by various kinds of cells. Exosomes contain biological molecules such as mRNA, proteins, and lipids that are originated from cells and they transport these molecules between cells. The cell-to-cell communication process, which is related to the immune system, affects transition of pathogens or growth of tumor cells and recent studies on exosomes have been focused on understanding its role and discovering biomarkers of diseases.

Exosomes are found in various kinds of body fluids, such as blood or urine, and urinary exosomes are usually originated from prostate or kidney cells. Closely related to prostate cancer (PCa), the size of PCa derived urinary exosomes is reported to be different from that of normal ones.

Flow field-flow fractionation (FlFFF) is an elution based analytical technique that separates sample components according to their sizes. In this study, urinary exosomes of controls and PCa patients were first retrieved by using ultracentrifugation and asymmetrical FlFFF (AF4) was adopted to sort out urinary exosomes according to their sizes. Exosomes in different sizes were collected and lipids within them were analyzed to discover any possible biomarker candidates. The overall lipid amounts were increased in PCa patient exosomes and lipids from small exosomes showed more changes than larger exosomes.

P-26

Comparative study on extraction method of fragrance allergens in water using GC-MS/MS

IN JA LEE*, Haksun Kwon, Chi-hwa An, Jae-Chan Ahn, Bogsoon Kim

Seoul Water Institute, Seoul Metropolitan Government, 04981, Korea

Products containing 26 of these compounds, which are fragrance allergens likely to cause contact allergies, are required under domestic cosmetic law to be labeled when their concentrations exceed 0.01% for rinse-off products (e.g. cleansers, shampoos), and 0.001% for leave-on products (e.g. lotions, deodorants) beginning in 2008. Fragrance allergens are continuously introduced into the environment via urban waste water effluents because they are important components of products used in daily life such as soaps, shampoos and lotions, so it is needed to develop the analysis to investigate those fragrance allergens.

Methods based on solid phase micro extraction(SPME) and liquid-liquid extraction(LLE) followed by GC-MS/MS have been studied for the analysis of 24 fragrance allergens excepting for 2 natural materials in water. Extraction conditions such as the kind of fiber, extraction temperature, type of solvent, amounts of sodium chloride were optimized using a multivariate approach.

In the case of using SPME, 15 of the 24 fragrance allergens were analyzed, and the correlation coefficient (r^2) of the calibration curve for quantification showed linearity of 0.9969 or more, and the method detection limits (MDL) and the limits of quantification (LOQ were 0.078 ~ 0.582 ug/L and 0.261 ~ 1.940 ug/L, respectively.

In the case of using LLE, 24 fragrance allergens were analyzed, and the correlation coefficient (r^2) of the calibration curve for quantification showed linearity of 0.9957 or more, MDL and LOQ were 0.020 ~ 0.138 ug/L and 0.065 ~ 0.440 ug/L, respectively.

It was concluded that the LLE pre-treatment method with low detection limit and more simultaneous analysis items was more effective to analyze fragrance allergens in water.

P-27

Isotopic analysis of uranium particles for NUSIMEP-7 using SEM-TIMS combined with simultaneous measurement

Jong-Ho Park[1,2] *, Kahee Jeong[3]

[1]*Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, 111 Daedoek-daero-989, Yuseong-gu, Daejeon, 34057, Korea*

[2]*Department of Radiochemistry & Nuclear Nonproliferation, University of Science and Technology, 217 Gajeong-ro, Yuseong-gu, Daejeon 34113, Korea*

[3]*Chemistry & Environment Group, Central Research Insitute, Korea Hydro & Nuclear Power, 70 Yuseong-daero-1312, Yuseong-gu, Daejeon 34101, Korea*

Four replicated U030 samples containing ultra-trace levels of uranium and five individual particles from a sample for the 7th Nuclear Signatures Interlaboratory Measurement Evaluation Programme (NUSIMEP-7) were analyzed to determine the uranium isotope ratios using scanning electron microscopy combined with thermal ionization mass spectrometry (SEM-TIMS). An advanced multiple ion counter (MIC) system was used for the complete simultaneous measurement of four uranium isotopes. The excellent agreement of $n(^{234}U)/n(^{238}U)$, $n(^{235}U)/n(^{238}U)$, and $n(^{236}U)/n(^{238}U)$ with certified values verified the applicability of SEM-TIMS with complete simultaneous measurement using the advanced MIC system to analyze uranium isotopes in individual microparticles. Further experimental study required for investigation of simultaneous measurement using the advanced multiple ion counter system is presented.

P-28

Targeted lipidomics approach applied to characterize the lipid metabolism of autophagic liver cells

Seung Cheol Park[1], Jae Won Lee[1], Ah Young Lee[2], Myung-Haing Cho[2], Kwang Pyo Kim[1*]

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

[2]*Laboratory of Toxicology, Research Institute for Veterinary Science and College of Veterinary Medicine, Seoul National University, Seoul, Republic of Korea.*

Intracellular lipids are essential to cells as an energy source, and their storage and utilization are critical to maintain cellular energy homeostasis. In particular, autophagy functions to regulate intracellular lipid stores and the levels of cellular lipids such as free fatty acids. Previous reports demonstrated that lipids have important roles to control the autophagy. However, it still remains to assess the correlation between autophagy and changes in lipid profile. The purpose of this study is to perform the comprehensive profiling of various lipids from liver cells in autophagy. In this study, LO2 cells were treated with rapamycin (RM) and chloroquine (CQ) to induce the autophagy and dysfunction of lysosome. The acculmalted autophagosomes in the drug-treated cells were subject to the target lipidome analyses based on UPLC-QqQ/MS. From the five groups including Control and RM-treated, CQ-treated, RM+CQ-treated, and DMSO-treated cells, neutral lipids, phospholipids, lysophospholipids, and sphingolipids were analyzed. In the use of optimal UPLC and MRM analysis, a total of 211 lipids were quantified from these samples. The lipid datasets obtained from five sample groups were then subjected into several statistical analyses. The general clustering trends of the five groups were visualized by PCA. They were differentiated in the PCA score plot. RM+CQ was scattered on far from other four groups indicating that the lipid profile of RM+CQ is different compared to other groups. Next, the data of neutral lipids, phospholipids, lysophospholipids, and sphingolipids were subjected to PCA and HCA. As a result, RM and RM+CQ have different profiles of neutral lipids and lysophospholipids compared to other three groups. Furthermore, CQ and RM+CQ showed the different profiles of sphingolipids. These indicated that the treatment of RM, CQ, and RM+CQ altered the lipid metabolism of liver cells. Moreover, three lipid classes including neutral lipids, lysophospholipids, and sphingolipids were mainly altered in autophagic cells compared to phospholipids. In conclusion, the target lipidomics approach was applied to characterize the lipid alteration of autophagic liver cells, and we could find the altered lipid classes from the RM, CQ, and RM+CQ treated samples.

P-29

Comparative analysis of human milk oligosaccharides by pasteurization and lyophilization

Ye Rin Jin[1,2], Nari Seo[1,2], Tuyen Nguyen[3], Nam Mi Kang[4], Jae Han Kim[3], and Hyun Joo An[1,2]*

[1]*Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

[2]*Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

[3]*Department of Food and Nutrition, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

[4]*College of Nursing Konkuk University,268 Chungwondae-ro, Chungju, 27478, Korea*

**E-mail: sugar@cnu.ac.kr Tel: 82-42-821-8547, Fax: 82-42-821-8541*

Microbial growth on human breast milk should be suppressed by heating and freezing processes. Major nutritional contents such as proteins, lipids, and carbohydrates undergo various influences during pasteurization or lyophilization. In particular, we have focused on the changes of human milk oligosaccharides (HMOs) after pasteurization and lyophilization steps.

HMOs are classified as a family of structurally diverse unconjugated glycans. Various structures of HMOs are closely relevant to catabolism and biological functions such that contribute to infant growth, organ development and immune maturation. Nevertheless, it is not yet proved that chemical stability of HMOs is affected by heating or freeze-drying.

Human milk samples from 3 mothers were pasteurized at 63℃ for 30 minutes and freeze-dried at -83℃ for 5 days, respectively. HMOs were enriched by solid-phase extraction with PGC cartridge and profiled by mass spectrometry. At first, compositions and structures of HMOs were assigned by MALDI-TOF/TOF MS. In addition, isomeric structures of HMOs were well separated and relatively quantified by PGC column-based LC/MS. As a result, more than 30 HMOs have been identified and quantified.

Therefore, we could conclude that pasteurization or lyophilization of human milk do not influence chemical properties of HMOs at all.

Acknowledgement

We are grateful for the support provided by the National Research Foundation (2015R1A2A1A15056046, 2015M3A9B5053960).

Reference

1. Totten, S. M. Wu, L. D. Parker, E. A. Davis, J. C. C. Hua, S. Stroble, C. Ruhaak, L. R. Smilowitz, J. T. German, J. B. Lebrilla, C. B., Rapid-throughput glycomics applied to human milk oligosaccharide profiling for large human studies, Analytical and Bioanalytical Chemistry, 30, 7925-7935 (2014)

P-30

Alteration of diacyl and ether phosphatidylcholines and phosphatidylethanolamines in the plasma and tissues of HBV mouse model

Sue Ah Noh[1], Jae Won Lee[1], Hyuck Jun Mok[1], Hong Seok Kang[2], Kyun-Hwan Kim[2], Kwang Pyo Kim[1*]

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

[2]Department of Pharmacology, School of medicine, Konkuk University, Seoul 143-701, Republic of Korea

Recently, lipidomics has been emerged as a systems-level analysis of lipids and factors that interact with lipids to find the crucial roles of lipids in biological samples. Among many lipid classes, phospholipids (PLs) have critical roles as cellular membrane components and lipid signaling. Many studies have revealed the correlation between the altered PL metabolism of diseases/disorders. In particular, phosphatidylcholines (PCs) and phosphatidylethanolamines (PEs) have been discussed as biomarkers for diseases, so that the profiling of PC and PE is critical for biomarker study. However, the ether forms including alkyl and alkenyl species of PC and PE were not detail profiled yet. In this study, we optimized the target profiling based on MRM for acyl and ether PCs and PEs from biological samples. By using UPLC-MS/MS, 41 PCs and 28 PEs including ether lipid were identified and quantitatively analyzed in mouse tissues and plasma. In the data analysis, we found that the levels of acyl and ether PCs and PEs differ depending on mouse brain, heart, liver and plasma. Furthermore, we applied this profiling method to profile the PC and PE of mouse model having hepatitis B virus (HBV). In the comparison of HBV model and control, their livers have different profiles of acyl and ether PCs and PEs. We identified significantly decreased 22 PCs and 1 PE including 9 ether PCs. And 2 PCs and 5 PEs were significantly increased.

P-31

UPLC-MS/MS Based Profiling of Eicosanoids in RAW264.7 Cells

Yu-Ri Choi[1], Jae Won Lee[1], Hyuck Jun Mok[1], Seung Cheol Park[1], Hyung Don Kim[2], Kwang Pyo Kim[1*]

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

[2]Department of Herbal Crop Research, National Institute of Horticultural and Herbal Science, RDA, Eumseong 369-873,

Although the pro-inflammatory and anti-inflammatory effects of various eicosanoids have been widely studied, changes in the levels of various eicosanoids during inflammation have not yet comprehensively studied. Thus, we designed two experiments in order to measure the levels of eicosanoids. We assessed the effect of lipopolysaccharide (LPS) treatment on the levels of eicosanoids in macrophage cells, and treated with LPS and 20(S)-ginsenoside-Rg3 (Rg3) for 12h, 24h. UPLC-MS/MS-based lipidomics analysis was used to profile various eicosanoids from macrophage cells treated with LPS and Rg3. The profiling data were statistically analyzed by principal component analysis, hierarchical clustering analysis, analysis of variance, and volcano plot. We have found that thirty-nine eicosanoids were upregulated, seven were down-regulated by LPS treatment in a concentration-dependent manner, and eighteen eicosanoids were recovered by Rg3 treatment.

P-32

Steroidal CYP enzyme activities in human amniotic fluid by GC-MS

Soyun Han[1,2], Ju-Yeon Moon[3], Jae-Hong Kim[2], Man Ho Choi[1]

[1]*Molecular Recognition Research Center, KIST*
[2]*College of Life Sciences and Biotechnology, Korea University*
[3]*Department of Pharmacy, The Catholic University of Korea*

Although the potential risk factors of preeclampsia are associated with placental oxidative stress and altered steroid metabolism, its pathogenesis has not fully been identified. To investigate whether human cytochrome P450 (CYP) enzymes are responsible to oxidative metabolism of endogenous steroids, gas chromatography–mass spectrometry in the selected-ion monitoring (GC–SIM/MS)-based steroid profiling was, firstly, developed for simultaneous quantification of CYP-mediated regioselective hydroxysteroids and their substrates, including 15 androgens, 7 estrogens, 4 progestins, 6 corticoids, and 8 sterols, with Oasis HLB™ solid-phase extraction. This CYP-mediated steroid signatures allows simultaneous assessment of CYP1A, CYP1B, CYP2C, CYP3A, CYP11B, CYP17A, CYP19A, and CYP21A. Then, the devised assay was applied to amniotic fluids obtained from patients with preeclampsia and normotensive controls. Due to its compositional changes of amniotic fluids along with gestational age according to the process of the fetal development, the assessment of steroidal CYP enzyme activities in amniotic fluids could serve as a useful tool for assessing the diagnostic biomarkers.

P-33

Characterization of site-specific N-glycoproteins in Dried Blood Spot by LC-MS/MS and customized database

Na Young Choi[1,2*], Eun Sun Ji[1], Gun Wook Park[1], Heeyoun Hwang[1], Ju Yeon Lee[1], Hyun Kyoung Lee[1,2], Jin Young Kim[1] and Jong Shin Yoo[1,2]

[1]*Biomedical Omics Group, Division of Bioconvergence Analysis, KBSI, Ochang, Korea*

[2]*Graduated School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea*

Glycosylation is one of the important post-translational modification of proteins, which have a variety of functions in a wide range of biological processes such as inflammation and immunization. Especially N-linked glycoproteins contain a variety of glycans attached to asparagine (N) residues of the polypeptide chain. Dried Blood Spot (DBS) sampling methods have a number of advantages which are easy to collection, transportation, and storage at room temperature compared with previous conventional sampling methods that store the blood in the liquid state at low temperature(-80 ℃). However, red blood cell-related proteins such as hemoglobin in complex DBS are non-glycoproteins that interfere with the analysis for glycoproteins.

In this study, we performed direct analysis of the N-glycoproteins through optimization of sample preparation from human serum without any depletion and enrichment processes. To optimize the sample preparation, we have tested denaturing conditions as well as desalting conditions before MS analysis. Through these test, we report the most efficient conditions for the analysis of glycopeptides. We applied the optimized condition to identify N-glycoproteins in DBS. We first found total 54 glycopeptides from 23 major glycoproteins in DBS using customized proteome database and confirmed by MS/MS spectra. Among them, 17 site-specific N-glycopeptides from 11 major glycoproteins including IgG directly quantified by LC-MS/MS with GPA system [1]. The quantified N-glycopeptides showed a similar retention time and CV% for quantitation was less than 30%. We were able to distinguish IgG isomers from the DBS and identify neutral fucosylated glycan structures from IgG and sialylated non-fucosylated glycan structures from 10 major quantified N-glycoproteins.

[1] Gun Wook Park., et. al; Scientific Report (2016) 6, 21175.

P-34

Platinum analysis in the kidney of mouse treated with the newly developed anticancer drugs

Sunghwa Choi[1], Eunji Song[1], Eunmi Choi[1], Jiyeon Kim[1], Youngmi Yang[1], Narae Keum[1,2], Minyoung Lee[1,3], Heh-In Im[4], Sang joon Lee[4], Youn Soo Sohn[5], Kyungsu Park[1*]

[1]Advaced Analysis Center, Korea Institute of Science and Technology,
[2]Department of chemistry, Yonsei University,
[3]Department of Chemistry, Graduate school, Kyung Hee University
[4]Center for Neuroscience, Brain Science Institute. Korea korea Institute of Science and Technology,
[5]C&Pharm, Rm 211 Science Building B, Ewha Womans University,

As most standard chemotherapy treatments are based on the platinum-based anti-cancer drugs without high selectivity for cancerous cells or tissues, these drugs have toxicity and side effects associated with killing normal, healthy cells.

This study was to determine the vivo excretion of newly developed anticancer drug Polyplatin by femtosecond LA-ICP-MS (femtosecond Laser-Inductively Coupled Plasma-Mass Spectrometry) that provides micron spatial resolution and excellent analytical sensitivity. Quantitative platinum distribution was verified using the ICP-MS on the organ of the mouse.

The progress of the experiment, Platinum content in the mouse kidney of 2, 12, 24, 72 hours after polyplatin administration was analyzed.

As a result, it was confirmed that platinum content decreased with time after polyplatin administration. we were able to provide basic data on excretion study of Pt anti-cancer drug development.

P-35

Analysis of inorganic element content compared to foreign fruits

Sunghwa Choi[1], Eunmi Choi[1], Jiyeon Kim[1], Youngmi Yang[1], Eunji Song[1], Narae Keum[1,2], Minyoung Lee[1,3], Kyungsu Park[1*]

[1]Advaced Analysis Center, Korea Institute of Science and Technology

[2]Department of chemistry,Yonsei University

[3]Department of Chemistry,Graduate school, Kyung Hee University

For the inorganic element content analysis, foreign fruits samples (Maqui berry, Cantaloupe melon, Elderberry) were collected.

Analysis of samples was analyzed according to the Korean Food Code.

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, satisfactory results were obtained below the Z-score 0.5.

Currently, the standard for domestic heavy metals is, In the case of Pb, 0.1 mg/kg of fruits, and 0.2 mg/kg of apples, mandarins and berry fruit. In the case of Cd, 0.05 mg/kg of fruits.

The average content of heavy metals in the foreign fruits is Pb>As>Sn>Cd. And no samples exceeded the domestic standard.

P-36

Chromium Speciation in Wooden Containers and Packing Materials Using HPLC-ICP-MS

Na-rae Keum[1,2*], Eun-mi Choi[1], Ji-yeon Kim[1], Young-mi Yang[1], Eun-ji Song[1], Sung-hwa Choi[1], Min-young Lee[1,3], Kyung-su Park[1*], Ki-Jung Paeng[2*]

[1]*Advanced Analysis Center, Korea Institute of Science and Technology*

[2]*Department of Chemistry, Graduate school, Yonsei University*

[3]*Department of Chemistry, Graduate school, Kyung Hee University*

In this study, chromium speciation from wooden containers and packing materials were carried out using High performance liquid chromatography-Inductively coupled plasma-Mass spectrometry (HPLC-ICP-MS). Chromium species as oxidation state have different effects to human body. Trivalent chromium is essential element for metabolism while hexavalent chromium has toxicity causing cancer. Therefore correct risk assessment of chromium is required to separate and determine each species.

HPLC-ICP-MS was introduced to chromium speciation. For optimizing the analytical condition, it was tested such as pH, kinds of analytical gases, organic modifier and flow rate of mobile phase. Then validation was carried out for taking confidence.

After confirm to method available, it was applied to real samples to measure migration from containers. Additionally, the spike test verified that the method was independent of the matrix effect. The results from using HPLC-ICP-MS were compared with quantified data from Ultraviolet-Visible spectrometry (UV-Vis).

P-37

Observations on human milk oligosaccharides affected by pasteurization or lyophilization

Ye Rin Jin[1,2], Nari Seo[1,2], Tuyen Nguyen[3], Nam Mi Kang[4], Jae Han Kim[3], and Hyun Joo An[1,2]*

[1]*Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

[2]*Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

[3]*Department of Food and Nutrition, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

[4]*College of Nursing Konkuk University, 268 Chungwondae-ro, Chungju, 27478, Korea*

**E-mail: sugar@cnu.ac.kr, Tel: 82-42-821-8547, Fax: 82-42-821-8541*

Pasteurization or lyophilization is occasionally used as pretreatment for human breast milk. In this regard, 500 microliters of milk and 5mg of milk powder were prepared to focus on the changes of human milk oligosaccharides (HMOs) after milk manufacturing processes.

HMOs are classified as a family of structurally diverse unconjugated glycans. Various structures of HMOs contribute to catabolism and biological functions such as infant growth, organ development and immune maturation. Still, it is not yet investigated that chemical stability of HMOs is affected by mild temperature-heating or freeze-drying.

Human milk samples from three mothers were pasteurized at 63℃ for 30 minutes or freeze-dried at -83℃ for 5 days, respectively. HMOs were enriched by solid-phase extraction with PGC cartridge and profiled by mass spectrometry. At first, compositions and structures of HMOs were assigned by MALDI-TOF/TOF MS. In addition, isomeric structures of HMOs were well separated and quantified by PGC column-based LC/MS. As a result, more than 30 HMOs have been identified and quantitatively determined.

The major species of neutral and acidic HMOs were identical between pasteurized and lyophilized samples from the same donor. Furthermore, ratios of each HMO type and total distribution of HMOs were similar between the two. Therefore, we could conclude that pasteurization or lyophilization of human milk do not influence chemical properties of HMOs at all.

Acknowledgement

We are grateful for the support provided by the National Research Foundation (2015R1A2A1A15056046, 2015M3A9B5053960).

Reference

1. Lawrence, R. A., Storage of human milk and the influence of procedures on immunological components of human milk, Acta Paediatrica, 88, 14-18 (1999)
2. Totten, S. M. Wu, L. D. Parker, E. A. Davis, J. C. C. Hua, S. Stroble, C. Ruhaak, L. R. Smilowitz, J. T. German, J. B. Lebrilla, C. B., Rapid-throughput glycomics applied to human milk oligosaccharide profiling for large human studies, Analytical and Bioanalytical Chemistry, 30, 7925-7935 (2014)

P-38

Development of LC-MS/MS method for quantitation of alpha-Galactosyceramide.

Soo Hyun Lee[1], Ki Young Choi[2] and Taegwon Oh[2]

[1]Department of Medical Record and Health Information Management, Kongju National University, 56 Gonju Daehak-ro Gongju-si Chungcheongnam-do, Korea

[2]Cellid, Inc., 1 Gwanak-ro, Gwanak-gu, Seoul, Korea

Selective, sensitive, and validated analytical methods for the quantitative evaluation of chemicals for new drug candidates are critical for the successful conduct of nonclinical and/or biopharmaceutics and clinical pharmacology studies. α-Galactosylceramide (GalCer) is a promising drug candidate as it has been identified as a ligand recognized by Vα14 natural killer T (iNKT) cells and that has been reported to show anti-tumor activiry and various immunological effects in infectious diseases, autoimmune disease and graft verse host disease in mice. In the present study, a confident liquid chromatography tandem mass spectrometry (LC–MS/MS) method has been developed for identification, confirmation and quantitation of GalCer. As application of established LC-MS/MS method, the stability of GalCer was evaluated with the method. For step forward, the method will be validated in accordance with the criteria defined in Bioanalytical method validation in Guidance for industry by FDA.

P-39

Development of new chemical separation method for uranium age-dating of UO_2 materials

Eun Ju Choi[1,2], Sang Ho Lim[1,2], Sun-Ho Han[1], Ranhee Park[1], Jinkyu Park[1], Chi-Gyu Lee[1]

[1]Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, Korea

[2]Radiochemistry & Nuclear Nonproliferation, University of Science & Technology, Korea

Age-determination of uranium samples is an important technique for nuclear forensics by analyzing a daughter-mother radionuclide pair such as $^{230}Th/^{234}U$, $^{231}Pa/^{235}U$, $^{232}Th/^{236}U$. $^{230}Th/^{234}U$ is one of the most commonly used isotope pair due to relatively rapid ingrowth of ^{230}Th in comparison with others and availability of high precision. For accurate and precise determination of $^{230}Th/^{234}U$ ratio, Th and U must be purified by removing interfering species from uranium samples prior to analysis as much as possible. Additionally, ^{232}Th impurities during chemical procedures should be minimized and well evaluated because standard ^{232}Th is used as a spike for isotope dilution technique.

In this study, we have developed new chemical separation method using UTEVA resin and optimized separation conditions. This new chemical separation method is expected to be more versatile than previous method using TEVA resin or ion exchange chromatograpy because it is possible to evaluate Pu age by analyzing $^{241}Am/^{241}Pu$ as well as $^{230}Th/^{234}U$ at the same time. For testing this method, we prepared simulated uranium samples. Elution curve and recovery yield were obtained from newly developed separation schemes. The optimal volumes of Th eluent (5 M HCl) was 6 mL and the recovery yield was 99.5 %. In addition we also verified this method with UO_2 reference materials and isotopic ratio measurements of $^{230}Th/^{234}U$ were performed using MC-ICP-MS equipped with desolvation system (Aridus-Ⅱ).

P-40

Simultaneous determination of chlorogenic acid isomers and metabolites in rat plasma using LC-MS/MS

Won-Gu Choi, Ju-Hyun Kim, Ju-Yeon Moon, Tae Yeon Kong and Hye Suk Lee*

Drug Metabolism and Bioanalysis Laboratory, College of Pharmacy, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Buchen-si, Gyeonggi-do, 420-743,

A selective, sensitive and reliable liquid chromatography-tandem mass spectrometry method for the simultaneous determination of chlorogenic acid, neochlorogenic acid, cryptochlorogenic acid, caffeic acid, caffeic acid 3-O-glucuronide, caffeic acid 4-O-glucuronide, and ferulic acid in rat plasma was developed. After liquid-liquid extraction with ethyl acetate as sample preparation, seven analytes were seperated on Halo C18 column with gradient elution of 0.1% formic acid in water and methanol. The analytes were quantified by an electrospray ionization tandem mass spectrometry in the selected reaction monitoring mode. The standard curves were linear over the concentration range of 0.5-200 ng/mL for chlorogenic acid and neochlorogenic acid, 2.5-1000 ng/mL for cryptochlorogenic acid, caffeic acid, caffeic acid 3-O-glucuronide, and caffeic acid 4-O-glucuronide, and 12.5-5000 ng/mL for ferulic acid, respectively. The intra- and inter-day coefficient variations and relative errors were 4.1 to 18.1% and -8.8 to 16.0% at LLOQ and were 2.0 to 12.5% and -10.0 to 10.4% at three QC concentrations. This method was successfully applied to the pharmacokinetic study of chlorogenic acid, cryptochlorogenic acid, neochlorogenic acid, caffeic acid, caffeic acid 3-O-glucuronide, caffeic acid 4-O-glucuronide, and ferulic acid after an oral administration of the extract of *stauntonia hexaphylla* leaf at a dose of 100 mg/kg in male Sprague-Dawley rats.

P-41

High Throughput Platform to Enirch Native Glycans on Therapeutic Glycoproteins using Liquid Handling System

Gyeong Mi Park[1,2], Youngsuk Seo[1,2], and Hyun Joo An[1,2*]

[1]*Graduate School of Analytical Science and Technology, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

[2]*Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea*

Glycosylation of biotherapeutics is critically associated with the stability, biological activity, half-life, and safety of drug. The glycosylation could be changed by production environment such as host cell system and culture conditions. Therefore, monitoring the glycosylation at each stage of manufacture process is a suitable approach to assess production quality for drugs. Automative high-throughput tools are currently developed and innovated to treat a large number of samples in a short time span and get high quality data by minimization of hands-on time. Here we have developed the automated analytical platform to enrich and fractionate native glycans using liquid handling system combined with 96-well microplate for a high-throughput manner. Human IgG used as a motif of therapeutic mAbs, a well known glycoprotein, was chosen to develop sample preparation procedure. Overall processes including protein denaturation by heating block, N-glycan release by PNGase F, and glycan purification and enrichment by solid phase extraction have been streamlined and optimized. Glycans were profiled by nanoLC chip/Q-TOF MS. We found total 24 glycans consisting of complex/hybrid type N-glycans w/wo sialic acid residues in both automated and manual treatment. The CVs of normalized peak intensities of top 10 N-glycans were less than 8.2 %, which indicates high comparability between two methods. Moreover, we validated the quantitative reproducibility for 5 different well positions in the 96-well plate. Three independent replicates experiments were performed per day. The Pearson correlation coefficient *R* between all samples was determined to be above 0.9. Glycan preparation using the automated platform showed to be rapid, reproducible, and reliable and it can be applied for real therapeutic glycoproteins.

P-42

Analytical method development and validation of for the quantification of 24S-, 25- and 27-hydroxycholesterols in the cerebrospinal fluid using LC-ESI/MS/MS with picolinic derivatization

Eunju Cha, Kang Mi Lee, Eun Sook Jeong, Ho Jun Kim, Oh-Seung Kwon, Jaeick Lee*

Doping Control Center, Korea Institute of Science and Technology, Hwarangno 14-gil 5, Seongbuk-gu, Seoul 136-791, Korea

The rapid and accurate quantitative determination of 24S-, 25- and 27-hydroxycholesterols (OHCs) in biological fluids such as cerebrospinal fluid (CSF) is highly challenging due to their low concentration. It is also difficult to obtain the complete chromatographic separation because OHCs have the same molecular weights and similar structures. Thus, a highly sensitive and selective analytical method is essential for the simultaneous quantitative determination of the OHCs concentrations. For this purpose, we developed a liquid chromatography-electrospray ionization tandem mass spectrometry (LC-ESI/MS/MS) with picolinyl ester (PE) derivatization method for the quantitative analysis of 24S-, 25-, and 27-OHCs in CSF. To enhance the sensitivity, three OHCs were converted to PE derivatives and analyzed to $[M+2 \cdot \text{picolinic acid} + Na]^+$. And targeted OHCs were successfully separated using C18 Kinetex column (100 x 2.10 mm, 2.6 μm) at 35 °C. The developed method was validated for the limit of detection (LOD), limit of quantification (LOQ), accuracy, precision, linearity and recorvery. As a results, LOD and LOQ were 0.3 ng/mL and 5 ng/mL for 24S- and 27-OHC, respectively. For 25-OHC, LOD and LOQ were 0.03 ng/mL and 0.5 ng/mL, respectively. The linear range was 0.1-5 ng/mL for 24S- and 27-OHC, and 0.03-1 ng/mL for 25-OHC. Precision and accuracy were 0.8%-7.7% and 94.5%-119.2%, respectively. Extraction recovery was 68.4%-105.0%, and correlation coefficients were greater than 0.99. In addition, this method was applied for the simultaneous quantitation of 24S-, 25-, and 27-OHC in CSF. Consequently, the present method using LC-ESI/MS/MS with PE derivatization showed sufficient intensity and good chromatographic resolution, which allowed for the quantification of trace amounts of OHCs, in this study.

This work was supported by an intramural grant from Korea Institute of Science and Technology.

P-43

Development of a screening method for multi-class prohibited substances by hybrid sample preparation and liquid Chromatography - Mass spectrometry in doping control

Yongseok Kim, Jaeick Lee, Junghyun Son, Ho Jun Kim, Kang Mi Lee, Ju-Hyung Park, Hophil Min, Changmin Sung, Oh-Seung Kwon, Ki Hun Kim*

Doping Control Center, Korea Institute of Science and Technology, Hwarang-ro 14-gil 5, Seongbuk-gu, Seoul 02792, Republic of Korea

In the field of doping control, as the number of prohibited substances is increasing rapidly, it requires a method which can detect them simultaneously for screening. This study reports a novel method by hybrid sample preparation consists of 'dilute and shoot' method and solid-phase extraction by weak cation exchange (WCX). Target compounds were extracted by a WCX cartridge and reconstituted with a diluted urine aliquot, then samples were analyzed by high performance liquid chromatography – triple quadrupole mass spectrometry. This method could analyze 260 target compounds at the concentration below the requirement level from The World Anti-Doping Agency (WADA), Some compounds such as meldonium with high polarity were detected, growth hormone-releasing peptides (GHRPs) which showed poor recovery in liquid-liquid extraction were also detected. The optimization of solid-phase extraction including cartridge washing and elution was preformed, 167 compounds showed more than 25% higher recovery compared to a result from a liquid-liquid extraction method. This hybrid sample preparation method with LC-MS could apply to screening of various classes of prohibited substances in doping control.

P-44

Metabolomic approach to the effect of co-administration of fenofibrate with atorvastatin in hyperlipidemic patients

Ji Soo Han[1,2], Sang-Hak Lee[3], Sang Yoon Choi[2], Geum-Sook Hwang[1,4]*

[1]*Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Book ah hyun-ro 150, Seoul, 120-140, Republic of Korea*

[2]*Dept of Life Sciences, Korea University, Seoul, 02841, Republic of Korea*

[3]*Division of Cardiology, Department of Internal Medicine, Severance Hospital, Yonsei University College of Medicine, 50-1 Yonsei-ro, Seodaemun-gu, Seoul 03722, Korea*

[4]*Department of Life Science, Ewha Womans University, Seoul 120-750, Republic of Korea*

Hyperlipidemia, a family of disorder characterized by abnormally increased concentration of lipids in the blood, is a prognostic sign of cardiovascular disease risk. Primary treatment objective in hyperlipidemic patients is to lower the level of LDL cholesterol by treating statins traditionally or triglycerides by treating fibrates. To compare the effect of atorvastatin (mono) and fenofibrate with atorvastatin (combo) drug therapy, we measured the levels of TG, HDL cholesterol and ApoA1 in serum of hyperlipidemic patients. Interestingly, the combo drug therapy was significantly decreased the level of TG and DG through profiling of lipids. Further, we performed metabolic profiling with 0 week and 12 week of serum obtained from hyperlipidemic patients treated with mono and combo drug using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/Q-TOF-MS). Partial least squares-discriminant analysis (PLS-DA) plots obtained from UPLC/Q-TOF MS analysis showed a unique clustering pattern in the combo therapy group. By multivariate analysis, we ascertained metabolic alteration in 12 week combo drug therapy group than other drug therapy group and identified the magnitude of reduction which was linked to combo drug therapy compared to atorvastatin alone. After statistical analysis, we observed the changed level of lipid metabolites through lipid analysis. Phosphatidylcholine (PC), lysophophatidylcholine (Lyso PC), lysophophatidylethanolamine (Lyso PE), sphingomylein (SM), ceramide (Cer), diacylglycerol (DG), and TG importantly contributed to the discrimination. Among the lipid metabolites, DG and TG were most significantly decreased in the combo drug therapy. This study suggests that LC/MS based metabolite profiling can be a useful tool to understand the effect of drug in altering the distribution of metabolites in hyperlipidemic patients. With this result, combo drug therapy may provide a new insight to therapeutic advantage by complementary benefits on the lipid profile for patients with hyperlipidemia.

P-45

Streamlined Analytical Platform for Primary structure characterization of Therapeutic Interfeon-beta-1a using LC-MS

Nayoung Yun[1, 2], Nari Seo[1,2], Unyong Kim[1,2], Hyun Joo An[1,2*]

[1]*Graduate School of Analytical Science Technology, Chungnam National University, Daejeon 305-764, Korea*

[2]*Asia-Pacific Glycomics Reference Site, Daejeon 305-764, Korea*

**E-mail: sugar@cnu.ac.kr, Tel: 82-42-821-8547, Fax: 82-42-821-8541*

Interferons (IFNs) are a group of cytokines that produced in response to the pathogens such as bacteria, virus, and parasites. In particular, IFN-β-1a having one N-glycosylation site is mainly used as the treatment agent for multiple sclerosis and condyloma acuminatum. Glycosylation of therapeutic proteins has critical roles such as biological activity, stability, plasma half-life, and immunogenicity. Therefore, glycan profiling is as important as peptide mapping to assess quality, safety, and potency of recombinant IFN for biosimilar or biobetter development. This study aims to develop the LC-MS based method for rapid primary structure(Amino acid sequence and glycan modification) characterization from IFN for efficient screening of recombinant glycoproteins during manufacturing processes. Here, tryptic peptide on IFN and intact IFN were enriched and separated on HPLC-C8 chip respectively then were detected each different Q-TOF MS methods. The platform was optimized to reduce the time, sample and solvent consumptions. The each LC-MS data were processed using MassHunter Qualitative Analysis B.07.01(Agilent Technologies) with Bioconfirm B.07.00 software (Agilent Technologies). In the sequence characterization of IFN by tryptic peptide analysis, we identified that the matched peptides cover 78% of IFN sequence. In intact IFN analysis, we profiled the 15 major glycan compositions of IFN that were occupied approximately 90% of relative abundance of glycan-level analysis. The developed analytical platform can be applied to screen IFN variants and/or biosimilars for both developmental and regulatory purposes.

P-46

Structural Analysis of Fucosylated N-glycan in Gastric Cancer using LC-QTOF MS/MS

Su Hee Kim*, Sung Hyeon Lee

GLYCAN Co., Ltd., Healthcare Innovation Park, 172 Dolma-ro, Bundang-gu, Seongnam 13605, Korea

Gastric cancer has one of the highest cancer mortality rates worldwide, largely because of difficulties in early-stage detection. Aberrant glycosylation in serum proteins is related with many human diseases including inflammation and various types of cancer. Aberrant glycosylation is desirable in order to improve the specificity and sensitivity for clinical use. Here, we combined protein-specific immunoaffinity purification, glycan release, and MS analysis to examine haptoglobin glycosylation of gastric cancer patients for glyco-markers. Interestingly, abundances of several tri- and tetra-antennary fucosylated N-glycans were increased in gastric cancer patients. Additionally, structural analysis via LC/MS/MS demonstrated that the fucosylated complex type N-glycans were mainly decorated with antenna fucose. In this study, we developed a targeted glycoproteomic approach using chip-based nano LC-QTOF MS and MS/MS following antibody-assisted targeted purification to discover glycan signatures of serum haptoglobin for gastric cancer. We could further obtain a specific structure of fucosylated molecules that are potential glyco-markers for gastric cancer via LC/MS/MS. The current study demonstrates that glycomic profiling of targeted serum haptoglobin via LC/MS and LC/MS/MS may be used as a powerful platform to monitor the specific glycosylation associated with gastric cancer.

P-47

Integrated omics for development of Nm23 activator, NMAC1

Jae-Jin Lee, Jin-Hwan Cho, and Kong-Joo Lee

Graduate School of Pharmaceutical Sciences, College of Pharmacy,
Ewha Womans University, Seoul, Korea 120-750

Nm23-H1 is the first identified metastasis suppressor gene. Nm23 has been implicated in various functions of metastasis by inhibiting multiple steps in the metastatic process. We have identified the Nm23 activator NMAC1. In triple-negative breast cancer cells, NMAC1 specifically inhibited Rac1 through Nm23-H1 activation. Transwell migration and matrigel invasion of MDA-MB-231 cells were inhibited by NMAC1. To investigate the regulation mechanism of NMAC1, we performed MS-based experiments. We have confirmed that NMAC1 binds to the C-terminal surface by a hydrogen / deuterium exchange mass spectrometer (HDX-MS). This interaction stabilized the C-terminal surface of Nm23-H1 by modifying the Kpn-loop dynamics. It is known that the NDPK activity requires the hexamerization of Nm23 which causes the Np23 activity of Nm23 to be lost by Kpn-loop deletion. To further investigate the cellular function of Nm23 and NMAC1, we performed an integrated omics that combines 2DE-PAGE-based proteomics, transcriptomics, and metabolism.

P-48

Degradation of redox-sensitive proteins is promoted by oxidation-induced conformational changes and ubiquitination

In-Kang Song, Jae-Jin Lee, Jin-Hwan Cho, and Kong-Joo Lee

College of Pharmacy and Graduate School of Pharmaceutical Sciences,
Ewha Womans University, Seoul 120-750, South Korea.

ROS (Redox oxidative species) are not only byproduct of respiration, but also key molecules of cell survival including signaling, proliferation, differentiation and apoptosis. However, cellular targets of ROS are still unclear. In this study, we identified the ROS target proteins in signaling pathway and their regulation mechanism employing 2D-gel electrophoresis and nanoUPLC-ESI-q-TOF tandem MS. We also found that redox sensitive proteins are readily oxidized to diverse modifications at reactive Cys residues, which regulate their stability. Oxidized redox sensitive proteins are readily ubiquitinated and then degraded via proteasome and autophagy. The molecular mechanism of protein degradation was investigated by confirming the ROS-induced structural changes employing hydrogen/deuterium exchange (HDX) mass spectrometry. The results suggest that redox sensitive proteins are regulated by oxidation induced ubiquitination and degradation as another means of quality control.
[Supported by the Global Research Lab Program (No. 2012045441). IK Song supported by BK21 Plus program].

P-49

The Plasma lipidomic profiling from patients with atrial fibrillation

Youngae Jung[1,2], Geum-Sook Hwang[1,3]*

[1]*Western Seoul Center, Korea Basic Science Institute, 150 Bugahyeon-ro, Seodaemun-gu, Seoul 03759, Korea*

[2]*Department of Life Science, Ewha Womans University, 52 Ewhayeodae-gil, Seodaemun-gu, Seoul, 03760, Korea*

[3]*Department of Chemistry and Nano Science, Ewha Womans University, 52 Ewhayeodae-gil, Seodaemun-gu, Seoul, 03760, Korea*

Atrial fibrillation (AF) is the most common arrhythmia in clinical practice, associated with a high risk of stroke, hospitalization and reduced quality of life. Although AF was known to be occurred by a complex interaction between various factors, the pathophysiology of AF has not been clearly elucidated. In present study, we performed the global lipid profiling to identify the altered plasma lipid metabolites in AF patients using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (QPLC/Q-TOF MS). In PCA score plots, AF patients could be clearly distinguished from healthy controls and specific lipid metabolites such as FFAs, LysoPC, LysoPE and PC changed in AF patients were confirmed to be responsible for this separation. In particular, we found a characteristic alteration depends on the degrees of unsaturation of fatty acids in the specific lipid classes including FFAs and phospholipids. This study demonstrated that FFAs including SFA, MUFA, and PUFA are elevated or reduced in the plasma samples of patients with AF, supporting the important role of inflammation in the pathogenesis of AF.

P-50

Glycomic profiling of serum haptoglobin using nano LC/MS and LC/MS/MS

Sung Hyeon Lee

GLYCAN Co., Ltd., Healthcare Innovation Park, 172 Dolma-ro, Bundang-gu, Seongnam 13605, Korea

Glycosylation changes have been reported in a wide variety of human diseases, including immune disorders and cancers, and even is associated with malignant transformation. Recently, a targeted glycoproteomic approach has gained considerable attention as a novel method for biomarker discovery to improve the specificity and sensitivity for clinical use. Here, we comprehensively investigated the indirect and direct glycomic profile of a target glycoprotein, serum haptoglobin (Hp) by chip-based nano LC-QTOF MS and MS/MS analysis following antibody-assisted purification. From the results of significant N-glycan variations between GC patients and healthy controls, we conclusively suggest that aberrant glycans of serum Hp are associated with patients with gastric cancer and might be a promising marker for GC screening/monitoring.

P-51

Analysis of perfluorinated compounds, brominated flame retardants, and insecticides in river water samples using LC-MS/MS

Hyeri Lee*, Bo-Mi Lee, Sohui Kim, Jong Beom Khan, Junbae Lee, and Se Uk Cheon

Geum River Environmental Research Center, National Institute of Environmental Research, Okcheon gun, 29027, Republic of Korea

A multiresidue analytical method was developed for perfluorinated compounds (PFCs), brominated flame retardants (BFRs), and insecticides in river water samples. For LC-MS/MS analysis, different instrumental conditions were established for each class of compounds. In order to reduce the background levels, the dedicated isolation column and the peek tubing were set up in LC-MS/MS. Method detection limit (MDLs) of PFCs, BFRs, and insecticides were 0.3 ~ 7.1 ng/L, 5.1 ~ 11.7 ng/L, and 3.0 ~ 3.7 ng/L, respectively. The water samples were collected in hydrophilic lipophilic balance (HLB) cartridges and then, the target compounds were eluted with methanol and ethyl acetate in sequence. The eluate was dried with gentle stream of nitrogen gas and reconstructed with methanol to be analyzed by LC-MS/MS. For the recoveries tests, distilled water samples were fortified with target compounds solution at 20 ng/L (PFCs), 100 ng/L (BFRs), and 40 ng/L (Insecticides), and eluted from HLB cartridges as mentioned above. The ranges of recoveries were 19.7 ~ 135 % (PFCs), 72.5 ~ 86.4% (BFRs), and 95.0 ~ 117.2 % (Insecticides) with coefficients of variation of less than 15%. The established method was applied to river water samples collected from Geum river main stream, So-ok stream, Juwon stream, Pumgok stream, and three dam sites in Daecheong Lake every month (March to October). The compounds of highest detection frequency were PFOA and dinotefuran (insecticide), whereas BFRs were detected only in March.

P-52

Simultaneous analysis of thiamine and biotin in infant formula by isotope dilution-liquid chromatography mass spectrometry

Jayeon Joo[1,2], Joonhee Lee[1*], Byungjoo Kim[1], Jeongkwon Kim[2]

[1]*Center for Organic Analysis, Division of Metrology for Quality Life, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, South Korea*

[2]*Department of Chemistry, Chungnam National University, Daejeon, 34134 Korea*

Thiamine and biotin are part of vitamin B complex and play a key role as a coenzyme in biochemical reaction in human body. A definite method for the analysis of water-soluble vitamins is necessary to produce reliable and SI traceable measurement data.

The aim of this study is to simultaneously determine thiamine and biotin in infant formula using isotope dilution-liquid chromatography mass spectrometry. Acid hydrolysis at room temperature was performed to extract thiamine and biotin in infant formula. Thiamine-[$^{13}C_3$] and biotin-[$^{2}H_2$] standard materials were spiked as internal standard. Waters X-bridge C18 column (4.6 x 150 mm, 3.5 μm) was selected for proper separation of thiamine and biotin, and 10 mmol/L ammonium formate in H_2O, pH 3.8 and methanol were decided as mobile phases. The post-column infusion method was used to study matrix effects originating from sample matrix in electrospray ionization mode.

For the quantification, selected reaction monitoring mode is applied to monitor the collisionally induced dissociation channels of m/z 265.1→122.0 and 245.1→227.1 for thiamine and biotin, respectively, and m/z 268.1→122.0 and 247.1→229.1 for corresponding isotope compounds. The repeatability and reproducibility test in infant formula showed less than 2 % of relative standard deviation.

An LC/MS/MS-based isotope dilution mass spectrometric method has been evaluated as a candidate reference method for the simultaneous determination of thiamine and biotin in infant formula.

P-53

Simple, Instant Determination of Fish and Seafood Freshness

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

Consumer acceptance and food safety are key concerns for wholesalers and retailers of fresh fish and seafood products. Although consumers provide the ultimate feedback on quality, suitable instrument-based methods can provide rapid analysis, objectivity, and low costs per sample, which are not always possible using human subjects. Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) is a very rapid, sensitive technique for assuring fish and seafood freshness. With detection limits matching those of the human olfactory system, minimal sample preparation, and direct analysis, SIFT-MS is a very effective technique for detecting spoiling of seafood early, enabling wide-scale freshness screening.

P-54

Simple, Instant Evaluation of Beef Freshness

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

Consumer acceptance and food safety are important concerns for suppliers of beef and other red meats. Although consumers provide the ultimate feedback on product quality, application of suitable instrumentation can provide rapid analysis, objectivity, and low costs per sample, which are not always possible using human subjects. Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) is a very rapid, sensitive technique for assuring freshness of beef and other red meats. With detection limits equivalent to those of the human olfactory system, minimal sample preparation, and direct analysis, SIFT-MS is a very effective technique for detecting spoiling of red meats, enabling wide-scale freshness screening.

P-55

Heavy Metal Content Comparison of Dried Fruit Chips in Korea Market Selling

Young-Mi Yang[1], Eun-mi Choi[1], Ji-yeon Kim[1], Eun-ji Song[1], Sung-hwa Choi[1], Na-rae Keum[1,2], Min-young Lee[1,3], Kyung-su Park[1*]

[1]*Advanced Analysis Center, Korea Institute of Science and Technology*

[2]*Department of Chemistry, Graduate School, Yonsei University*

[3]*Department of Chemistry, Graduate School, Kyung Hee University*

The purpose of this study was to analyze heavy metals contents of Dried Fruit Chips in Korea Markets.

According to Korea Food Code, samples were digested by microwave digestion system. This study analyzed for Pb, Cd, As and Sn by using ICP-MS (Inductively Coupled Plasma Mass Spectrometer.

Validation Study for established method were carried out by evaluation linearity, limit of detection, limit of quantification, accurary, precision and quality management using a Certified Reference Material(CRM).

The study found out that Results of Pb, Cd were lower than the national standard specification of Pb 0.1mg/kg (Apple, Tangerine, Berry fruit 0.2 mg/kg) and Cd 0.05 mg/kg in fruits.

P-56

A Comparative Study of Heavy Metal Concentration in Nut products.

Eun Ji Song[1], Young Mi Yang[1], Sung Hwa Choi[1], Ji Yeon Kim[1], Eun Mi Choi[1], Narae Keum[1,2], Min young Lee[1,3], Kyung Su Park[1*]

[1]*Advanced Analysis Center, Korea Institute of Science and Technology*

[2]*Department of Chemistry, Yonsei University Graduate School*

[3]*Department of Chemistry, Graduate School, Kyung Hee University*

The purpose of this study was comparison of the heavy metal analysis in nut products.

Nut products in this study mean tigernuts, brazilnuts. Purchased markets are Korean markets.

According to Korean Food Standards Codex, samples were digested by microwave digestion system. This study analyzed for Pb, Cd and As by using ICP-MS (Inductively Coupled Plasma Mass Spectrometer), ICP-OES (Inductively Coupled Plasma Optical Emission Spectrometer).

We evaluate linearity, Limit of Detection, Limit of Quantification, Accuracy and Preision to verification of analysis mathod using a Cerfified Reference Material.

Safety standard of Pb in nut products is 0.1 mg/kg. And Cd in nut products is 0.3 mg/kg.

P-57

Changes of the flavonoid glycosides during different stage of tea-processing in green and black tea (*Camelia sinensis*)

Min-Ki Lee[1], Heon-Woong Kim[1], Seon-Hye Lee[1], Young Jin Kim[1], Hyun-Ah Jung[2], Jeong-Sook Choe[1], Jung-Bong Kim[1]*

[1]*National Academy of Agricultural Science, Rural Development Administration, 166, Nongsaengmyeong-ro, Iseo-myeon, Wanju-gun, Jeollabuk-do, Republic of Korea*

[2]*Department of Food Science and Human Nutrition, Chonbuk National University, 567 Baekje-daero, deokjin-gu, Jeonju-si, Jeollabuk-do, Republic of Korea*

In most studies were focused on analysis of bioactive ingredients in green tea and different fermentation types of tea infusion including oolong, black and white tea. Thus, the purpose of this study is to investigate flavonoid glycosides in green and black tea during different tea-processing stages. A total of twenty-four flavonoid glycosides were identified in green tea and its fermented products using UPLC equipped with diode array detector (flava-3-ols, 280 nm; flavonols, 350 nm) and ESI-MS. Among the flavonoids in green and black teas, (-)-epigallocatechin 3-*O*-gallate (EGCG) and (-)-epicatechin 3-*O*-gallate (ECG) which have been known for strong bioactivities were predominant compounds (over 74% of total flavonoids in green tea). Total contents of catechins and flavonols in green tea were steadily increased during green tea-processing stages. After roasting stage, especially, EGCG and ECG were remarkably increased in green tea. On the other hands, EGCG and ECG were considerably decreased after fermentation stage in black tea-processing stages. Theaflavins as catechin derivatives were consistently increased in black tea according to degree of fermentation. In the case of flavonols, total contents were slightly decreased in black tea-processing stages. Therefore, tea-processing of green and black teas as flavonoid rich sources was important to enhance their active ingredients for future tea industry and research.

Keywords: *Camellia sinensis*, Tea-processing stages, Flavonoids, UPLC-DAD-QTOF/MS

P-58

Analysis of isoflavone patterns by food processing conditions in Korean soybean (*Glycine max* L.) varieties using UPLC-DAD-QTOF/MS

Heon Woong Kim, Min Ki Lee, Seon Hye Lee, Young-Jin Kim, Hwan Hee Jang, Sung Hyen Lee, Jeong-Sook Choe, Jung Bong Kim*

National Institute of Agricultural Sciences, RDA, 166, Nongsaengmyeong-ro, Iseo-myeon, Wanju

Isoflavones is most important and abundant secondary metabolites in aspects of human health benefits from a leguminous plant. In this study, the chemical informs about 24 individual isoflavones were constructed from seeds, sprouts and leaves of soybean (*Glycine max* L.) based on literature sources and analytical data. A total of eighteen isoflavone glycosides including daidzein 7-*O*-glucoside (daidzin, *m/z* 417, $[M+H]^+$) were identified in Korean soybean varieties using ultra performance liquid chromatography with diode array detection and quadrupole time of flight/mass spectrometry (UPLC-DAD-QTOF/MS) on the basis of constructed isoflavone library. Among these, genistein 7-*O*-(6"-*O*-malonyl)glucoside (6-*O*-malonylgenistin, *m/z* 519, $[M+H]^+$) were confirmed as major component in soybean seeds. Malonyl glycosides were changed to non-acylated glycosides as well as acetyl glycosides by heat and pressure in food processings. Especially, 4"-*O*-acetyldaidzin, 4"-*O*-acetylgenistin and 4"-*O*-acetylglycitin elucidated as new compounds by food processing of soybean seeds.

P-59

Characterization of flavonoid glycosides from Korean common sage (*Salvia plebeia* R. Br.) by UPLC-DAD-QTOF/MS

Seon-Hye Lee[1], Heon-Woong Kim[1], Min-Ki Lee[1], Young Jin Kim[1], Youn-Soo Cha[2], Jeong-Sook Choe[1], and Jung-Bong Kim[1*]

[1]*National Academy of Agricultural Science, Rural Development Administration, 166, Nongsaengmyeong-ro, Iseo-myeon, Wanju-gun, Jeollabuk-do, Republic of Korea*

[2]*Department of Food Science and Human Nutrition, Chonbuk National University, 567 Baekje-daero, deokjin-gu, Jeonju-si, Jeollabuk-do, Republic of Korea*

Common sage (*Salvia plebeia* R. Br.) was great importance to contain bioactive compounds in the pharmacological and clinical studies. *S. plebeia* R. Br. cultivated in Korea was analyzed to investigate different flavonoid types using ultra-performance liquid chromatography-diode array detector-electrospray ionization-quadrupole time of flight mass spectrometry (UPLC-DAD-ESI-QTOF/MS). A total sixteen flavonoids were identified and classified into flavones and flavanones according to their UV spectrums and ion fragment patterns. Individual flavonoids were composed of glucose at 5- or 7- position with basic structures including apigenin, luteolin, hispidulin, nepetin, and some flavanones. In flavone glycosides, 6-hydroxyluteolin 7-*O*-glucoside (2452.7 mg/100 g dry weight, DW) was presented highest contents followed by hispidulin 7-*O*-glucoside (2281.0), nepetin 7-*O*-glucoside (2002.6). These three major flavone contents were accounted for 58.4% of total flavonoids. Especially, apigenin aglycone and apigenin 7-*O*-glucoside were separated first in *S. plebeia* R. Br. The six flavanones containing the hydroxyl- and methoxy- groups were determined, among them 5,7,3′,4′- tetrahydroxy-6-methoxyflavanone 7-*O*-glucoside was found highest level (938.3 mg/100 g DW). 5,6,7,3′,4′- pentahydroxyflavanone 7-*O*-glucoside and 5,6,7,4′-tetrahydroxyflavanone 7-*O*-glucoside were presumed to be newly identified compounds, based on the literature review with compiled MS and NMR data of *S. plebeia*.

Keywords: *Salvia plebeia* R. Br., Flavonoids, 6-Hydroxyluteolin, UPLC-DAD-QTOF/MS.

P-60

Comparison of flavonoid characteristics between blueberry (*Vaccinium* spp.) and raspberry (*Rubus* spp.) in South Korea using UPLC-DAD-QTOF/MS

Young Jin Kim[1], Heon-Woong Kim[1], Min-Ki Lee[1], Seon-Hye Lee[1], Hwan-Hee Jang[1], Yu-Jin Hwang[1], Jeong-Sook Choe[1], Youn-Soo Cha[2] and Jung-Bong Kim[1*]

[1]*Department of Agro-food Resources, National Institute of Agricultural Sciences, Wanju, 55365, Korea*

[2]*Department of Food Science and Human Nutrition, College of Human Ecology, Chonbuk National University, Jeonju, 561756, Korea*

Flavonoids in the fruit of seven highbush blueberry (*Vaccinium* spp.) varieties ('Darrow', 'Chandler', 'Bluegold', 'Nelson', 'Bluecrop', 'Elizabeth', and 'Legacy') and four different areas (Jeongeup, Sunchang, Gochang, and Gwangyang) of raspberries (*Rubus* spp.) cultivated in South Korea were investigated using UPLC-DAD-QTOF/MS. Total 29 flavonoids of these berries were identified comparison of UV spectra and mass spectral analysis with chemical library based on literature sources. In blueberries, all flavonoid derivatives were shown flavonol with kaempferol, quercetin, isorhamnetin, myricetin, and syringetin aglycones. Quercetin, quercetin 3-*O*-arabinofuranoside (avicularin), quercetin 3-*O*-(6"-*O*-malonyl)glucoside, and isorhamnetin 3-*O*-robinobioside were reported to the first time in blueberries. All flavonoids in raspberries consist of quercetin aglycone and its glycosides. The mean of total flavonoid contents in blueberries [143.0 mg/100g dry weight (DW)] were 1.5-fold higher than raspberries (95.4 mg/100g DW). The greatest flavonoid contents in blueberry were quercetin 3-*O*-galactoside (hyperoside, up to 76.1 mg/100g DW). On the other hand, quercetin 3-*O*-glucuronide (up to 55.5 mg/100g DW) was found highest contents in raspberries, and it was not detected in blueberries. The identification of flavonoids in berries can support potential beneficial human health effects.

keywords: *Vaccinium* spp., *Rubus* spp., Flavonoids, UPLC-DAD-QTOF/MS

P-61

Rapid screening of 29 sulfonamide diuretics in dietaty supplements based on extracted common ion chromatogram and neutral loss scan by UHPLC-Q/TOF MS

Nam-Yong Ki, Wonwoong Lee, Jisu Hur, Keon-Hee Ko, Jongki Hong*

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

Growing number of the abuse of diuretics in dietary supplements has become a global problem due to wide distribution and serious negative health effect. In this study, rapid screening method combined with simple sample preparation was developed for detection and confirmation of 29 sulfonamide diuretics by ultra-high performance liquid chromatography quadrupole / time of flight mass spectrometry (UHPLC-Q/TOF-MS). Simple cleanup using liquid-liquid partition was effectively eliminated significant interferences from dietary supplements. The separation of 29 sulfonamide diuretics was achieved within 10 min using 2.6 ㎛ fused-core C18 particles in a 100 x 2.1 mm column with mobile phase (A : 10 mM ammonium formate in water; B : 100 % acetonitrile). The MS/MS spectra of sulfonamides were preferentially interpreted to find common ion and neutral loss fragment. As results, common fragment ion at *m/z* 77.9650 $[SO_2N]^-$ and neutral molecule loss of SO_2NH were observed. These characteristic fragmentations could be used as rapid screening of sulfonamide diuretics and diagnostic ion for elucidation of new emerging sulfonamide class drugs in dietary supplements. Screening of sulfonamides in supplements was rapidly performed by extracted common ion chromatogram (ECIC) of m/z 77.9650 and neutral loss scan of SO_2NH based on narrow mass window within mass tolerance ±5 ppm, avoiding false positive and/or negative results. Overall calibration curves within dynamic range for all targets were shown to be linear correlation coefficient $R^2 > 0.995$ and limits of detection ranged 0.08-11.18 ng/mL for all sulfonamides. The developed method will be helpful for the protection of the abuse of sulfonamide diuretics in dietary supplements, ensuring public health and consumer safety.

P-62

Simultaneous analysis of the 3 PFASs in rat plasma and tissues using UPLC-MS/MS: Application to pharmacokinetics and tissue distribution

Sook-Jin Kim, Dong-Seok Lee, Hea-Young Cho*

College of Pharmacy, CHA University, 335 Pangyo-ro, Seongnam-si, 13488, Korea

Perfluoroalkyl and polyfluoroalkyl substances (PFASs) including perfluorooctanoic acid (PFOA), perfluorooctanesulfonic acid (PFOS) and perfluorohexane sulfonic acid (PFHxS) are widely used in many manufacturing and various industrial applications. The PFASs was known to cause neurotoxicity, hepatotoxicity, and reproductive and developmental toxicities. The aim of this study was to develop and validate a simultaneous determination method of PFOA, PFOS, and PFHxS for rat plasma and tissues using a UPLC-MS/MS system. The analytes and internal standards (IS) were simply extracted by liquid-liquid extraction after protein precipitation with acetonitrile. UPLC analysis was carried out under the following conditions: a Kinetex® 2.6 μm C_8 100 Å column, mobile phase of methanol and 5 mM ammonium acetate buffer with gradient elution, and a flow rate of 0.3 mL/min. The three analytes were detected using electrospray ionization tamdem mass spectrometery with multiple reaction monitoring (MRM) mode. The chromatograms showed good resolution, selectivity, and no interference in rat biological samples. The standard curves for PFOA, PFOS, and PFHxS in rat plasma and tissue samples were linear over the ranges concentration of 1–10,000 ng/ml with correlation coefficients greater than 0.994. Precision and accuracy with inter- and intra-batch coefficients of variation (CVs) were not exceeding ±15%. The validated simultaneous determination method of the 3 PFASs was accepted criteria of the international guidance and successfully applied to characterize the pharmacokinetics and tissue distribution of PFOA, PFOS and PFHxS in rats after a single oral or IV administration. The 3 PFASs were highly distributed in the liver and kidney.

UPLC-MS/MS, PFASs, Pharmacokinetics, tissue distribution, Rat

P-63

MS/MS fragmentations of biotoxins and simultaneous determination of diarrhetic shellfish toxins in bivalves by UPLC-ESI-MS/MS combined with time segment polarity switching mode

Myoung Eun Lee, Wonwoong Lee, Jongki Hong*

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

Diarrhetic shellfish poisoning (DSP) is a gastrointestinal illness caused by intake of shellfish contaminated with DSP toxins. Especially, five typical DSP biotoxins such as okadaic acid (OA), dinophysistoxin-2 (DTX-2), yessotoxin (YTX), dinophysistoxin-1 (DTX-1) and pectenotoxin-2 (PTX-2) have been frequently occurred in Korea. We developed ultra-performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS) to determine trace amounts of marine biotoxins in bivalves. Analysis of these toxins in bivalves is confronted with several limitations due to their low concentration and physiochemical properties and the coexistence of lipid matrices. Extraction of biotoxins from bivalves was carried out by ultrasonication using methanol. For the cleanup of extract, three methods (liquid-liquid partition, freezing lipid filtration, and freezing lipid filtration combined with SPE) were readily examined with the observation of lipid contents by fast atom bombardment-MS. As result, freezing-lipid filtration and SPE cleanup was shown to be the best effective lipid elimination method. During freezing-lipid filtration, about 90% of the lipids extracted from the bivalves were easily removed without any significant losses of marine toxins. For further cleanup, Strata-X-SPE cartridge could successfully purified biotoxins from remaining interferences using 0.1% ammonium hydroxide in methanol. Also, these biotoxins could be simultaneously determined by UPLC-ESI-MS/MS combined with time segment polarity switching mode, based on high separation capacity between acidic toxins (OA, DTX-1 and 2, YTX, and homo-YTX) and neutral toxin (PTX-2) under optimized UPLC conditions. Method validation through certified reference materials (CRMs) and spiking experiments was carried out to determine the recovery, precision, accuracy, and limits of detection (LOD) and quantification (LOQ) of the method. The overall recovery was above 86% in the spiked mussel sample at EU permitted level (160 μg/kg and 1000 μg/kg). The developed method was successfully applied for the determination and quantification of marine toxins in several kinds of bivalves collected from Korean fishery markets, ensuring food safety.

P-64

Glycan signatures of human saliva

Hantae Moon[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*

In recent years, saliva has received particular attention among researchers especially in the field of forensic sciences. Saliva encountered at crime scene is one of the most significant evidence and thus, the identification of saliva from other human fluids and non-human fluids is an essential prerequisite prior to further crime investigation. Conventional methods including enzymatic amylase and starch-iodine test to determine and distinguish saliva have low sensitivity in trace samples and lack of specificity due to cross-reaction with other fluids. In order to overcome these weaknesses in conventional methods, various studies have been attempted based on biochemical components. Glycosylated proteins, which are highly sensitive to the biochemical environment, are a major constituent in saliva and play an important and vital role in maintenance of oral health. Here, we have explored the possibility if glycan can be used as a bio-signature to identify and differentiate human saliva compared with other fluids. Briefly, N-glycans in human saliva (7 males and 11 females) were enzymatically released and enriched by solid phase extraction with a porous graphitized carbon cartridge. Human saliva N-glycans were carried out by nano LC-PGC chip/Q-TOF MS and –MS/MS. We could determine highly fucosylated N-glycans as a saliva-specific molecule.

P-65

The importance for van der Waals potential for accurate collision cross section calculations

Jong Wha Lee[1,2], Hugh I. Kim[2]*

[1]*Dept of Chemistry, Pohan University of Science and Technology, 77 Cheongam-Ro, Pohang 37673, Republic of Korea*

[2]*Dept of Chemistry, Korea University, 145 Anam-ro, Seoul 02841, Republic of Korea*

Ion mobility spectrometry (IMS) is a gas-phase separation tool based on collisions between ions drifting in an electric field and neutral buffer gas filling the IMS cell. Mobility of ions in IMS is directly related to their collsion cross section (CCS), which holds the information on ion structure in the gas phase. Combined with theoretical tools for estimating ion CCS, IMS can be used for structural investigation of ions in the gas phase. Naturally, accuracy of the theoretical calculations is crucial for such application. However, no single method currently available can be used for predicting the CCS of a wide range of ions.

Ion CCS is determined by the intermolecular interactions between the ion and neutral buffer gas molecules. For ions in helium, the van der Waals interaction is regarded to be the most important intermolecular interaction. However, limited number of studies have studied the correct representation of ion-neutral van der Waals interactions for accurate CCS calculations. Here we combine the van der Waals interaction potentials and parameters of molecular mechanics force fields for accurate prediction of ion CCS. We show that rather than specific parameters describing van der Waals interaction distance and energy, the form of the potential is the most important factor that determine the accuracy of CCS calculations for a wide range of ions. Among those tested, the combination of the Buckingham potential and the parameters of the general Amber force field (GAFF) or Merck Molecular Force Field (MMFF94) resulted in errors of less than 4% for all the ions studied here. This is the highest-accuracy calculation method currently available. We expect our study to advance fundamental understanding on ion-netural interactions for accurate CCS calculations and enhance the application of IMS for characteriazation of ion structures in the gas phase.

P-66

The effect of Sodium and Potassium ions for sucrose detection by comparing charcoal, DHB and CHCA matrices in MALDI-MS analysis

Jihyun Paek, Dabin Lee, Yeoseon Kim, Sooyeon Chae, Jeongkwon Kim*

Dept. of Chemistry, Chungnam National University, Deajeon, 34134, Korea

Matrix-assisted laser desorption/ionization (MALDI) is one of the most commonly used soft ionization method for the determination of large molecules such as proteins or peptides. MALDI conventionally uses organic matrices such as 2,5-dihydroxybenzonic acid (2,5-DHB) and α-cyano-4-hydroxycinnamic acid (α-CHCA). However, organic matrices usually break up under laser irradiation. Moreover, the product of the matrices have signal interferences with high intensity in the low molecular weight ranges (m/ƶ<500). Many alternative matrices such as activated charcoal, carbon nanotubes, and porous silicon surface have been used to overcome the interferences of matrix-related ions. In this investigation, sucrose which has molar mass of 342.29, was analyzed using 2.5-DHB, CHCA, and charcoal. Among the three matrices, charcoal was found to be best since it provides the highest sucrose peak intensity and the lowest interferences. However, when using charcoal matrix and sodium ion addition, it was observed that sucrose was cleaved into glucose generating [glucose + Na]$^+$ peak. Therefore, it was necessary to explore new method for the detection of only intrinsic sucrose by MALDI. Lowering the laser intensity decreases the glucose peak intensity to only a certain extent and changing the additive cation from Na^+ to K^+ successfully removed the glucose peak. The addition of K^+ cation was found to be an efficient way for the determination of sucrose.

P-67

Metabolic profiling of *Cirsium* species during floral budding and full flowering

Min-Sun Kim[1], Geum-Sook Hwang[1,2*]

[1]*Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Seoul 120-140, Republic of Korea*

[2]*Department of Life Science, Ewha Womans University, Seoul 120-750, Republic of Korea*

Cirsium species are members of the Compositae family that grow wild and have been used for many years as a food source and traditional folk medicine. In this study, we examined metabolic changes associated with flowering stages of *Cirsium* species using ultra-performance liquid chromatography (UPLC)-quadrupole time-of-flight (QTOF) mass spectrometry. The levels of phenolic acids and most flavonoids in the phenylpropanoid pathway were increased at the full flowering stage. However, the levels of coumaric acid, kaempferol, and pectolinarigenin revealed different patterns between *Cirsium* species. As these results, high amount of phenolic acids and flavonoids at flowering stage is expected to increase various physiological activities of plants, including antibacterial, antioxidative, and anti-inflammatory properties. This approach could be applied to explore the metabolic pathway associated with vegetative cycle phases and could confirm the optimal harvest time was determined by an increased content of bioactive compounds in plant.

P-68

Reactive paper spray ionization mass spectrometry for the analysis of the conjugated ketones

Soobin Choi, Sangwon Cha

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

Paper spray ionization (PSI) is an ambient ionization method which utilizes a triangular paper tip as a sampling base as well as an electrospray tip. In PSI, sample solution is usually deposited onto a paper tip and dried. Analytes in a sample spot are then extracted, transported to the end of the paper tip, and finally ionized by applying an electrospray solution and high voltage on a paper tip. In case an electrospray solution contains a reactant which can readily react with target analytes, *in situ* derivatization of target analytes can occur during PSI processes and this method is referred to as reactive PSI. In this presentation, we demonstrated reactive PSI mass spectrometric analysis of conjugated ketones including quinones and isothiazolones. The reactant for this application was cysteamine which readily reacts with a conjugated ketone *via* Michael addition reaction. Since the reaction product has an amine group which can be easily protonated, sensitivity was greatly enhanced by this approach. In addition, conjugated ketones could be selectively detected by monitoring the specific fragment ions of the reaction products.

P-69

Real-time Resolution of Analytes, without Chromatographic Separation

Ji Hoon.Lee, Romertta.Kim, Jung-Tae.Park

ATFRONTIER. Younglin Bldg. 60 Anyangcheondongro, Dongan-gu, Anyang-si, Gyeonggi-do, 14042, korea

Syft Technologies have developed a triple ion SIFT-MS instrument that offers real time high-resolution analysis of volatile analytes, without the need for chromatographic separation. The use of three ions and the relatively soft Chemical Ionisation (CI) method of ion generation allows accurate and confident identification and quantification of analytes, even among analytes with similar reaction chemistries.

P-70

Serial lectin affinity chromatography for comparative serum glycoproteomics on colon cancer biomarker discovery

Jinwook Lee, Wonryeon Cho*

Department of Bionanochemistry, Wonkwang University, Iksandearo 460, Iksan, 54538, South Korea

There is a great interest in categorizing the blood plasma proteomes to find disease-related proteins. Most of these proteins exist in post-translationally modified isoforms. Among them, sialylation is known to be aberrant in tissue and plasma of cancer patients in addition to the branching ratio of bi-antennary to multi-antennary glycans. This study suggests a way for recognizing proteins bearing sialylated glycan branches and the relative degrees to which branching ratios changed in association with cancer, based on the differential binding affinity of branched glycans to Con A. In order to get the best results from colon cancer plasma and healthy group plasma using self-packed Con A and SNA serial affinity chromatography, efficient detection method in LC-MS was also designed and examined with iTRAQ Labeling.

P-71

Study of variations in human saliva N-glycans

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*

For the past decades, saliva glycans attract the attention as a potential biomarker for insight of health state in clinical and forensic field owing to advantages of saliva: easy access, simple storage, and non-invasive collection. Glycosylation, one of the most common PTMs, plays an important role in a wide range of biological processes. Saliva glycosylations are altered in the physiological and pathological situations by diseases, external environment, and chemical materials. Although several studies had been reported for diagnosis of health states by montitoring of saliva glycans, variation study for effects of individual and environmental differences is insufficient. In this study, we investigated 1) inter-individual variations in saliva N-glycans among subjects (n=18), 2) intra-individual variations in saliva N-glycans collected on different days (1, 2, 7, and 30 days) within a given person, and 3) environmental variations in N-glycans degradations during storage of saliva (1, 2, 3, and 7 days) on room temperature. N-glycans were enzymatically released from individual saliva by PNGase F then these were purified and enriched by PGC-SPE. Saliva N-glycans were fully characterized by nano LC chip/Q-TOF MS. Inter- and intra-individual and environmental variations were examined through comparisons of composition and relative abundances in each glycan profile. This study may help design the experiments and evaluate the saliva glycan candidates for biomarker discovery study.

P-72

Effect of Ca(II) on the conformation and aggregation process of alpha-synuclein

Jong Yoon Han, and Hugh I. Kim

Deptartment of Chemistry, Korea University, Seoul 02841, Korea

Parkinsons's disease (PD) is a neurodegenerative disease, characterized by aggregation of alpha-synuclein (αSyn). To understand factors affecting αSyn to form abnormal aggregates, chemical compounds and metal ions have been investigated *in vitro*. Among them, Ca(II), one of the most crucial metal ions in life, was shown to promote αSyn aggregation and it has been considered to have a relationship with PD. Ca(II) was observed to interact with C-terminal domain of αSyn and their binding affinity was measured (K_d ~ 1 mM). However, how the interaction affects the aggregation process of αSyn is not clearly understood. In this study, we investigated the effect of Ca(II) on the conformation and aggregation process of αSyn using mass spectrometry (MS), small-angle X-ray scattering (SAXS), and transmission electron microscopy (TEM). Our results showed that interaction between Ca(II) and C-terminal of αSyn promotes conformational change of αSyn into extended structure. The conformation change is considered as a cause of increased rates of αSyn aggregation. Furthermore, we observed that Ca(II) can affect the aggregation process during nucleation and elongation steps, and even mature fibril. Our study will provide physicochemical understanding of interaction between αSyn and Ca(II) and the aggregation process of αSyn.

KSMS

【 협력업체 】

Thermo Fisher Scientific Korea

Waters Korea

Dong-il SHIMADZU crop.

Agilent Technologies Korea

SCIEX Korea

BRUKER Korea

Goojung Chromatech Inc.

AT Frontier

TAESHIN BIO SCIENCE