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2017 한국질량분석학회

여름정기학술대회 및 총회

2017 KSMS Summer Conference

2017년 8월 23일(수) -25일(금) 12:00~

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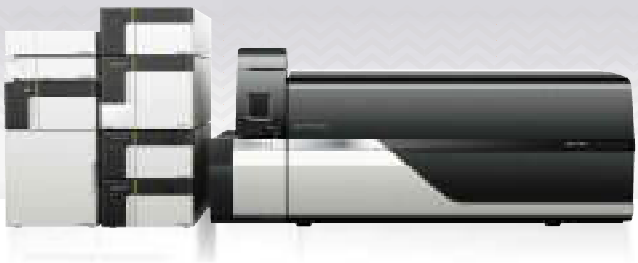

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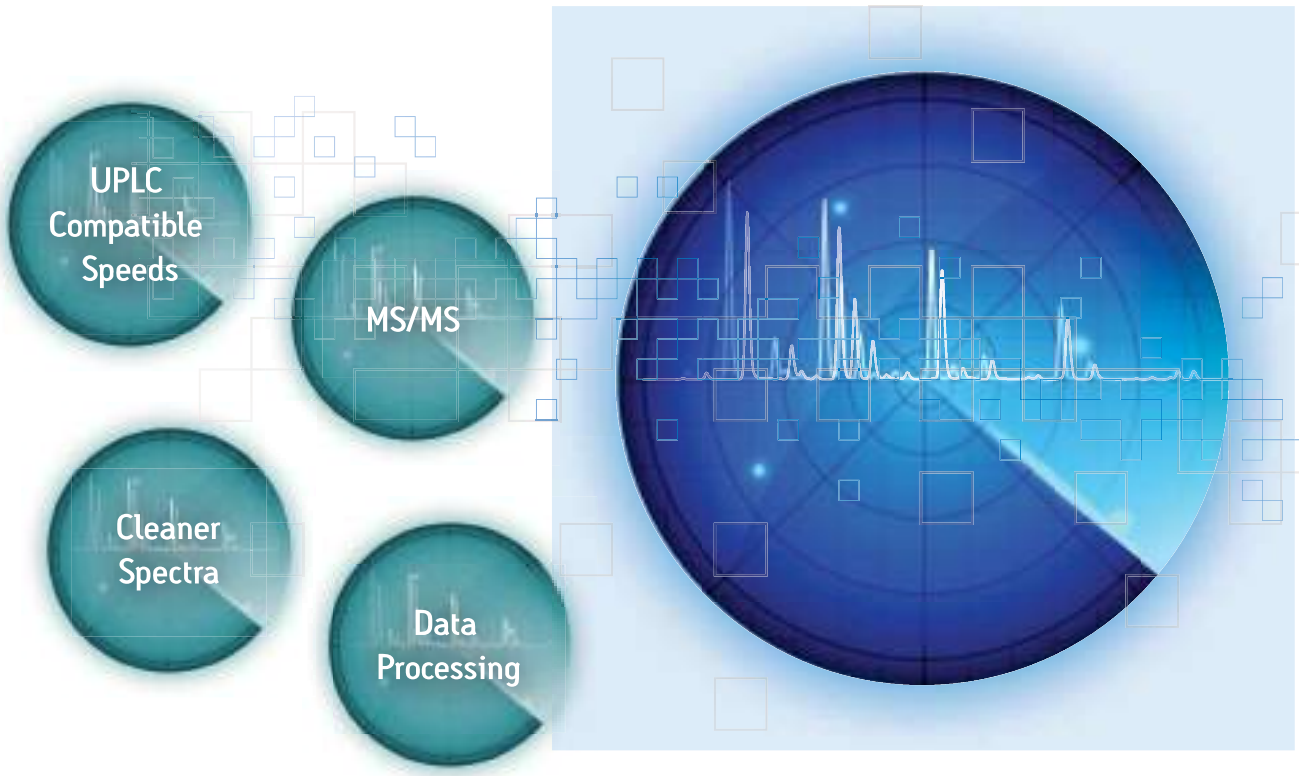

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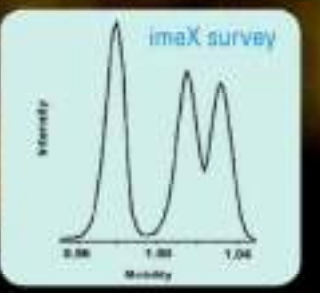

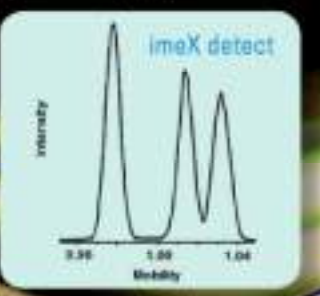

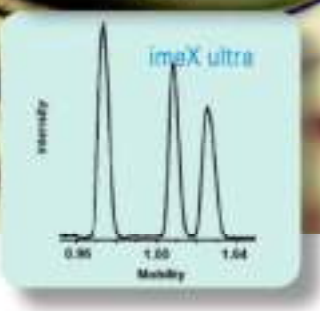

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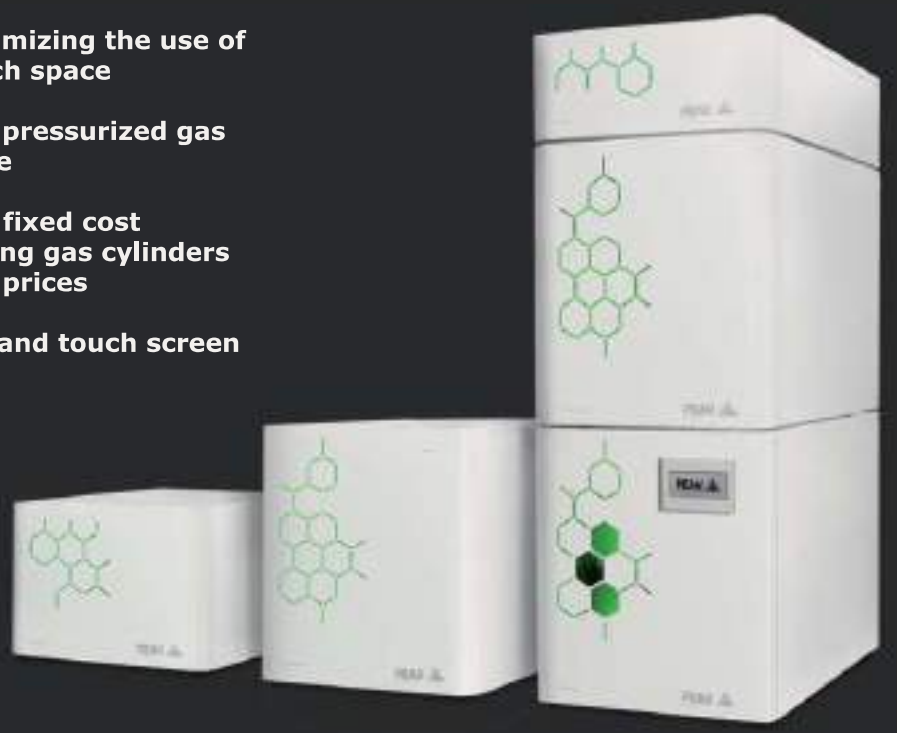

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제품명	제품번호	용량
Acetonitrile + 0.1% Formic acid (v/v) for LC-MS	1.59002.1000	1L
	1.59002.2500	2.5L
	1.59002.4000	4L
Acetonitrile + 0.1% Acetic acid (v/v) for LC-MS	1.59004.2500	2.5L
	1.59004.4000	4L
Acetonitrile + 0.1% Trifluoroacetic acid (v/v) for LC-MS	1.59014.2500	2.5L
	1.59014.4000	4L
Water with 0.1% Formic acid (v/v) for LC-MS	1.59013.2500	2.5L
	1.59013.4000	4L
Water with 0.1% Acetic acid (v/v) for LC-MS	1.59007.2500	2.5L
	1.59007.4000	4L
Water with 0.1% Trifluoroacetic acid (v/v) for LC-MS	4.80112.2500	2.5L
	4.80112.4000	4L

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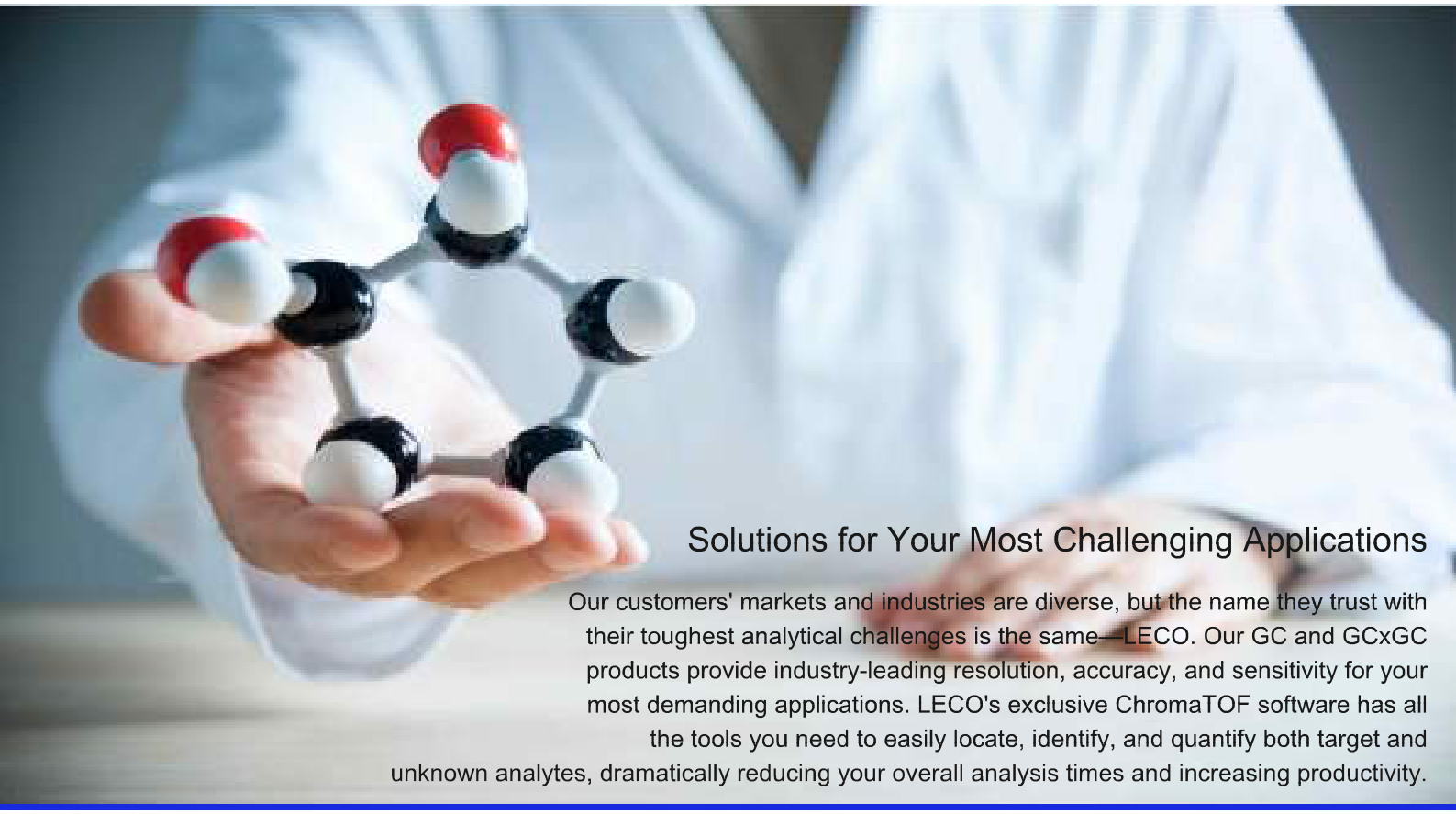

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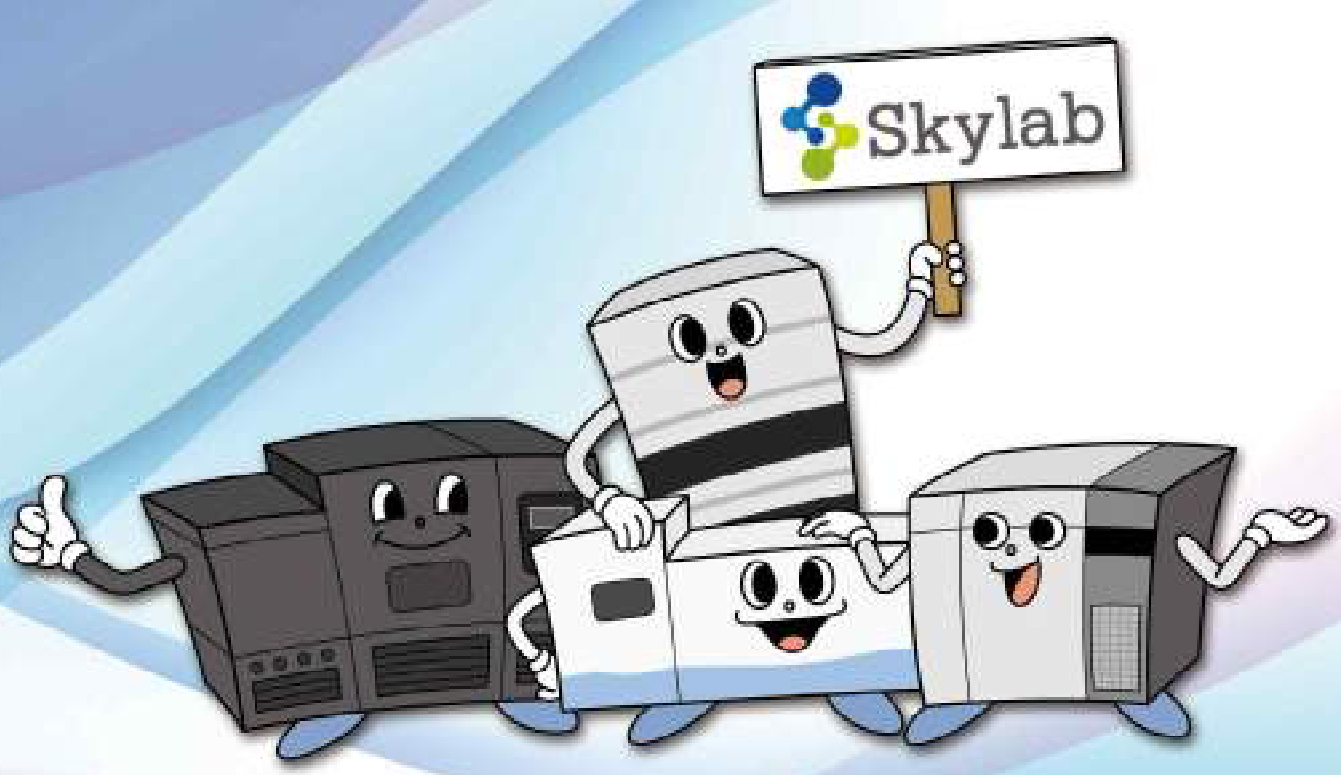

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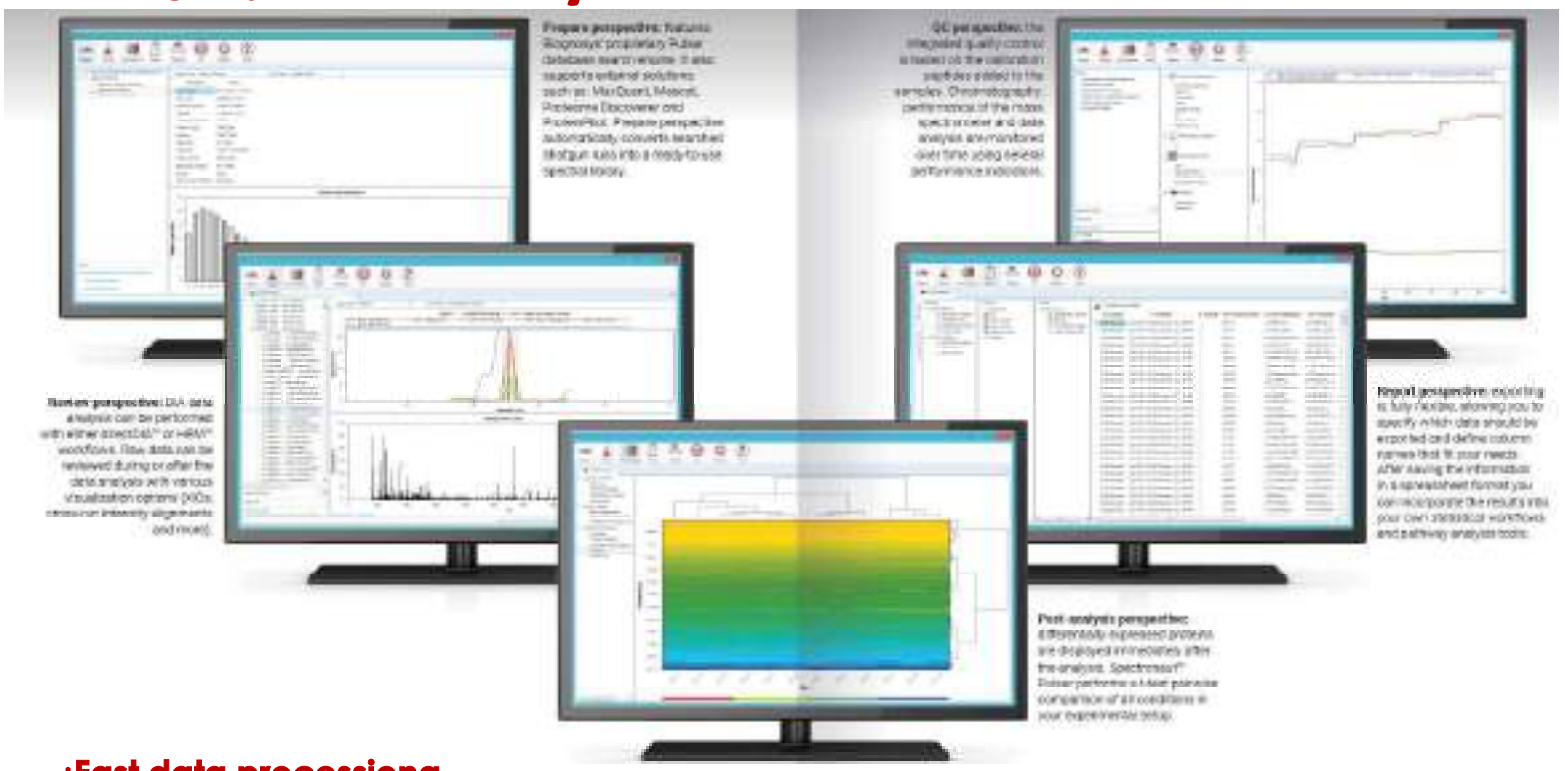

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<회장>

문명희 (연세대학교)

<조직위원>

강덕진 (한국표준과학연구원)
권용일 (강남권산부인과)
김광표 (경희대학교)
김병주 (한국표준과학연구원)
김영환 (한국기초과학지원연구원)
김정권 (충남대학교)
김준곤 (고려대학교)
김진영 (한국기초과학지원연구원)
김태영 (광주과학기술원)
김현식 (한국기초과학지원연구원)
박종호 (한국원자력연구원)
변용관 (국방과학연구소)
소헌영 (동일시마즈)
송규석 (한국원자력연구원)
신승구 (포항공과대학교)
안현주 (충남대학교)
오한빈 (서강대학교)
유종신 (한국기초과학지원연구원)
이재익 (한국과학기술연구원)
임용현 (한국표준과학연구원)
정봉철 (한국과학기술연구원)
차상원 (한국외국어대학교)
최만호 (한국과학기술연구원)
표희수 (한국과학기술연구원)
한상범 (중앙대학교)
한상윤 (가천대학교)

안내 사항

2017년 한국질량분석학회 여름정기학술대회 및 총회에 참가하신 회원 여러분 환영합니다

■ **현장등록**

8월23일(수), 12:00 ~ 24(목), 17:00

■ **Plenary Sessions**

Plenary Lecture: 24일(목), 10:00

■ **Special Sessions**

Special Lecture: 25일(금), 11:10

■ **Short Course**

23일(수), 13:00 ~ 17:10

이름표를 꼭 패용해 주시기 바랍니다.

1. Introduction to Mass Spectrometry
2. Practical Applications of Mass Spectrometry

■ **Symposium Sessions**

24일(목)

SYM1 (12:50 ~ 14:50, 영주홀A)
SYM2 (12:50 ~ 14:50, 영주홀B)
SYM3 (12:50 ~ 14:50, 백록홀A)
SYM4 (15:00 ~ 17:00, 영주홀A)
SYM5 (15:00 ~ 17:00, 영주홀B)
SYM6 (15:00 ~ 17:00, 백록홀A)

25일(금)

SYM7 (08:50 ~ 10:50, 영주홀A)
SYM8 (08:50 ~ 10:50, 영주홀B)

■ **기기전시**

23일(수) ~ 25(금),
제주도 제주국제컨벤션센터 1F 로비 부스전시장소

■ **포스터게시 및 철거**

게시: 24일(목), 10:00 까지
철거: 25일(금), 12:00 이후

■ **Poster Session**

포스터 발표자는 24일(목) 10:50 ~ 11:50 까지
포스터 앞에 대기하여 질문에 응해야 합니다.
포스터 일련번호를 부착하였으니 해당번호에 포스터를 부착해 주시고 발표해 주시기 바랍니다.

홀수: 10:50 ~ 11:20 발표

짝수: 11:20 ~ 11:50 발표

■ **전체만찬**

24일(목), 19:00 ~ 20:30

제주도 제주국제컨벤션센터(ICC) 델리지아 / 3F

■ **공지사항**

》정회원 참석자께서는 총회참석이 불가한 경우, 등록대에 비치된 위임장을 작성하여 등록데스크로 제출해 주시기 바랍니다.

》행사기간내 이름표를 꼭 패용해 주시기 바랍니다.

》제주국제컨벤션센터 모든 건물은 금연구역입니다.

》세션 중에는 핸드폰을 진동 혹은 무음으로 해 주십시오.

》세션 중에는 발표가 방해되지 않도록 사진촬영은 자제하여 주십시오

행사장 안내

▶행사장 안내

201 홀	Short Course 1
202 홀	Short Course 2
영주홀 A	Symposium 1, 4, 7
영주홀 B	Symposium 2, 5, 8
백록홀 A	Symposium 3, 6
영주홀 A+B	Brief Oral Presentation-1
백록홀 A	Brief Oral Presentation-1
영주홀 A+B	Plenary Lecture
영주홀 A+B	Special Lecture

201 홀	User Meeting-1
202 홀	User Meeting-2
203 홀	User Meeting-3
영주홀 A	Luncheon Seminar I Sponsoring Session I
영주홀 B	Luncheon Seminar II Sponsoring Session II
백록홀 A	Luncheon Seminar III Sponsoring Session III
1F 로비	Poster Session

행사장 안내

▶전시부스 안내

A-1 **Waters Korea**	**B-1** **Agilent Technologies Korea**	**C-1** **Thermo Fisher Scientific Korea**	**D-1** **ASTA Inc.**
A-2 **AB SCIEX KOREA**	**B-2** **Bruker Korea Co., Ltd.** **SCINCO Co., LTD.** **Euro Science Co., Ltd**		**D-2** **Scion Instruments Korea Co., Ltd.**
A-3 **Goojung Chromatech Inc.**	**B-3** **Dong-il SHIMADZU Corp.**		**D-3** **SMAnalytical**
			D-4 **PeakmanSP Co., Ltd**
			D-5 **SHODEX LC/MS COLUMNS**
			D-6 **LECO KOREA**
			D-7 **YoungSeong Techpia**
			D-8 **PerkinElmer**
			D-9 **ATFrontier**
			D-10 **Skylab(Neo Power Tech)**
			D-11 **Merck**

프로그램

August 23 (Wednesday)

TIME	P R O G R A M		
12:00 ~	Registration		
	SHORT COURSE (Organizer: 김진영 (한국기초과학지원연구원) & 한상윤 (가천대학교))		
	Introduction to Mass Spectrometry (Room: 201호)	**Practical Applications of Mass Spectrometry (Room: 202호)**	
13:00 ~ 14:15 (75 min)	Introduction to Mass Spectrometry 차상원 (한국외국어대학교)	Practical Aspects of Chromatography and Mass Spectrometry 이재익 (한국과학기술연구원)	
	Coffee Break		
14:30 ~ 15:45 (75 min)	Ionization Methods Focused on ESI, APCI and APPI 김성환 (경북대학교)	Practical Applications of MS_Tandem Mass Spectrometry 김태영 (광주과학기술원)	
	Coffee Break		
16:00 ~ 17:15 (75 min)	Mass Analyzers in Mass Spectrometry 박종호 (한국원자력연구원)	Interpretation of Mass Spectra 오한빈 (서강대학교)	
	Coffee Break		
17:20 ~ 18:40 (80 min)	**User Meeting-1** (Sponsored by Thermo Fisher Scientific Korea) **(Room: 201호)**	**User Meeting-2** (Sponsored by Waters Korea) **(Room: 202호)**	**User Meeting-3** (Sponsored by Agilent Technologies Korea) **(Room: 203호)**

August 24 (Thursday)

TIME	PROGRAM		
08:50 ~ 09:50 (60 min)	Organizer: 차상원 (한국외국어대학교)		
	Brief Oral Presentation of Selected Posters-1 (Chair: 김민식 (경희대학교)) **(Room: 영주홀 A+B)**	**Brief Oral Presentation of Selected Posters-2** (Chair: 이홍희 (한국표준과학연구원)) **(Room: 백록홀 A)**	
10:00 ~ 10:50 (50 min)	**Plenary Lecture** Prof. Vicki Hopper Wysocki (The Ohio State University (OSU)) (Organizer: 문명희 (KSMS 회장)) **(Room: 영주홀 A+B)**		
SYMPOSIUM			
10:50 ~ 11:50 (60 min)	**POSTER SESSION** (Organizer: 김정권 (충남대학교)) **(1F 로비)**		
11:50 ~ 12:40 (50 min)	**Luncheon Seminar I** (Sponsored by Agilent Technologies Korea) **(Room: 영주홀 A)**	**Luncheon Seminar II** (Sponsored by Waters Korea) **(Room: 영주홀 B)**	**Luncheon Seminar Ⅲ** (Sponsored by Thermo Fisher Scientific Korea) **(Room: 백록홀 A)**
SYMPOSIUM			
12:50 ~ 14:50 (120 min)	**SYM1: Bio-medical & Clinical Mass Spectrometry** Keynote Speaker: Prof. Susumu Uchiyama (University of Osaka) (Organizer: 안현주(충남대학교 분석과학기술대학원) 박세훈(성균관대 의대 서울삼성병원)) **(Room: 영주홀 A)**	**SYM2: MS Fundamentals & Elemental Analysis** (Organizer: 박종호(한국원자력연구원) 이경석(한국표준과학연구원)) **(Room: 영주홀 B)**	**SYM3: New Trends in Mass Spectrometry** Keynote Speaker: Prof. Ron M.A. Heeren (Maastricht University) (Organizer: 차상원(한국외국어대학교) 오한빈(서강대학교)) **(Room: 백록홀 A)**
SYMPOSIUM			
15:00 ~ 17:00 (120 min)	**SYM4: Pharmaceutical Mass Spectrometry** (Organizer: 이재익(한국과학기술연구원) 최용석(단국대학교)) **(Room: 영주홀 A)**	**SYM5: MS for Omics Ⅰ** (Metabolomics and Lipidomics) Keynote Speaker: Prof. Gavin E. Reid (The University of Melbourne) / Prof. Guowang Xu (Dalian Institute of Chemical Physics, Chinese Academy of Sciences) (Organizer: 김태영(광주과학기술원) 권성원(서울대학교)) **(Room: 영주홀 B)**	**SYM6: Food & Agriculture** (Organizer: 한상범(중앙대학교) 김영준(서울과학기술대학교)) **(Room: 백록홀 A)**

17:10 ~ 17:40 (30 min)	**'2017 KSMS General Meeting'** **(Room: 백록홀 A)**		
17:50 ~ 18:40 (50 min)	**Sponsoring Session I** (Sponsored by AB SCIEX Korea) **(Room: 영주홀 A)**	**Sponsoring Session II** (Sponsored by Dong-il SHIMADZU Corp.) **(Room: 영주홀 B)**	**Sponsoring Session Ⅲ** (Sponsored by Bruker Korea Co., Ltd) **(Room: 백록홀 A)**
19:00 ~ 20:30 (90 min)	**Conference Banquet** (Organizer: 이재익 (KIST)) **(델리지아 (3F))**		

August 25 (Friday)

TIME	P R O G R A M	
08:50 ~ 10:50 (120 min)	**SYM7: Energy & Environmental** Keynote Speaker: Prof. Young Jin Lee (Iowa State University) (Organizer: 서정주(한국기초과학지원연구원) 김성환(경북대학교)) **(Room: 영주홀 A)**	**SYM8: MS for Omics Ⅱ** (Proteomics and Glycomics) Keynote Speaker: Prof. Lance Wells (University of Georgia) (Organizer: 강덕진(한국표준과학연구원) 임재민(창원대학교)) **(Room: 영주홀 B)**
11:10 ~ 11:50 (40 min)	**Special Lecture** 김현식 (한국기초과학지원연구원) (Organizer: 문명희 (KSMS 회장)) **(Room: 영주홀 A+B)**	
11:50 ~ 12:30 (40 min)	**Poster Award & Closing Remarks** **(Room: 영주홀 A+B)**	

세부프로그램

WEDNESDAY Afternoon, AUGUST 23

SHORT COURSE
13:00 - 17:15

Introduction to Mass Spectrometry (201 호)

13:00 - 14:15	**Introduction to mass spectrometry** 차상원 (한국외국어대학교)
14:30 - 15:45	**Ionization methods focused on ESI, APCI and APPI** 김성환 (경북대학교)
16:00 - 17:15	**Mass analysers in mass spectrometry** 박종호 (한국원자력연구원)

Practical Applications of Mass Spectrometry (202 호)

13:00 - 14:15	**Practical aspects of chromatography and mass spectrometry** 이재익 (한국과학기술연구원)
14:30 - 15:45	**Practical applications of MS_Tandem mass spectrometry** 김태영 (광주과학기술원)
16:00 - 17:15	**Interpretation of mass spectra** 오한빈 (서강대학교)

BRIEF ORAL PRESENTATION OF SELECTED POSTERS - 1

8:50 – 09:50

Session 1 - 영주홀 A+B

Organizer: 차상원 (한국외국어대학교) / Chair: 김민식 (경희대학교)

08:50–08:53 Determination of ethnic differences in human saliva proteome by the construction and the characterization of the Korean whole saliva proteome
조하라 (단국대학교)

08:53–08:56 Lipids profiling of *Drosophila melanogaster* heads using electrospray ionization mass spectrometry (ESI-MS)
장현준 (충남대학교)

08:56–08:59 Derivatization of myoglobin after microwave-assisted acid hydrolysis
이다빈 (충남대학교)

08:59–09:02 Investigation of various liquid chromatography mass spectrometry (LC/MS) methods for comprehensive ganglioside profiling
최수빈 (한국외국어대학교)

09:02–09:05 Clinical application of multi hormones in human serum by liquid tandem mass spectrometry
이호운 ((재)씨젠의료재단)

09:05–09:08 Phospholipid quantification and enhancement of cardiolipin profiling based on isotope-labeled methylation by nUPLC-ESI-MS/MS
이종철 (연세대학교)

09:08–09:11 Comprehensive proteomics of 2D-/3D-cultured adipocyte cell and its co-cultured with macrophage using a nLC-ESI-MS/MS
이선영 (경희대학교 / 한국표준과학연구원)

09:11–09:14 Protein Sequence Analysis by TEMPO-assisted Free Radical Initiated Peptide Sequencing (FRIPS) Mass Spectrometry
이재웅 (서강대학교)

09:14–09:17 Establishing an analysis method of anticancer drugs to study cellular uptake and efficiency of combination therapy
민경서 (고려대학교)

09:17–09:20 Label-free quantitative strategy for non-human sialic acid using MRM-MS
고재경 (충남대학교 분석과학기술대학원)

09:20–09:23 Global N-glycoproteome analysis in the course of human neural stem cell differentiation
송민영 (한국기초과학지원연구원)

09:23–09:26 Qualitative determination of steviol and its glycosides in *Stevia rebaudiana* by liquid chromatography tandem mass spectrometry
김성년 (한국기초과학지원연구원)

09:26–09:29 Quantitation of glycans in yeast using metabolic isotope labeling with isotopic glucose by mass spectrometry
김지연 (창원대학교)

09:29–09:32 A sandwich-type HBsAg immunoassay using ICP-MS with metal-doped nanoparticles
김찬미 (단국대학교)

09:32–09:35 Profiling of a wide range of neurochemicals in human urine by ultra performance liquid chromatography-tandem mass spectrometry combined with *in situ* selective derivatization
이원웅 (경희대학교)

BRIEF ORAL PRESENTATION OF SELECTED POSTERS - 2

8:50 – 09:50

Session 2 - 백록홀 A

Organizer: 차상원 (한국외국어대학교) / Chair: 이홍희 (한국표준과학연구원)

08:50–08:53 Identification of prostate cancer specific signature in cell lines based on proteomic analysis
박아름 (을지대학교)

08:53–08:56 Development and validation of an analytical procedure for the total mercury in oyster and tuna using isotope-dilution inductively coupled plasma mass spectrometry
김휘진 (과학기술연합대학원 대학교 / 한국표준과학연구원)

08:56–08:59 Effects of acetonitrile amounts on bovine serum albumin and myoglobin tryptic digestion in gentle mixing or microwave
김여선 (충남대학교)

08:59–09:02 Optimization of paper spray ionization for sensitive protein analysis
박태민 (한국외국어대학교)

09:02–09:05 Development of a structural characterization method of lignin oligomers using pseudo-LC-MS3 analysis
송우영 (광주과학기술원)

09:05–09:08 Glycomics-based Forensic Platform for the Identification of Human Saliva
박진영 (충남대학교 분석과학기술대학원)

09:08–09:11 MATLAB-based Software Development for Screening Illegal Drugs and Analogues Identification Using LC-MS/MS Data
장인애 (서강대학교)

09:11–09:14 Competitive Homo- and Hetero- Self-assembly of Amyloid-β 1-42 and 1-40 in the Early Stage of Fibrillation
허채은 (고려대학교)

09:14–09:17 Rapid and sensitive carbapenemase assay using LDI-MS based on a parylene-matrix chip
박종민 (연세대학교)

09:17–09:20 Development of an on-line proteolysis and glycopeptide enrichment method using enzyme immobilized thermo-sensitive porous polymer membrane enzyme reactor (μPPMER) and nanoflow liquid chromatography-tandem mass spectrometry
양준선 (연세대학교)

09:20–09:23 Development of relative quantification method for lipidome by using $^{2}H_2O$ partial metabolic labeling
김종현 (광주과학기술원)

09:23–09:26 Simultaneous quantification of the four coumarins including one active metabolite in human plasma by UHPLC-MS/MS: Application to pharmacokinetics
천성문 (차 의과학대학교)

09:26–09:29 Evaluation of a set of calibrants for more accurate measurement of collision cross section (ccs) of polycyclic aromatic hydrocarbon compounds
임동완 (경북대학교)

09:29–09:32 Characterization of weathered oil by paper spray ionization and estimation of the oxidation degree of spilled oils depending on the chemical class distribution
김동휘 (경북대학교)

09:32–09:35 Estimation of Elemental Compositions for Additives in Polymers Using Newly Developed EI/CI Ion Source without Venting MS
이동건 (동일시마즈)

THURSDAY Morning / Afternoon, AUGUST 24

PLENARY LECTURE

영주홀 A+B

Chair: 회장 문명희 (연세대학교)

10:00 – 10:50

10:00-10:50 **Native MS: Development of SID/IMMS and SID/HRMS**
Vicki Hopper Wysocki (The Ohio State University (OSU))

POSTER SESSION

1F 로비홀

Chair: 김정권 (충남대학교)

10:50 – 11:50

10:50-11:50 **Poster Session**

KEYNOTE SPEAKER

THURSDAY Afternoon, AUGUST 24

SYM-1: Bio-medical & Clinical Mass Spectrometry (영주홀 A)

12:50-13:20 **Biophysical characterizations of antibody drugs by mass spectrometry**
Susumu Uchiyama (The University of Osaka)

SYM-3: New Trends in Mass Spectrometry (백록홀A)

12:50-13:20 **Accelerating MultiModal Molecular Imaging: Innovations in structural elucidation.**
Ron M.A. Heeren (Maastricht University)

SYM-5: MS for Omics Ⅰ (Metabolomics and Lipidomics) (영주홀B)

15:00-15:30 **Illuminating the Structural Diversity of the Lipidome: Ultraviolet Photodissociation Tandem Mass Spectrometry for Comprehensive Lipid Characterization**
Gavin E. Reid (University of Melbourne)

15:30-16:00 **Integrated Omics Approach Centered on Mass Spestrometry-based Metabolomics to Decipher Mechanism Implicated in Human Diseases**
Guowang Xu (Dalian Institute of Chemical Physics, Chinese Academy of Sciences)

THURSDAY Afternoon, AUGUST 25

SYM-7: Energy & Environmental (영주홀A)

08:50-09:20 **Real-Time Monitoring of Molecular Products in Thin-Film Fast Pyrolysis of Glucose-based Carbohydrates**
Young Jin Lee (Iowa State University of Science and Technology)

SYM-8: MS for Omics Ⅱ (Proteomics and Glycomics) (영주홀B)

08:50-09:20 **Glycomic and Glycoproteomic Mass Spectrometry Approaches**
Lance Wells (University of Georgia)

SYMPOSIUM 1 & 2 & 3

12:50 – 14:50

SYM-1: Bio-Medical & Clinical Mass Spectrometry (영주홀 A)

Chairs: 안현주 (충남대학교 분석과학기술대학원) & 박세훈 (성균관의대 삼성서울병원)

12:50-13:20 **Biophysical characterizations of antibody drugs by mass spectrometry**
Susumu Uchiyama (The University of Osaka)
: Keynote speaker

13:20-13:40 **Glycan Markers for Ovarian Cancer with High Sensitivity and High Specificity**
권용일 (강남권산부인과)

13:40-14:00 **Dissection of Adaptive Drug Resistance Mechanism Harnessing Mass Spectrometry-based Proteomics**
김재영 (충남대학교 분석과학기술대학원)

14:00-14:20 **Glycomic Profiling of Targeted Serum Haptoglobin for Gastric Cancer Using Nano LC/MS and LC/MS/MS**
김정회 (KAIST 생명과학과)

14:20-14:40 **Clinical Application of LC/MS/MS for Drug Counseling in Pregnant Women**
박은석 (제일병원 마더세이프 & 진단검사의학과)

SYM-2: MS Fundamentals & Elemental Analysis (영주홀 B)

Chairs: 박종호 (한국원자력연구원) & 이경석 (한국표준과학연구원)

12:50-13:10 **Inorganic element analysis in various fields using fsLA and ICP-MS**
박경수 (한국과학기술연구원)

13:10-13:30 **Determination of naturally occurring radioactive materials by $LiBO_2$ fusion and ICP-MS**
임종명 (한국원자력연구원)

13:30-13:50 **Analysis of Various Samples Using TOF-SIMS at KBSI Busan Center**
진종성 (한국기초과학지원연구원)

13:50-14:10 **Development of food matrix CRMs for elemental analysis**
허성우 (한국표준과학연구원)

14:10-14:30 **Sources Identification of Pb in Marine Environments around the Korean Peninsula**
최만식 (충남대학교)

14:30-14:50 **Applications of mass spectrometry on polar snow and ice core samples**
이강현 (극지연구소)

SYM-3: New Trends in Mass Spectrometry (백록홀 A)

Chairs: 차상원 (한국외국어대학교) & 오한빈 (서강대학교)

12:50-13:20	**Accelerating MultiModal Molecular Imaging: Innovations in structural elucidation.** Ron M. A. Heeren (Maastricht University) : Keynote speaker
13:20-13:40	**Paper Spray Ionization and Paper Spray Chemical Ionization –Sensitive Ionization Methods for the Analysis of Spilled Oils** 김성환 (경북대학교)
13:40-14:00	**Elemental imaging and quantification of thermally conducting polymer containing fiber-type SiO_2 fillers using LIBS and laser ablation ICP-MS** 임흥빈 (단국대학교)
14:00-14:20	**ToF-SIMS Study of Tissue Samples** 이태걸 (한국표준과학연구원)
14:20-14:40	**Development of MALDI IMS and its application in cancer diagnosis** 오주연 (㈜아스타)

SYMPOSIUM 4 & 5 & 6
15:00 – 17:00

SYM-4: Pharmaceutical Mass Spectrometry (영주홀 A)

Chairs: 이재익 (한국과학기술연구원) & 최용석 (단국대학교)

15:00-15:20	**Metabolomic approaches based on chromatography hyphenated mass spectrometry** 홍종기 (경희대학교 약학대학)
15:20-15:40	**LC-MS/MS Determination of Residual Carbonyl Compounds in Dietary Supplement using Fluorogenic Derivatization** 이용문 (충북대학교 약학대학)
15:40-16:00	**Laser desorption/ionization (LDI) mass spectrometry based on nanomaterials for biomedical applications** 변재철 (연세대학교)
16:00-16:20	**Quality Characterization and Evaluation Using Mass Spectrometry in Biosimilar Development** 이경훈 (셀트리온)
16:20-16:40	**Developments of automated high-throughput sample preparation methods using glycan-specific affinity capturing for glycosylated proteome analysis** 이후근 (가천대학교 약학대학)
16:40-17:00	**Analysis of Homogeneous and Heterogeneous Antibody-Drug Conjugates (ADCs) for Bioanalytical and Pharmacokinetics Analysis Platforms** 진종화 (KBIO 신약개발지원센터)

SYM-5: MS for Omics Ⅰ(Metabolomics and Lipidomics) (영주홀 B)

Chairs: 김태영 (광주과학기술원) & 권성원 (서울대학교)

15:00-15:30	**Illuminating the Structural Diversity of the Lipidome: Ultraviolet Photodissociation Tandem Mass Spectrometry for Comprehensive Lipid Characterization** Gavin E. Reid (University of Melbourne) : Keynote speaker
15:30-15:50	**Integrated Omics Approach Centered on Mass Spestrometry-based Metabolomics to Decipher Mechanism Implicated in Human Diseases** Guowang Xu (Dalian Institute of Chemical Physics, Chinese Academy of Sciences) : Keynote speaker
16:00-16:20	**Revisiting the Metabolism and Bioactivation of Ketoconazole Using LC–MS-Based Metabolomics** 김주현 (가톨릭대학교)
16:20-16:40	**Free Fatty Acids as biomarkers in Pulmonary Fibrosis** 유현주 (울산의대 서울아산병원)
16:40-17:00	**Recent advances in steroid signatures to monitor endocrine diseases evaluated by GC-MS/MS** 문주연 (가톨릭대학교 약학대학)

SYM-6: Food & Agriculture (백록홀 A)

Chairs: 한상범 (중앙대학교) & 김영준 (서울과학기술대학교)

15:00-15:20	**Chemical Fingerprints and their applications** 민지숙 (국립과학수사연구원 대구과학수사연구소)
15:20-15:40	**Development of Certified Reference Materials for Accurate Determination of Fluoroquinolone Antibiotics in Chicken Meat** 형석원 (한국표준과학연구원)
15:40-16:00	**Simultaneous and Rapid Analysis of 500 Pesticide Multiresidues in Crops Using GC-MS/MS and LC-MS/MS** 이종화 (서울대학교)
16:00-16:20	**Analysis of functional nutrients in human milk from three Asian countries** 김재한 (충남대학교)
16:20-16:40	**Risk Prevention and Management of Pesticides Residues in the Food Industry** 고광용 (CJ 제일제당)
16:40-17:00	**Discrimination of Geographical Origins of Rice and Ginseng Using a Mass Spectrometer-Based Electronic Nose** 문지영 (국립농산물품질관리원 시험연구소)

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SYMPOSIUM 7 & 8

08:50 – 10:50

SYM-7: Energy & Environmental (영주홀 A)

Chairs: 서정주 (한국기초과학지원연구원) & 김성환 (경북대학교)

08:50-09:20 **Real-Time Monitoring of Molecular Products in Thin-Film Fast Pyrolysis of Glucose-based Carbohydrates**
Young Jin Lee (Iowa State University of Science and Technology)
: Keynote speaker

09:20-09:40 **Rapid, real-time and simultaneous quantification of volatile organic compounds with Selected Ion Flow Tube Mass Spectrometery (SIFT-MS)**
임운혁 (한국해양과학기술원)

09:40-10:00 **Comparing discrimination capabilities of fluorescence spectroscopy versus FT-ICR-MS for sources and hydrophobicity of sediment organic matter**
허 진 (세종대학교)

10:00-10:20 **Ultra-High Resolution FT-ICR Mass Spectrometry for Analaysis of Fine Aerosol ($PM_{2.5}$)-derived Organic Substances**
장경순 (한국기초과학지원연구원)

10:20-10:40 **Applications and Results of Ambient Aerosol Measurement using High Resolution Time of Flight Aerosol Mass Spectrometery**
이태형 (한국외국어대학교)

SYM-8: MS for Omics Ⅱ (Proteomics and Glycomics) (영주홀 B)

Chairs: 강덕진 (한국표준과학연구원) & 임재민 (창원대학교)

08:50-09:20 **Glycomic and Glycoproteomic Mass Spectrometry Approaches**
Lance Wells (University of Georgia)
: Keynote speaker

09:20-09:30 **Ultraplexed MS1-based accurate protein quantification**
김종서 (서울대학교 기초과학연구원 (IBS) RNA 연구단)

09:30-09:50 **Multiplexed parallel reaction monitoring assays for protein tyrosine kinases**
김혜정 (KBIO 신약개발지원센터)

09:50-10:10 **MS based Glycoproteome Analysis Using IQ-GPA and Its Applications**
김진영 (한국기초과학지원연구원)

10:10-10:30 **Integrative Multi-Omics of Th1 Differentiation**
김민식 (경희대학교)

SPECIAL LECTURE

영수홀 A+B

Chair: 문명희 (연세대학교)

11:10-11:50 **Instrumentation for Mass Spectrometry**

김 현 식 (한국기초과학지원연구원 / 전임회장)

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BRIEF ORAL PRESENTATION

Brief Oral 1-1

[P-013]

Determination of ethnic differences in human saliva proteome by the construction and the characterization of the Korean whole saliva proteome

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

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

Since the early 2000s, global analyses of the saliva proteome have been performed to identify more than 3,000 proteins in human saliva. While ethnic differences in the human plasma proteome have been recently reported, such studies on human saliva in this aspect have not been previously reported. Thus, here, in order to determine ethnic differences in the human saliva proteome, the construction and the characterization of the Korean whole saliva (WS) proteome through nLC-Q-IMS-TOF analyses of WS samples collected from eleven healthy South Korean male adult volunteers were carried out. As a results, a Korean WS proteome catalogue indexing 480 proteins was built for the first time. Among 480 proteins, 226 distinct Korean WS proteins, not observed in the integrated human saliva protein dataset were identified, and significant gene ontology distribution differences in the Korean WS proteome compared to the integrated human saliva proteome were also determined. Thus, ethnic differences in the human saliva proteome became evident by these observations. Additionally, the potential value of ethnicity-specific human saliva proteins as biomarkers for diseases highly prevalent in that ethnic group was confirmed by finding 35 distinct Korean WS proteins likely to be associated with the top 10 deadliest diseases in South Korea. Finally, the present Korean WS protein list can serve as the first level reference for future proteomic studies on Korean saliva.

Brief Oral 1-2

[P-147]

Lipids profiling of *Drosophila melanogaster* heads using electrospray ionization mass spectrometry (ESI-MS)

Hyun Jun Jang[1,2], Jeong Hyang Park[3], Joon Sig Choi[2], Sohee Yoon[1*]

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

[3]*Department of Brain & Cognitive Sciences, DGIST, Daegu, 42988, Republic of Korea.*

Drosophila is a widely used disease-induced animal model because of its remarkable similarity to human diseases in degenerative brain diseases. Electrospray ionization mass spectrometry (ESI-MS) is commonly used approaches for the lipid analysis. In this study, we first attempted to establish lipid analysis of control *Drosophila* for the detection of lipid biomarkers of degenerative brain diseases.

The whole body or head of *Drosophila* is often used in biological analysis, but we have attempted to define the lipid distributions in whole head and in each part of *Drosophila* head. First, we dissected the *Drosophila melanogaster* head into phosphate buffered saline (PBS), brain and outer peel, respectively, and extracted lipids from each part. ESI-MS was then performed to compare lipid species and distributions between in the brain, the peel, PBS, and whole head.

Phosphatidylcholines were mainly detected in the brain, whereas triacylglycerols (TAG) were abundantly detected in the peel and in PBS solution. Some phospholipids detected as negative ions showed a significantly different distribution in each part. According to the lipid composition in lipid-dissolved PBS solution during the dissection, it can be suggested that TAG is abundantly distributed outside the brain in *Drosophila* head, while only small amount of the lipid presents in the brain. This means that meaningful lipid biomarker candidates found only in the brain may be suppressed when analyzing the whole head.

Brief Oral 1-3

[P-144]

Derivatization of myoglobin after microwave-assisted acid hydrolysis

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

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

Bottom-up approach using microwave-assisted acid hydrolysis of proteins has been used in protein sequence analysis. Microwave-assisted acid hydrolysis of proteins can be performed with a small amount acid such as hydrochloric acid (HCl), formic acid (FA), acetic acid or phosphoric acid in a microwave oven for an hour incubation. Acid hydrolysis using a small amount acid cleaves proteins exclusively at C-terminal of aspartic acid. A mixture of dilute HCl and 2 % FA can make protein cleaved into polypeptide ladders, where C-terminals of aspartic acids are cleaved by 2 % FA and polypeptide ladders are generated by dilute HCl.

In this study, we will look for the most appropriate derivation method to confirm peptide sequences of the polypeptide ladders. Derivatization of peptides with N-acetoxysuccinimide or *O*-methylisourea was performed after microwave-assisted 2 % formic acid hydrolysis. When acetylation that attachs acetyl group at amino group of lysine residues and N-terminals of peptides using N-acetoxysuccinimide was performed, the number of unobserved mass peaks was increased because of lower intensity of the derivatized peptides. Another derivatization such as guanidination that converts amino group of lysine residues and N-terminals of peptides to guanidine groups using *O*-methylisourea was also performed to look for the most appropriate derivation method. Detailed results will be presented during the session.

Brief Oral 1-4

[P-149]

Investigation of various liquid chromatography mass spectrometry (LC/MS) methods for comprehensive ganglioside profiling

Soobin Choi and Sangwon Cha*

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

Gangliosides, major acidic glycosphingolipids in mammals, contain sugar chains with a variety of sialic acid residues. There are hundreds of variations in ganglioside structures based on compositions and structures of oligosaccharide head groups as well as compositions of ceramide cores. In addition, gangliosides are extremely labile molecules. These often make it difficult to perform reliable ganglioside profiling by liquid chromatography mass spectrometry (LC/MS). Therefore, we tested and evaluated various LC methods including conventional reversed phase LC, ion-pairing LC, and hydrophilic interaction chromatography (HILIC) for analyzing gangliosides. In this evaluation process, we focused on optimizing separation conditions for resolving structural isomers of disialogangliosides, designated to GD1a and GD1b, which are known to be major species in mammal brains. Based on the results through this investigation, an effective and sensitive LC/MS condition for ganglioside profiling was suggested.

Brief Oral 1-5

[P-072]

Clinical application of multi hormones in human serum by liquid tandem mass spectrometry

Houn Lee, Hyojin Kim, Jinsun Jung, Hanseul Suh, Heejung Jang, Eunha Oh

R&D office, Seegene Medical Foundation, 320, Cheonho-daero, Seongdong-gu, Seoul, ***Korea***

Cortisol and DHEA are powerful physiological hormones that are important to health. DHEA antagonizes the effects of cortisol. It is a precursor for sexual hormones, which are testosterone and the estrogens. This method is to develop simultaneous analysis using LC-MS/MS in 5 hormones: cortisol, DHEA, testosterone, progesterone, and E2. 6 serum samples were analyzed by LC-MS/MS during 5 days as interday and intraday analysis. The samples were treated with MTBE for LLE. E2 was measured with a derivative reaction of DMIS. This analysis was successfully validated according to the guideline from KFDA. Also, the analysis demonstrated a linearity in a range of 1-400 μg/L (R2>0.99) for cortisol, 0.1-10 μg/L (R2>0.99) for testosterone, 0.05-20 μg/L (R2>0.99) for progesterone, 0.5-30 μg/L (R2>0.99) for DHEA, and 5-500 pg/mL (R2>0.99) for E2. A lower limit of detection was 0.161 μg/L for cortisol, 0.023 μg/L for testosterone and progesterone, 0.116 μg/L for DHEA, and 1.450 pg/mL for E2. Cross-validation between ELISA and LC-MS/MS showed a high correlation (R>0.97) and both the accuracy and precision (88.9-110.5%) were measured by recovery analysis during 5 days in low (CV<20%), medium, and high concentration (CV<10%). Carryover and Quality control were also validated (CV<20%). Accordingly, even though automated ELISA analysis is faster, LC-MS/MS analysis is more sensitive, accurate and cost-effective. Moreover, this method makes simultaneous quantification of multiple compounds possible.

Brief Oral 1-6

[P-018]

Phospholipid quantification and enhancement of cardiolipin profiling based on isotope-labeled methylation by nUPLC-ESI-MS/MS

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

Dept of Chemistry, Yonsei University, 50 Yensei-ro, Seodaemun-gu, Seoul, 03722, South Korea

A main concern in the accurate lipidomic analysis by LC-ESI-MS is to maintain high reproducibility in quantification against the fluctuation in ionization, especially since different types of lipid species have different ionization efficiencies. In this study, an isotope-labeled methylation (ILM) method for quantitative analysis for phospholipids (PLs) using nanoflow LC-ESI-MS/MS was developed to improve the quantification. The ILM method is based on methylation (H-methylation:CH_3, D-methylation: CHD_2) of the phosphate or carboxyl group of PLs using (trimethylsilyl)diazomethane, which serves as a methylation reagent. Two methylated lipid pairs have the same ionization efficiency and elute simultaneously by LC. A relative quantitation is achieved by directly comparing the peak areas of these two methylated lipids. The methylation efficiency values were higher than 96% for most PL classes under acidic condition. For the evaluation of the ILM method, the nUPLC-ESI-MS/MS analysis of PL in selected reaction monitoring (SRM) mode was performed by varying the mixing ratio of the H-/D-methylated PL standards and good linear relationships were observed with an error value of less than 6.6% in average.

As a result, 83 PLs without including PCs and PEs were quantified by applying the ILM method to the lipid extracts of the DU145 cell line with and without D-allose treatment. This method has demonstrated that identification/quantification of lipids, especially phosphatidic acid and cardiolipin, were significantly improved compared to the conventional quantification without ILM.

Brief Oral 1-7

[P-019]

Comprehensive proteomics of 2D-/3D-cultured adipocyte cell and its co-cultured with macrophage using a nLC-ESI-MS/MS

Sun Young Lee,[1,2] Kwonseong Kim,[2] Jongki Hong,[1] Sung Bum Park,[3] Ki Young Kim,[3] Dukjin Kang[2]

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[2]*Center for Bioanalysis, Division of Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 34113, Korea*

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Adipocytes play a role in regulating the fat storage, and lead to obesity, type II diabetes, and inflammation-related diseases via both hypertrophy and hyperplasia. In general, the cellular proteomics of adipocytes has been carried out by means of which the cellular proteome from adipocyte cell is obtained through a two dimensional (2D)-cultured strategy and followed by shotgun proteomics, thereby excavating a key protein that regulates metabolic mechanism in adipocyte cells. However, 2D-cultured cellular proteomics is still insufficient to exactly represent that of real tissue in living body. In order to deeply understand the metabolic mechanism of adipocytes, there is necessary to make the environment that is similar to real tissue. In this study, we developed 3D-cell culture system for 3T3-L1 cell lines and co-cultured ones with macrophage and investigated on the difference of cellular proteome between 2D- and 3D-cultured systems. To do this, each protein sample was isobarically labeled using an iTRAQ-8plex, pooled equally, and performed tandem mass spectrometric analysis. As the results, we quantified a total of 4190 proteins in duplicate runs and find out proteins having a different quantities between 2D- and 3D-cultured adipocytes. In 3D-cultured adipocyte cells, the levels of proteins that are implicated in adipogenesis such as fatty acid binding protein, fatty acid synthase, and acetyl-CoA carboxylase were up-regulated, compared to that of 2D cultured-ones.

Brief Oral 1-8

[P-003]

Protein Sequence Analysis by TEMPO-assisted Free Radical Initiated Peptide Sequencing (FRIPS) Mass Spectrometry

Jae-ung Lee and Han Bin Oh*

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The TEMPO-based FRIPS method has been previously shown to be a powerful tandem mass spectrometry tool for peptide sequencing. However, it has not been applied to sequencing proteins; top-down analysis. We have made efforts to extend this method into small protein ubiquitin (8.6 kDa). To get an ubiquitin sample conjugated with only one o-TEMPO-Bz-C(O)- radical site at the N-terminus, initially seven primary amines of lysine (K) were blocked by guanidination and then conjugated with o-TEMPO-Bz-C(O)- reagent. The modified ubiquitin ions were isolated and fragmented by CID and HCD for each charge state using an LTQ-Orbitrap™ mass spectrometer. It was found that the radical ions resulted from the release of the TEMPO radical were generated regardless of the types of collisional energy and charge states. Also, various types of fragmented ions like a-/x-, b-/y-, and c-/z- could be identified in the similar way to the TEMPO mediated FRIPS. This demonstrates that TEMPO mediated FRIPS is applicable to the top-down analysis.

Brief Oral 1-9

[P-164]

Establishing an analysis method of anticancer drugs to study cellular uptake and efficiency of combination therapy

Areum Hong, Gyeong Seo Min, Hugh I. Kim*

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As the incidence of cancer increases steadily, development and relevant pharmacokinetics/pharmacodynamics study of anticancer drugs has long been in the spotlight. According to previous clinical researches, most of the anticancer drugs are used as combination, not as single drug for maximizing efficiency. To develop effective combination of anticancer drugs, understanding how combination therapy works better than single drug is crucial. However, related researches have been focused on mainly drug combination efficiency in clinical investigation. Therefore, we aim to study cellular uptake and efficiency of combination therapy for cancer cells. Firstly, we selected combination of anticancer drugs to treat neuroblastoma and neuroblastoma cell lines, SK-N-SH and SH-SY5Y. To search proper drug treating condition to cell, cell viability tests of each drug in the combination were conducted. Also, we developed quantitation method using mass spectrometry for drug in cell culture media to study any differences in drug uptake depending on drug treatment, combination or single drug. As a result, we optimized solvent condition for drug ionization efficiency and pretreatment method of culture media to quantify small molecules including anticancer drugs. Based on these results, we are currently working on the correlation between drug efficiency and time-based cellular uptake after treating drug combination.

Brief Oral 1-10

[P-099]

Label-free quantitative strategy for non-human sialic acid using MRM-MS

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

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

The surface of most vertebrate cells is decorated with a layer of sugar chains known as the glycosylation. Sialic acids expressed as outer terminal units on the sugar chains play fundamental roles in cell–cell and cell–microenvironment interactions. One particular sialic acid called N-Glycolylneuraminic acid (Neu5Gc) could not be synthesized in humans due to an inactivated *CMAH* gene. However, exogenous Neu5Gc from dietary sources (particularly red meats), and biotherapeutics produced from CHO cell is often detected in human. Especially, it is observed at even higher levels in some human cancers. Therefore, the screening of non-human sialic acid is getting attention in biotherapeutics as well as clinical research. Neu5Gc is traditionally analyzed using HPAEC-PAD or RP-HPLC requiring derivatization steps with poor sensitivity. In this study, we developed label-free method for specific and sensitive detection of Neu5Gc based on mass spectrometry. Mouse plasma containing plenty of Neu5Gc was enzymatically treated with PNGase F to release N-glycans, followed by chemical hydrolysis to liberate Neu5Gc selectively. The Neu5Gc was chromatographically separated and analyzed by PGC-UHPLC/triple quadrupole (QqQ). MRM transitions and instrument parameters were optimized with Neu5Gc standard. The limits of detection (LOD, $S/N \geq 3$) for these compounds were at low-femtomole levels (20 fmol), and the limits of quantitation (LOQ, $S/N \geq 10$) were at high-femtomole levels (200 fmol). The NeuGc standard represents good linearity ($R^2 > 0.99$ for over 4 orders of magnitude). Using this linear regression equation, the total NeuGc in mouse plasma content was determined to be 10 ± 0.1 (Mean ± SE) pmol. This platform will be applied in clinical research and QA/QC in biotherapeutics.

Brief Oral 1-11

[P-090]

Global N-glycoproteome analysis in the course of human neural stem cell differentiation

Min-Young Song, Da Kyeong Park, Hyun Kyeong Lee, Gun Wook Park,
Ju Yeon Lee, Jin Young Kim, Jong Shin Yoo*, and Young Hye Kim*

Biomedical Omics Group, Korea Basic Science Institute, Cheongju-si, 28119, Republic of Korea

Neural stem cells self-renew and differentiate into neurons and glia cells. Human neural stem cells (hNSCs) have a great potential to repair neurological diseases but their therapeutic development is hampered by lack of well-defined markers to identify neural lineage cells and to estimate neural fate. During hNSC differentiation, cell surface glycoproteins play key roles not only in cell adhesion and migration but also in determining cell fates such as proliferation and differentiation. The present study thus aims at a comprehensive characterization of surface glycoproteins in the course of neuronal differentiation. We identified and quantified the N-glycopeptides derived from undifferentiated and 3-week differentiated hNSCs by combining membrane fractionation, hydrophilic interaction chromatography (HILIC), and nano LC-MS/MS, followed by bioinformatic analysis using the in-house software named GlycoProteome Analyzer (IQ-GPA). From the undifferentiated and differentiated hNSCs, a total of 120 N-glycopeptides containing 220 glycoforms on 97 glycoproteins were identified with FDR 1%. Among them, 110 glycoforms of 59 glycoproteins and 76 glycoforms of 38 glycoproteins are more abundant in undifferentiated and differentiated hNSCs, respectively. Many of these differentially expressed glycoproteins are known to be involved in neuronal cell adhesion, migration, differentiation, and regulation of transport. Our comprehensive glycoproteomic dataset presented here provides valuable information for understanding of neuronal differentiation process and development of potential neural cell lineage markers.

Brief Oral 1-12

[P-132]

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

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

Brief Oral 1-13

[P-023]

Quantitation of glycans in yeast using metabolic isotope labeling with isotopic glucose by mass spectrometry

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Glycosylation is one of the most common protein post-translational modifications (PTMs). Typically, glycans are attached to proteins at asparagine residues and serine/threonine residues so called N-glycans and O-glycans. These plays significant role in many biological functions such as cell differentiation, cell development, tumorigenesis and metastasis, and inflammation etc. Because changes in the expression levels of these glycans affect many physiological functions, it is important to analyze changes in glycans expression levels by quantitative analysis. Therefore, mass spectrometry-based quantitative analysis of glycans has been developed. Many quantitative analysis of glycan by mass spectrometry typically have been used by labeling methods such as reductive stable isotope labeling, IDAWG, and so on.

Herein, we applied metabolic isotope labeling strategy for glycan quantitation in yeast (*Saccharomyces cerevisiae*). We used the Metabolic Isotope Labeling of Polysaccharides with Isotopic Glucose (MILPIG) method to label the light (^{12}C) or heavy ($^{13}C_1$) glucose on glycans of yeast. We quantitatively analyzed isotopic labeled glycans in yeast by mass spectrometry.

Key words: Glycan, Yeast, MILPIG, Mass Spectrometry

Brief Oral 1-14

[P-042]

A sandwich-type HBsAg immunoassay using ICP-MS with metal-doped nanoparticles

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Hepatitis B virus (HBV) causes acute and chronic infection cirrhosis and liver cancer and Hepatitis B surface antigen (HBsAg) is its basic marker used to screen for the infection. In this work, sandwich-type immunoassay using ICP-MS is developed for the detection of HBsAg. For details, the sandwich-type conjugates employing metal-doped magnetic nanoparticles (MNPs) and metal/dye-doped silica nanoparticles (SNPs) were produced through the immunoreaction of selected proteins and the concentration of the target was determined through the ratiometric quantification of the doped metals using ICP-MS. For this, both Cs-doped Fe_3O_4 MNPs and Eu/RhBITC-doped SNPs for target extraction and tagging as a probe, respectively, were synthesized and immobilized with the antibodies of HBsAg. Feasibility of quantification was shown from the calibration curve plotted the intensity ratio of Eu/Cs vs. the concentration of target. For future work, this method will be applied to real samples and multiplex detection with other viruses by exchanging doped metal in the probe nanoparticles.

Brief Oral 1-15

[P-016]

Profiling of a wide range of neurochemicals in human urine by ultra performance liquid chromatography-tandem mass spectrometry combined with *in situ* selective derivatization

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Development of a reliable analytical method of neurochemicals in biological fluids is important to discover potential biomarkers for the diagnosis, treatment and prognosis of neurological disorders. However, neurochemical profiling of biological samples is challenging because of highly different polarities between basic precursors and acidic metabolites, low physiological levels, and high matrix interference in biological samples. In this study, an ultra-performance liquid chromatography-tandem mass spectrometry (UPLC-MS/MS) method combined with *in situ* selective derivatization for comprehensive profiling of 20 neurochemicals in urine was developed for a wide range of neurochemicals. *In situ* selective derivatization greatly improved the peak capacity on a reversed-phase C18 column and sensitive mass detection in LC-ESI-MS/MS-positive ion mode due to reduction of the distinct physicochemical properties between acidic and basic neurochemicals. The MS/MS spectra of neurochemicals exhibited specific ions, such as losses of amine, methanol, or methyl formate molecules from protonated molecules, enabling selection of appropriate multiple reaction monitoring (MRM) ions for selective and sensitive detection. The developed method was validated in terms of linearity, limit of detection (LOD) and limit of quantification (LOQ), precision, accuracy, and recovery. The correlation coefficients (R^2) of calibration curves were above 0.9961. The ranges of LODs and LOQs were 0.1–3.6 ng/mL and 0.3–12.0 ng/mL, respectively. The overall precision and accuracy were 0.52–16.74% and 82.26–118.17%, respectively. The method was successfully applied to simultaneously profile the metabolic pathways of tyrosine, tryptophan, and glutamate in Parkinson's disease patient urine (PD, n = 21) and control urine (n = 10). Significant differences ($P \leq 0.01$) between two groups in the activity of phenylethanolamine *N*-methyltransferase (PNMT) and alcohol dehydrogenase (ADH) were observed. In conclusion, this method provides reliable quantification of a wide range of neurochemicals in human urine and would be helpful for finding biomarkers related to specific neuronal diseases.

Keywords: neurochemicals, human urine, *in situ* selective derivatization, LC-MS/MS-MRM, profiling analysis, Parkinson's disease

Brief Oral 2-1

[P-140]

Identification of prostate cancer specific signature in cell lines based on proteomic analysis

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Various studies have been being performed to search for new diagnostic biomarker to be able to more accurately and specifically diagnose diseases. However, it is difficult to detect and distinguish between diseases, because most of the candidate markers and tumor-specific signature are not expressed in specific disease as well as are presented in other diseases.

Prostate gland has a unique characteristic and increase mitochondrial energy metabolism (i.e., the Krebs cycle and electron transport chain) when normal prostate cells turn into cancer cells. Thus, we attempted to find a prostate cancer-specific signature presenting in this unique environment.

We performed proteomics analysis to compare altered proteins of each cell lines: RWPE-1, LNCaP, Du145 and PC3. Liquid chromatography tandem mass spectrometry (LC-MS/MS) was used to identify proteins in each of cell lines. Notably, mitochondrial energy metabolism pathways related to the Krebs cycle and electron transport chain were highly prevalent among the proteins that were more than 1.2-fold up-regulated in the three prostate cancer cell lines, compared with normal cell line. We analyzed main transcription factor that regulates mitochondrial energy metabolism and selected YY1 among the top-ranked transcription factors. In addition, the expression of genes related to the Krebs cycle and electron transport chain was decreased in prostate cancer cell lines treated with NP-001 which is YY1 inhibitor, compared to the untreated controls. These results suggested that YY1 is a key and specific transcription factor regulating mitochondrial energy metabolism in prostate cancer cell lines.

Brief Oral 2-2

[P-030]

Development and validation of an analytical procedure for the total mercury in oyster and tuna using isotope-dilution inductively coupled plasma mass spectrometry

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Mercury is one of the highly toxic element and can accumulate in human body along the food chain in environment so that its accurate analysis in sea foods is important for food safety and environment monitoring. In this study, an analytical procedure for the total mercury in oyster and tuna has been developed based on the isotope-dilution inductively coupled plasma mass spectrometry (ICP-MS) using mercury-200 isotope as enriched spike to achieve the highest accuracy. Analytical issues in ICP-MS for mercury such as low recovery, severe memory effect, and high matrix effects have been also studied in detail. Pressurized microwave-assisted acid digestion with concentrated nitric acid was utilized for sample dissolution. Then, the mass fraction of total mercury was obtained from the isotope ratios of mercury-202 over mercury-200 which were measured by ICP-MS. Equilibrium between mercury isotopes naturally existed and spiked was fulfilled during sample preparation. Memory effects could be ignored by using 0.1 % 2-mercaptoethanol as washing solution. Signal reductions with less than 50 % were observed in ICP-MS measurements after sample preparation even though quantitative recovery. Matrix effects such as dependence of signal intensity on the nitric acid concentration were attributed to the signal reduction. The analytical procedure developed in this study can be applied to certification of total mercury contents in relevant CRMs.

Brief Oral 2-3

[P-143]

Effects of acetonitrile amounts on bovine serum albumin and myoglobin tryptic digestion in gentle mixing or microwave

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Protease can be used in protein digestion. Trypsin, one of the most common proteases, cleaves exclusively at C-terminus of amino acid Lysine and Arginine in protein. Moreover, organic solvents are often added for the trypsin digestion to modify native proteins to denatured proteins, and this tendency makes it effective to digest proteins. In this study, we investigate the digestion efficiency of trypsin for bovine serum albumin and myoglobin digestion with different amounts (0 %, 10 %, 20 %, 30 %, 40 %, and 50 %) of acetonitrile (ACN) in tryptic digestion. Digested peptides were analyzed using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) and the sequence coverage was calculated as an indication of trypsin activity. As a result, we concluded the best tryptic digestion results were obtained when the samples containing 10 % ACN were digested with gentle mixing (500 rpm) at 37 ^{o}C. In addition, we discovered microwave yields similar sequence coverage in 37 ^{o}C and 55 ^{o}C. More detailed experimental procedures and results will be provided during the session.

Brief Oral 2-4

[P-148]

Optimization of paper spray ionization for sensitive protein analysis

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Paper spray ionization (PSI) is an ambient extractive ionization method for mass spectrometry (MS). PSI utilizes a planar triangular-shaped paper as a sampling base as well as an electrospray tip. By using PSI MS, proteins can be ionized in a similar way to electrospray ionization and its ionization softness has been demonstrated by detecting noncovalent protein complexes. In this study, we optimized experimental parameters of PSI for sensitive analysis of proteins. Optimization was performed against various sizes of proteins including insulin, ubiquitin, cytochrome C, carbonic anhydrase, and bovine serum albumin. Experimental parameters such as spotting methods, types of solvent, water content in spraying solvents, and types of papers were subjected to optimization. Through this optimization processes, it was found that most parameters investigated in this study greatly affected protein signal intensities and their charge state distributions (CSDs). For example, water content was inversely related to protein signal intensity and a paper tip coated with amine derivatized microparticles generated higher CSDs than a conventional filter paper tip. In addition, it was also found that an optimal water content of a spraying solvent could be related to a size of a given protein.

Brief Oral 2-5

[P-176]

Development of a structural characterization method of lignin oligomers using pseudo-LC-MS3 analysis

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Lignin is the second most abundant biopolymer which is a component of the plant cell wall and also a precursor of lignans, phenolic plant metabolites. Structural characterization of lignin is crucial for understanding the biosynthetic perturbations of the plant cell wall and plant metabolism of phenolic derivatives. Lignin is synthesized by oxidative radical coupling among three kinds of monomers. However, analysis of the lignin structure is challenging because the coupling of the lignin monomers having delocalized radicals generates highly diverse types of chemical bonding.

Here, a new method has been developed for concrete structural characterization of lignin oligomers using liquid chromatography-quadrupole time-of-flight mass spectrometry (LC-QTOF-MS) analysis. This method provides multi-stage fragment ion information by two serial collisionally-induced dissociation events for characterization of the large lignin oligomers. First, a lignin mixture extracted from wood chip was analyzed by untargeted LC-MS2 coupled with a UV detector at 280 nm for the specific detection of the aromatic group. The peaks on the total ion chromatogram having UV absorption at 280 nm were considered to be lignin candidates, and their m/z values and retention times were recorded. A pseudo-LC-MS2 analysis was performed on the same sample with the same chromatographic conditions. The pseudo-MS2 fragment ions that had not been detected on the untargeted LC-MS2 were filtered out to remove fragment ions from co-eluting matrix components. Using the list of the filtered pseudo-MS2 fragment ions, a retention time-labeled pseudo-LC-MS3 target list was generated. Next, the scheduled, targeted pseudo-LC-MS3 analysis was performed. From the collected MS2 and MS3 fragment ion information, the structure of the lignin was determined by inspecting both unit- and bond-specific fragment ions.

Brief Oral 2-6

[P-152]

Glycomics-based Forensic Platform for the Identification of Human Saliva

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Saliva found at crime scenes is one of the important evidences and thus, the identification of human saliva from other human fluids and non-human fluids is an essential prerequisite prior to further crime investigation. In previous study, we determined that significant level of fucosylation and highly fucosylated N-glycan were specific features to identify human saliva from other body fluids. Herein, we developed glycomics-based forensic applicable platform for the identification of human saliva using dried saliva spot (DSS), because most saliva encountered at crime scenes is dryness and a trace amount. Briefly, DSS were prepared by spotting of human saliva on a protein saver card and then dried at ambient temperature. N-glycans were enzymatically released by PNGase F from DSS and enriched by PGC-SPE. Saliva N-glycans were characterized by MALDI-TOF/TOF MS. N-glycan profiles of DSS showed high correlation with N-glycans found in previous study by solution-based method. Indeed, highly fucosylated N-glycan and significant level of fucosylation as specific signatures of human saliva were equally observed from glycan profiles in DSS with similarity even in a trace amount. We also evaluated reproducibility of glycans profiles of DSS in terms of instrumental and experimental replications. This study can be useful to expand glycomic-based method for human saliva identification in practical application at crime scenes.

Brief Oral 2-7

[P-001]

MATLAB-based Software Development for Screening Illegal Drugs and Analogues Identification Using LC-MS/MS Data

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Illegal drugs and analogues, for example, erectile dysfunction drugs, analgesics, diuretics, weight loss compounds, and psychotropic drugs, are widely spread in the online markets, particularly advertised as health supplements. To eradicate these illegal drugs and analogues from the illegal market places, a variety of analytical screening tools are now being used, and LC-MS/MS-based method has been recognized as one of the most powerful screening tool. In screening these illegal drugs, identifications of them are generally based on the database search in which the exact masses of the precursor molecules and their fragments are documented. However, for illegal compounds that are not listed in the database, it is not possible to identify them. To address this issue, we are now developing a new approach in which in-silico chemical compounds are catalogued in the expanded database. This new software are now still in the development stage and the main part of this on-going project will be discussed in detail in the conference.

Brief Oral 2-8

[P-154]

Competitive Homo- and Hetero- Self-assembly of Amyloid-β 1-42 and 1-40 in the Early Stage of Fibrillation

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Amyloid-*β* 1-42 (A*β*42) and 1-40 (A*β*40) peptides, whose self-assembly process has been linked with the formation of amyloid plaques in Alzheimer's disease, exist as a mixture in human fluids. For this reason, heteromeric self-assembly of A*β*42 and A*β*40 has been widely investigated to understand the influence of this mixture in A*β* fibrillation. However, understanding the role of heteromeric self-assembly in A*β* fibrillation is still unclear due to the heterogeneous cross-interactions between A*β*42 and A*β*40. In this research, we demonstrated the influence of the cross-interaction of A*β*42 and A*β*40 in the early stage of fibrillation. We monitored the fibrillation process of A*β*42, A*β*40 and their 1:1 mixtures using thioflavin T (ThT) assay and electrospray ionization mass spectrometry (ESI-MS). Then, we further investigated the preference for homo- and hetero- oligomerization of A*β*40 and A*β*42 using ion mobility spectrometry (IMS) along with solution small-angle X-ray scattering (SAXS) and molecular dynamics (MD) simulations. A*β*42 and A*β*40 have no significant preference for homo- versus hetero-oligomerization when forming small oligomers. However, because of the different conformations induced by A*β*42 and A*β*40, the cross-interaction is gradually attenuated as oligomerization proceeds. Thus, our results suggest that the competitive self-assembly of A*β*42 and A*β*40 plays a crucial role in disturbing homo-oligomerization of A*β*42 in the early stage of fibrillation.

Brief Oral 2-9

[P-075]

Rapid and sensitive carbapenemase assay using LDI-MS based on a parylene-matrix chip

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Carbapenem is the strongest β-lactam antibiotics and acts as inhibitors of the enzymes that catalyze formation of peptidoglycan in the cell wall of bacteria. Recently, the emergence of carbapenem-resistant bacteria seriously threatens this class of lifesaving drugs. Therefore, rapid detection of carbapenemase-producing enterobacteriaceae (CPE) is very important to prevent spread of these strains. Carbapenemase is an important enzyme that are produced by CPE and catalyze the hydrolysis of carbapenem. Typically, MALDI-TOF MS is not appropriate for small molecule analysis because organic matrices make a lot of noise at low m/z range. Parylene-matrix chip was developed for reduce matrix noise, and used to analyze small molecules. Recently, the Parylene-matrix chip has been used for analysis of penicillin-resistant bacteria. The applicability of the Parylene-matrix chip was demonstrated in a quantitative β-lactamase assay that required the quantification of penicillin (*m/z*: $[PEN+H]^+$ = 335.1 and $[PEN+Na]^+$ = 357.8), as well as its hydrolyzed product, penicilloic acid (*m/z* : $[PA+H]^+$ = 353.1). In this study, the Parylene-matrix chip was used in the carbapenemase assay. The assay measured the hydrolysis of 4 carbapenems such as doripenem, ertapenem, imipenem, and meropenem into their hydrolyzed form. Finally, MALDI-TOF MS based carbapenem susceptibility test was carried out with different 60 isolates using Parylene-matrix chip.

Brief Oral 2-10

[P-017]

Development of an on-line proteolysis and glycopeptide enrichment method using enzyme immobilized thermo-sensitive porous polymer membrane enzyme reactor (μPPMER) and nanoflow liquid chromatography-tandem mass spectrometry

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Protein N-glycosylation is one of post-translational momdifications (PTMs) in which glycans are attached covalently to nitrogen atom in asparagine (asn, N). Since glycosylation of proteins plays essential roles in protein folding and various functions of proteins, it is important to analyze glycoproteins in biological samples. For the selective isolation/purification of glycoproteins, lectin immobilized methods have been commonly utilized. In this study, dual micro-scale thermo-sensitive porous polymer membrane enzyme reactors (μPPMER) have been utilized for on-line proteolysis followed by enrichment of glycopeptides prior to nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS/MS).

A thermo-sensitive porous polymer membrane, Ps-co-MAn-NIPAM, was synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization and it was coated on nylon membrane by breath figure method. Trypsin and concanavalin A (ConA) was immobilized on the coated membrane for proteolysis and glycopeptide capture, respectively, and each of membrane was inserted in PPMER module. Dual PPMER modules were connected to nLC-ESI-MS/MS system and proteolysis efficiency with glycopeptides enrichment selectivity by temperature were evaluated. In addition, human plasma and urine samples were analyzed in the most optimized glycopeptide enrichment condition and glycoproteins were identified for performance evaluation of on-line dual PPMER module.

Brief Oral 2-11

[P-165]

Development of relative quantification method for lipidome by using $^{2}H_2O$ partial metabolic labeling

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Liquid chromatography-mass spectrometry (LC-MS) combined with stable isotope labeling is a powerful technique for identification and quantification of lipids. However, relative quantification of lipids is not well established and only a few isotope-labeled derivatization methods have been applied limitedly to lipids containing a reactive functional group like an amine or phosphate group. Metabolic isotope labeling of lipid has also rarely been attempted since no common metabolic pathway covering all categories of lipid exists. In order to overcome this limitation, we employed $^{2}H_2O$ in developing a novel method for relative quantification of lipidome based on partial isotope labeling. The method relies on subtle changes in the isotopic envelope shape derived from deuterium incorporation into lipid to figure out the relative abundance of unlabeled and labeled lipids in a mixture. A total of 216 lipids from HeLa cells were identified by using LipidBlast database in positive and negative ion modes. Relative quantification of 190 lipids that do not contain an amine or phosphate group including monoacylglycerol, diacylglycerol, triacylglycerol, monogalactosyldiacylglycerol, and digalactosyldiacylglycerol could be achieved. Efficiency of the relative quantification method was evaluated by varying the mixing ratio of unlabeled and labeled lipids. Out of the 190 lipids, 96 lipids (51%) could be classified as confident relative quantification on the basis of their peak intensities and the degrees of deuterium incorporation. Our approach expands the scope of relative quantification of lipid and is also expected to be applicable to higher organisms for which little metabolic isotope labeling method is available.

Brief Oral 2-12

[P-087]

Simultaneous quantification of the four coumarins including one active metabolite in humans by UHPLC-MS/MS: Application to pharmacokinetics

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Coumarins in Cham-dang-gwi, responsible for pharmacological effects in arthritis, cold, headache and premenstrual syndrom, are composed of decursin, decursin angelate and nodakenin. The aims of this study are to develop simultaneous determination of the four coumarins including decursinol as an active metabolite in human plasma using UHPLC-MS/MS and to characterize the pharmacokinetic profile of the components after oral administration of *Angelica gigas* root extract powder (1.12 mg as decursin, 4.37 mg as decursin angelate and 21.79 mg as nodakenin) to human. Chromatography separation was performed on dual columns of Kinetex® C18 column and Capcell core C18 column with mobile phase consisting of water and methanol at flow rate of 0.3 mL/min using gradient elution. Liquid-liquid extraction using methanol was employed for sample preparation. MRM operated in the negative ion mode was adopted in MS detection, and the precursors to the product ion transition values of m/z 329.14→228.9, 329.9→228.8, 409.43→246.7 and 246.8→212.9 were used to measure decursin, decursin angelate, nodakenin and decursinol.

The linear calibration curves were fitted over the the range of 0.05-50 ng/mL for four components, with the correlation coefficient greater than 0.998. The inter- and intra-day accuracy was between 90.6-108.24%, and the precisions were within 11.2% for all components. The method was applied to the pharmacokinetic study of four components after ususal dosing to Korean subjects.

Brief Oral 2-13

[P-040]

Evaluation of a set of calibrants for more accurate measurement of collision cross section (ccs) of polycyclic aromatic hydrocarbon compounds

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Ion mobility spectrometry (IMS) can provide collision cross section (CCS) values that can be used to elucidate chemical structures. For the structural elucidation, accurate measurement of CCS values is crucial. To obtain CCS values, the obtained IMS spectra must be calibrated by using adequate calibrants. Polyalanine has been widely used as a calibrant for CCS. Polyalanine has been used to obtain the CCS values of PAH molecules. However, polyalanine may not be an ideal calibrants for PAH molecules because of the following reasons. First, polyalanine is ionized by electrospray ionization but PAH are typically analyzed by atmospheric pressure photo ionization. The ionization source must be switched between analysis and calibration. Second, the structure of polyalanine can be different from that of PAHs. Therefore, it is reasonable to expect that using a set of PAH calibrants and use it for the analysis PAH would provide more accurate data. In this study, CCS values of PAH compounds were newly measured and the values were combined with the previously reported CCS values (http://depts.washington.edu/bushlab/ccsdatabase). Based on the CCS values, a new set of PAH calibrants were suggested. The set of calibrants were used for external and internal calibration of standard compounds and crude oils. The obtained results were compared with the one calibrated with polyalanine. More accurate CCS values were obtained with the new set of calibrant.

Brief Oral 2-14

[P-122]

Characterization of weathered oil by paper spray ionization and estimation of the oxidation degree of spilled oils depending on the chemical class distribution

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Mass spectrometry has been wildly used as a powerful technique to analyze complex mixtures, providing information on the chemical composition and structures through the molecular weight. For the successful mass spectrometric analysis, it is necessary to select the proper ionization technique depending on the sample properties and instrument performance such as resolving power, accuracy and sensitivity. For environmental or biological samples, the amount of sample consumed also has to be considered as important as those factors. In this study, paper spray ionization mass spectrometry (PSI-MS) was applied to characterize the photo-oxidized and spilled oils. PSI is fast and convenient ionization method for the direct analysis of complex mixtures. It is shown that PSI is a sensitive ionization technique that can be operated up to 20 minutes with 50 μg of oil sample. It can detect down to femtograms of analytes. And the linearity was tested in a range of 2 picogram ~ 2 nanogram using a standard material.

Brief Oral 2-15

[P-158]

Estimation of Elemental Compositions for Additives in Polymers Using Newly Developed EI/CI Ion Source without Venting MS

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GC-MS offers a wealth of fragmentation data and a thorough, highly useful mass spectral library; therefore, it is used for identifying unknown compounds. In cased where a compound detected is not registered in the mass spectral library, the positive chemical ionization (CI) method is required to acquire the molecular weight from protonated ion. However, this requires venting the MS and an exchange of ion sources when switching ionization methods.To solve the problem, we developed the new EI/CI common use ion source called SMART EI/CI ion sourcewhich can switch the EI and CI methods without downtime. In this study, we estimate elemental composition of additives in polymers using SMART EI/CI ion source with MassWorks™ software.

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PLENARY LECTURE

Plenary Lecture

Native MS: Development of SID/IMMS and SID/HRMS

Vicki Hopper Wysocki

Ohio State University

Characterization of the overall topology and inter-subunit contacts of protein complexes, and their assembly/disassembly and unfolding pathways, is critical because protein complexes regulate key biological processes, including processes important in understanding and controlling disease. Conventional structural biology methods such as X-ray crystallography and nuclear magnetic resonance provide high-resolution information on the structures of protein complexes. However, other emerging biophysical methods that provide lower resolution structural data (e.g. stoichiometry and subunit connectivity) on the structures of the protein complexes are also important. Native mass spectrometry is an approach that provides critical structural information with higher throughput on low sample amounts. The power of native MS increases when coupled to ion mobility (IM-MS), a technique that measures rotationally averaged collisional cross sections and thus direct information on conformational changes, or to high resolution mass spectrometry (HRMS). We have implemented SID in Q-IM-TOF, Orbitrap, and FTICR instruments. This presentation illustrates surface-induced dissociation/ion mobility (SID/IM MS) and SID HRMS in Orbitrap and ICR for characterization of topology, intersubunit connectivity, and other structural features of multimeric protein complexes. Data for a number of protein-partner complexes are under investigation, where the partner can be small molecule ligand, protein, DNA, or RNA.

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SPECIAL LECTURE

Special Lecture

Instrumentation for Mass Spectrometry

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As a member of KSMS, my research interests have been focused largely on the development of mass spectrometers. Initially my instrumentation activities were heading to the performance improvements of an extremely high field Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) and several new technologies to enhance the resolution and sensitivity were developed and patented. But, those new technologies cannot be adopted in domestic manufacturing companies in Korea. In addition, it is not easy to keep improving those advanced technologies in our research environments without industrial demands and feedbacks. Facing those difficulties, my research direction was changed to support and encourage the domestic manufacturing companies of mass spectrometers. In that way, research institutes can support industrial partners and also find the consumer's demands from those partners for good circulation relationship of mutual cooperation between research and industrial sectors. Current trends of instrumentations for mass spectrometry are composed of achieving high performance and miniaturization. The instrumentation research activities in our laboratory will be described based on those demands and our readiness. To establish the healthy domestic industrial environments, a variety of technical supporting activities such as operation of open laboratory and display room, performance evaluations and improvement project for newly developed domestic equipment will be introduced to assist the domestic manufacturers of mass spectrometers.

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SYMPOSIUM

Symposium-1-A

<KEYNOTE SPEAKER>

Biophysical characterizations of antibody drugs by mass spectrometry

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Stoichiometry and dissociation constant (K_D) are biophysical parameters that represent d*G*, thus clarifying these parameters are essential for understanding biological phenomena and also prediction of drug efficacy. We have been engaged in developments of biophysical methods for accurate determination of K_D and stoichiometry for protein-protein interactions in solution. Analytical ultracentrifugation combined with native mass spectrometry is a powerful approach to identify distribution states of a protein-protein interaction even when more than 5-6 different stoichiometric complex exists in solution. Study on antibody and antigen interactions including anti-TNF monoclonal antibodies-TNF interactions will be introduced.

One of the main issues of therapeutic proteins is degradation during transportation and storage. We have studied chemical and physical stabilities of antibody drugs, including development of analytical methods, stability prediction, and formulation optimization. Chemical modifications including deamidation, racemization, and oxidation are assessed by mass spectrometry. Oxidations of amino acid residues can be effectively reduced via optimized formulation with proper container and closure system. Aggregation of antibody is major concern of physical stability, while regions responsible for aggregation can be identified hydrogen deuterium exchange mass spectrometry. Recent research on the stability of therapeutic proteins with future perspectives will be described. [References] Krayukhina, et al., *mAbs* **2017,** *9*, 664-679.; Kabe, Y., et al., *Nature Comm.* **2016**, *7*, 11030.; Amano, M., et al., *J. Pharm. Sci.* **2016**, *105*, 623-629.; Ohto, U., et al., *Nature* **2015**, *520*, 702-705.; Uchiyama, S. *Biochim Biophys Acta.* **2014**, *1844*, 2041-2052.; Amano, M., et al., *Anal. Chem.* **2014**, *86*, 7536-7543. Amano, M., et al., *Anal. Chem.* **2011**, *83*, 3857-3864. Oda M., et al., *FEBS. J.* **2006**, *273*, 1476-1487.

Symposium-1-B

Glycan Markers for Ovarian Cancer with High Sensitivity and High Specificity

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Glycosylation is the most common post-translational modification of protein, highly sensitive to the biochemical environment, and has been implicated in many diseases including cancers. Because the biosynthesis of oligosaccharides depends on several highly competitive processes, variations in the concentration of specific glycosyl transferases could produce completely different products. For this reason, monitoring changes in glycosylation and global glycan profiling of human serum has already led to several potential markers. In this study, we have applied high-throughput, automated sample preparation system to Korean ovarian cancer serum for the discovery of glycan marker. N-linked glycans are observed and several are identified as potential markers for ovarian cancer.

Ovarian cancer patient (n=144) containing all stages (I-IV) and healthy control (n=202) serum samples were treated using streamlined automation system. In parallel, commercial sera (n=134) were processed to determine technical and analytical reproducibility. Serum (25 □ L) was treated with PNGase F at 37oC for 10min to release N-linked oligosaccharides using microwave reactor. Released glycans were purified and fractionated using automated solid phase extraction (SPE) and solvents of varying polarity to partition them into highly anionic and neutral components. Minimum sample handling and automation not only increases the speed but also overcomes many of problems caused by human bias and variations in techniques. The samples were fractionated into three and each was analyzed by mass spectrometry. The fractions are then analyzed directly by nano LC-chip Q-TOF MS. Masses of N-linked glycans were profiled and compared for marker discovery.

Markers were determined using the intensity and the frequency of the compositions. Total 27 glycan compositions were identified for potential N-glycan biomarkers. The frequency or intensity of a number of markers was increased (positive marker) or decreased (negative marker) as clinical stage changes. Each positive and negative markers are related on biological synthesis pathway. The results illustrate the use of glycan biomarkers to detect ovarian cancer with sensitivity and specificity.

Symposium-1-C

Dissection of Adaptive Drug Resistance Mechanism Harnessing Mass Spectrometry-based Proteomics

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While molecular targeted therapies have shown promises in cancer patient care, therapy resistance and tumor recurrence still remain major hurdle. One way cancer cells can escape from targeted agents is through their ability to evade drug effects by rapidly rewiring signaling networks. Harnessing mass spectrometry, we conducted a system-level profiling of drug-induced alterations in ATP-binding proteomes and phosphoproteome to discover novel mechanisms involving adaptive responses and drug resistance. First, we profiled global phosphotyrosine proteome alterations induced by DDR2 inhibitor dasatinib in DDR2-mutant lung cancer cells. We found dasatinib enhances tyrosine phosphorylation in a panel of receptor tyrosine kinases, including EGFR, MET and IGF1R and pharmacological inhibition of those RTK enhances dasatinib efficacy. Second we mapped global ATP-binding proteomes perturbed by two clinical MEK inhibitors, AZD6244 and MEK162, in a panel of KRAS mutant lung cancer cells. The activity-based protein profiling revealed diverse kinome responses, indicating each cell adapts to MEK inhibition in unique ways. Despite the heterogeneity of kinome responses, decreased probe labeling of mitotic kinases and increase of kinases linked to autophagy were identified to be common responses. Collectively, these studies demonstrate the utility of phosphoproteomics and activity-based protein profiling to identify novel adaptive resistance mechanisms, further to develop rational drug combinations

Symposium-1-D

Glycomic Profiling of Targeted Serum Haptoglobin for Gastric Cancer Using Nano LC/MS and LC/MS/MS

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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 associated with many human diseases including inflammation and various types of cancer. Serum-based global glycan profiling using mass spectrometry has been explored and has already led to several potential glycan markers for several disease states. However, localization of the 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. Age-and sex-matched 60 serum samples (30 cancer patients and 30 healthy controls) were used to profile and quantify haptoglobin N-glycans. A T-test based statistical analysis was performed to identify potential glyco-markers for gastric cancer. Interestingly, abundances of several tri-and tetra-antennary fucosylated N-glycans were increased in gastric cancer patients. Additionally, structural analysis via LC/MS/MS indicated that the fucosylated complex type N-glycans were primarily decorated with antenna fucose, which can be categorized as sialyl-Le a or sialyl-Le x type structures. This platform demonstrates quantitative, structure-specific profiling of haptoglobin glycosylation for the purposes of biomarker discovery for gastric cancer.

Symposium-1-E

Clinical Application of LC/MS/MS for Drug Counseling in Pregnant Women

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In the absence of proper counseling and appropriate labeling, many pregnant wemen miss out on vital information about their medication; including the dosage regimen and possible side effects. This lack of information could be especially harmful to expecting mothers. Effective interventions are required to increase the knowledge of pregnant women regarding the safe use of medications during pregnancy. Accurate pharmacokinetic evaluation of the drug in the body should be performed to ensure proper drug counseling and intervention. For this reason, we are conducting the practical application of LC / MS / MS through the case study of "A selective and sensitive detection of multiple retinoids and acitretin in human serum with LC-MS/MS" which is currently being studied for effective counseling of Isotretinoin drugs.

Isotretinoin (Accutane), is a prescription medication used to treat juvenile and adult acne, often used by women during childhood. Careful management is needed when women of childbearing age use this or similar drugs. Since ingesting these types medications during pregnancy due to misinformation can lead to misperception. Unnecessary drug exposure during pregnancy may result in adverse effects, hospitalization and even serious congenital disabilities including deformities of the heart, face, and brain.

Proper counseling, in turn, could be beneficial to prevent any medication related adversity during pregnancy such as miscarriages, minimize the spread of misleading information of harmful substances from one pregnant woman to another and provide a healthy birth experience.

Recently, there have been more cases of counseling for Isotretinoin in MotherSafe to create a safe childbirth environment for expecting mothers by providing information on hazardous substances in materials. MotherSafe, a maternity drug counseling center, has been operating or of hospitals with multiple locations in, Ulsan, Seoul, Busan, Gwangju, Daejeon, Daegu South Korea with the support from the Department of Health and Human Services since 2010. The next step in providing effective counseling of Isotretinoin drugs is to incorporate the clinical application of Liquid chromatography-tandem mass spectrometry (LC-MS/MS) to accurately measure the concentration of medication in the body and provide appropriate counseling based on the findings.

Symposium-2-A

Inorganic element analysis in various fields using fsLA and ICP-MS

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Typical methods for analyzing heavy metals include destructive analysis using AAS, ICP-OES and ICP-MS equipment, and non-destructive analysis methods such as XRF and XPS equipment, etc. which are directly analyzed using X-ray. Destructive analysis has the advantage of accurate qualitative and quantitative analysis, but it requires a long pretreatment process such as acid decomposition. In the case of the non-destructive analysis method, it is possible to perform the analysis directly without a long pre-treatment process. However, since there are not many kinds of accurate reference materials having similar matrix, it is difficult to analyze accurately and there is a limit to analyze trace elements.

Recently, studies using fsLA-ICP-MS (femtosecond Laser Ablation-Inductively Coupled Plasma-Mass Spectrometer) which has high detection sensitivity and resolution by coupling ICP-MS with a femtosecond laser that produces particles uniformly with resolution in μm.

Using fsLA-ICP-MS, In the field of food, we analyzed the grains and rice which are attracted to excellent nutrition, In the BIO field, the tissues of mice treated with anticancer drugs, In the field of materials, biodiesel tracking and soil were analyzed in fiber and environment.

As a result, various analytical results were obtained in various fields.

Symposium-2-B

Determination of naturally occurring radioactive materials by $LiBO_2$ fusion and ICP-MS

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The concern regarding the radioactivity of naturally occurring radioactive materials has been growing over the last decade. In particular, radiation exposure in the industry when handling raw materials (e.g., coal mining and combustion, oil and gas production, metal mining and smelting, mineral sands (REE, Ti, Zr), fertilizer (phosphate), and building materials) has been brought to the public's attention. As new legislation has come into force implementing radiation safety management for the use of naturally occurring radioactive materials (NORM), it is necessary to establish a rapid and accurate measurement technique. Measurement of ^{238}U and ^{232}Th using conventional methods encounter the most significant difficulties for pretreatment (e.g., purification, speciation, and dilution/enrichment) or require time-consuming processes. To decide the proper handling options, a rapid and accurate analytical method that can be used to evaluate the radioactivity of radionuclides (e.g., ^{238}U, ^{232}Th, and ^{40}K) should be developed and validated. A measurement technique using ICP-MS allows radioactivity in many samples to be measured within a short time period with a high degree of accuracy and precision. However, since the pretreatment process consequently plays an important role in the measurement uncertainty, the development and validation of the method should be performed.

In this study, a series of experiments were conducted for vadidation of measurement techniques for NORM (e.g., ^{238}U and ^{232}Th) using ICP-MS for raw materials and by-products. A sample digestion process for ICP-MS was used for $LiBO_2$ fusion and $Fe(OH)_3$ co-precipitation. For an evaluation of the accuracy and precision of each method, various certified reference materials (CRMs) were analyzed using an established process.

Symposium-2-C

Analysis of Various Samples Using TOF-SIMS at KBSI Busan Center

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At KBSI Busan Center, TOF-SIMS has been established since 2014, and various research samples are being analyzed and supported by many researchers. The model is a product of ION-TOF GmbH with TOF.SIMS 5. Vacuum system maintains ultra high vacuum up to 5.0 x 10^{-10} torr. Analysis ion beam can measure imaging mode as well as spectrometry using Bi cluster liquid metal ion gun. We use Cs ion source for easy anion analysis and O_2 ion source for cation analysis for depth analysis. In particular, Ar clusters are used for surface analysis and depth analysis of organic materials including polymers.

Surface spectrocopy mode provides elemental and molecular information, with ppm sensitivity and mass resolution of over 10,000. In surface imaging mode, parallel mass detection is possible from ^{1}H to polymer with lateral resolution of less than 100 nm. Also, it is possible to analyze the depth profiling mode to obtain the depth direction information of the sample. It is characterized by depth resolution of less than 1 nm, information of thin layers of 1 nm to > 10 nm, and analysis of insulator samples using charge compensation method. The data thus obtained can also be used for 3D image analysis.

I would like to introduce the analysis results of various samples analyzed at Busan Center. Of course, I will announce except for the samples of customers who want to treat the company as confidential. In the future, I hope that many researchers will use TOF-SIMS to obtain good analytical results on surface analysis, image mapping and depth distribution of various samples.

Symposium-2-D

Development of food matrix CRMs for elemental analysis

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Elemental analysis in food and its related product is an important part of quality assurance, regulatory compliance and product development. Ingestion of Toxic elements and essential elements from food related to nutrition, disease. They are need to determination of toxic, trance and essential elements in food to verified to help determine heath effect of food.

In this presentation, we report developments of several food matrix CRMs for elemental analysis to help to testing and method validation for elements in food analysis. We certify toxic elements for comtaminant regulation as well as essential elements for nutrition from food matrix. We introduce international proficiency test programme (APLAC-APMP Joint PT programme) which is jointly coordinated by KRISS and KOLAS. KRISS provide CRMs for test materials before CRM release and certified values for KCRV values.

Symposium-2-E

Sources Identification of Pb in Marine Environments around the Korean Peninsula

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Environmental Pb levels have decreased significantly after the phase-out of leaded gasoline, but Pb remains an important contaminant in various marine environments and is affected by other Pb sources such as coal burning, wastes, batteries, paints and chemicals, nonferrous metal refineries, and miscellaneous industrial effluents. Especially, since the seas around the Korean peninsula are located downwind direction from Chinese mainland, it is one of quite important subjects in the environmental management plans to discriminate and proportionate the Pb sources. Pb ores have different isotope ratios from the surrounding rocks and other ores because Pb isotope ratios in the crust have evolved over time depending on the half-life of their parent isotopes, and no uranium (U) or thorium (Th) is found in Pb ores (e.g., galena) formed in the past. Therefore, Pb isotopes are used to identify the sources of natural or anthropogenic Pb in marine materials, including seawater, sediments, marine aerosols, settling particles, mussel tissues, and shells.

This study presents the results of case studies about the source identification of natural and anthropogenic Pb in sediments of several marine environments around the Korean peninsula including bays (Chunsu & Garorim, Ulsan), the western coast, the Yellow Sea shelf, and the Ulleung Basin. The key results in each case study are as follows; 1) Geum river derived and Han river derived particulate Pb were transported into the Chunsu and Garorim bays, respectively, but in the innermost tidal flat of the Garorim bay, Pb from Seosung mine was found, 2) imported ores from Australia, Peru and USA were identified as major Pb sources from non-ferrous metal refineries and ship-building facilities, respectively, in Ulsan bay, 3) Pb in coastal sediments near the river mouths around the Yellow Sea represents the ore origin in nearby river drainage basin and can be discriminated among rivers, 4) atmospheric Pb from Chinese coal burning and leaded gasoline has been preserved in Ulleung basin sediments.

Symposium-2-F

Applications of mass spectrometry on polar snow and ice core samples

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Snow and ice core samples recovered from polar region have provided valuable information on past climate and environmental changes. That information has been mainly come from various proxy records measured by mass spectrometries.

Primarily, past changes in atmospheric temperature are reconstructed from hydrogen and oxygen isotope ratios in polar snow and ice core samples analyzed by isotope ratio mass spectrometry (IR-MS). When water evaporates, light isotopes of oxygen and hydrogen are enriched in water vapor, while heavy isotopes preferentially fall during precipitation. For the glacial period, low air temperature caused large precipitation before it reached a polar region, and thus water stable isotopes of polar snow became light. On the other hand, during the inter-glacial period, more water vapor can reach a polar region with heavier water stable isotopes. Using this, in the late 1960s, the first record of glacial-interglacial changes were reconstructed from Greenland deep ice core. Since then, a number of ice core records have been reported in both polar regions and they have revealed the global climate changes for the past 800,000 years.

Secondly, trace metals records of ice cores determined by inductively coupled plasma mass spectrometry (ICP-MS) have shown changes in atmospheric input of those elements corresponding to various environmental changes. The ice core records of representative crustal elements such as aluminum (Al), barium (Ba), iron (Fe) and scandium (Sc) have represented the changes in natural dust input depending on climate change. Bismuth (Bi) peaks are strong evidence for large volcanic eruptions. Heavy metals such as cadmium (Cd), copper (Cu), lead (Pb) and zinc (Zn) have shown that the anthropogenic air pollution occurred in hemispheric scale even during ancient Greek and Roman period. However, most of those elements exist in extremely low concentrations of pg g^{-1} level. Therefore measurements of trace metals in polar snow and ice are still hard challenges. In order to avoid contamination of samples, ice cores are carefully decontaminated by mechanical chiseling, all sample vessels are cleansed with nitric acid for more than several months before using them and whole analytical processes are performed in a clean laboratory by trained researchers wearing clean garment.

Pb and strontium (Sr) isotope ratios have been analyzed from ice cores using thermal ionization mass spectrometry (TIMS). Those non-traditional isotopic data, together with rare earth elements, are very useful tools for source identification of air mass. Recently, it is known that climate changes are closely related to changes in air circulation, but detailed mechanisms are not fully understood. In this regard, ice cores can provide records of past climate changes and source region transitions simultaneously. Unfortunately, trace metals isotope ratios in ice core samples have not been widely reported because very few laboratories can properly treat analytical samples. In addition, TIMS measurement is time consuming. Therefore, at present, new analytical method for isotopic ice core data using multi-collector inductively coupled plasma mass spectrometry (MC-ICP-MS) is being developed. MC-ICP-MS can be applied for more various elements which are known to be fractionated by various natural and anthropogenic processes. Therefore, if MC-ICP-MS is successfully applied to ice core measurement, it is expected to reconstruct not only sources transitions but also changes in other geochemical processes corresponding to climate changes.

Symposium-3-A

<KEYNOTE SPEAKER>

Accelerating MultiModal Molecular Imaging: Innovations in structural elucidation.

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State-of-the-Art molecular imaging with MS now enable high resolution tissue screening that provides direct insight into tissue metabolism. Applications have penetrated various research domains from drug metabolism to the visualization of molecular signaling pathways in cancer. In this lecture we will demonstrate how mass spectrometry based multimodal molecular imaging can be used to reveal the cellular phenotypes. We will discuss the development and application of new MS based chemical microscopes that target biomedical tissue analysis in various diseases as well as other chemically complex surfaces. There is a clear need to add analytical structural separation utilizing ion mobility of gas phase ion chemistry. We will demonstrate how to elucidate the way in which local environments can influence molecular signaling pathways on various scales. The integration of this pathway information in a surgical setting is imminent, but innovations that push the boundaries of the technology and its application are still needed. The imaging MS community is driving translational molecular imaging research and these needed developments rapidly forward.

More and more researchers realize that a single technology provides only a subset of the molecular information needed to obtain an in depth understanding of a clinical problem. Multimodal approaches enable the study of clinical samples at a variety of molecular and spatial scales. The molecular complexity on the genome, proteome and metabolome level all needs to be taken into account. The distribution of several hundreds of molecules on the surface of complex (biological) surfaces can be determined directly in complementary imaging MS experiment with different desorption and ionization strategies. High throughput, high resolution MALDI techniques offer three dimensional molecular data on the tissue level. Ambient desorption and ionization techniques complement MALDI in their capabilities to reveal different molecular signatures that can be employed for direct tissue typing in molecular pathology. State-of-the-art molecular imaging mass spectrometry has evolved to bridge the gap between different disciplines such as MRI, PET, fluorescence imaging and histology. The combination with tools from structural biology makes it possible to perform imaging experiments at length scales from cells to patients

Symposium-3-B

Paper Spray Ionization and Paper Spray Chemical Ionization –Sensitive Ionization Methods for the Analysis of Spilled Oils

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It is well known that sensitivity of mass spectrometry (MS) analysis is critically dependent on the choice of ionization method and the choice should be made depending on the sample properties. Electrospray ionization (ESI), atmospheric pressure photoionization (APPI), and atmospheric pressure chemical ionization (APCI) are commonly used atmospheric pressure ionization (API) techniques. ESI is commonly used for molecules with high polarity and APPI and APCI are used to analyze low/non-polar compounds. For the samples requiring high sensitivity, nano-electrospray ionization (nano-ESI) has been successfully used. However, nano-ESI is prone to clogging because very narrow spray tip has to be used. In addition, there is no available technique that has high sensitivity like nano-ESI and can ionize low/non-polar compounds. Thus, we propose that paper spray chemical ionization (PSCI) can be used to analyze low/non-polar aromatic molecules with sensitivity comparable to that of nano-ESI. PSCI is developed based on paper spray ionization (PSI). The key differences between the experimental conditions for PSI and PSCI are in the choice of solvent and applied voltage. Further details are explained in the following sections. Non-polar solvent such as dichloromethane and high voltage (6~7 kV) are used for PSCI.

We think that PSI and PSCI are complementary technique that can be applied for environmental sample. For an example, it can be successfully applied to study humic or spilled oil samples. In this presentation, development of PSCI, advantage of PSI and PSCI over conventional ionization technique and the application of PSI and PSCI for environmental will be presented.

Symposium-3-C

Elemental imaging and quantification of thermally conducting polymer containing fiber-type SiO_2 fillers using LIBS and laser ablation ICP-MS

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In this work, analytical methods for the determination of Zn in polycarbonate (PC) conducting polymers containing fiber-type SiO_2 fillers were studied. Since Zn compounds combined with SiO_2 fibers represent important fillers substituting for hazardous organic retardants containing halogen compounds in various electrical products, a rapid, reliable analytical method is urgently required for practical application. Particulary, the feasibility of laser-ablation (LA)-ICP-MS and laser induced-breakdown spectroscopy (LIBS) was studied to be used for quality control in the manufacturing process, for which reference materials are required. To accomplish this, a new sample treatment process was developed based on dry ashing for decomposition followed by acid dissolution and Si removal. The concentration of Zn in the dissolved solution was determined by standard addition spiked with In as an internal standard using inductively coupled plasma–mass spectrometry (ICP-MS). Although the mapping images showed inhomogeneity, the intensities of both ablation techniques showed reasonable correlations with the concentrations of Zn obtained using the developed analytical method, which indicates that both have excellent potential for screening and quantification of the conducting polymers, even if fiber-type SiO_2 filler is present.

Symposium-3-D

ToF-SIMS Study of Tissue Samples

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Matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) has been used for molecular identification of proteins in the discovery of disease-related biomarkers as a key platform technique in proteomics. ToF-SIMS on the other hand has been used to analyze small biomolecules such as amino acids, peptides, vitamins and drugs because the collisional cascade process cannot produce secondary ions with a molecular weight of over m/z 2,000 without the use of noble metals or MALDI matrixes.

Here, we will show our recent ToF-SIMS data of tissue samples obtained by using various primary ion beams and sampling methods, and discuss the potential capability of ToF-SIMS to study for –omics, particularly lipidomics for tissue study.[1-5]

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Symposium-3-E

Development of MALDI IMS and its application in cancer diagnosis

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Imaging mass spectrometry (IMS) based on matrix-assisted laser desorption ionization (MALDI) is an emerging technique to identify molecules and map their distributions within a pathological tissue section. Unlike other biological imaging methods, MALDI imaging is capable of analyzing multitudes of unlabeled species in a single measurement.

A MALDI-TOF system of reflector geometry was developed for high spatial resolution by employing a dedicated laser beam optics with variable focal spot size (12 μm ~ 160 μm) and a precision sample translation stage. An intriguing feature of our IMS is a modular epi-fluorescence microscope implemented to observe the MALDI ionization source on the same measurement platform. More comprehensive and evident molecular information is allowed by the near-infrared (NIR) imaging of fluorescently tagged molecules with superior sensitivity, not being hampered by autofluorescence.

Preliminary experiments were carried out with tumor tissues, demonstrating the potential of simultaneous MALDI-IMS and NIR fluorescence imaging as a useful tool to facilitate the discovery of new biomarkers for hypoxia and efficient therapeutic targets of a tumor.

Symposium-4-A

Metabolomic approaches based on chromatography hyphenated mass spectrometry

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Metabolomics, commonly known as metabolic profiling or metabonomics, is a fast growing field in biomedical research and offers a powerful and promising approach for a broad range of applications. Metabolomics focuses on deriving the concentrations and fluxes of low molecular weight metabolites (<~1 kDa) in bio-fluids, cells or tissue, plants, and related samples, and this information provides enormous detail on biological systems and their current status. Mass spectrometry (MS) is one of most powerful and commonly used analytical methods in metabolomics. In this presentation, metabolomics approaches based on GC/MS and LC/MS will be briefly introduced in line with the development of analytical methodology. Some of applications in our metabolomic studies included chemical profiling of neurotransmitters and short-chain fatty acids to discover toxicology biomarkers for the diagnosis of diseases and therapeutic prediction.

Symposium-4-B

LC-MS/MS Determination of Residual Carbonyl Compounds in Dietary Supplement using Fluorogenic Derivatization

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Many studies have raised concerns regarding food due to carbonyl compounds released by various sources, including the burning of oils, animal fats and vegetables [1]. The presence of low molecular mass carbonyls in dietary supplement is undesirable because they can be responsible for unpleasant organoleptic properties in some health implications. These carbonyls can bind in vivo to biological nucleophiles, resulting in toxic mutagenic and carcinogenic effects. You can include the purpose of the research and the main results. In recent years, the popularity of dietary supplements has soared worldwide, as they are believed to be safer and healthier than synthetic drugs and free of side effects. In the present work, we propose an analytical method for the sensitive determination of the six of carbonyl compounds in dietary supplement, such as formaldehyde, acetaldehyde, formaldehyde, acetaldehyde, propionaldehyde, acetone, 2-butanone and benzaldehyde. However, direct LC-MS analysis of short-chain aldehydes without derivatization is hindered by poor chromatographic performance and low ionization efficiency. Carbonyl compounds were derivatized with fluorescein 5 -thiosemicarbazide (FTSC) yielding the corresponding thiosemicarbazones [2], which were separated by liquid chromatography and detected by tandem mass spectrometry (MS/MS). On the basis of the MS fragmentation analysis, the characteristic ion fragments for FTSC-carbonyl compounds and the IS were observed at m/z 389.9 and m/z 347.8, respectively (Figure 1). The predominant ion at m/z 389.9 was chosen for the quantitation, and an ion at m/z 347.8 was used as the confirmative ion for FTSC-carbonyl compounds. In this mass spectrometry method, each compound has the same product ion at m/z 389.9. Therefore, chromatographic separation should be completely accomplished before the sample is introduced into the MS/MS system. To determine the applicability of this method, we quantified many kinds of carbonyl compounds, including formaldehyde, acetaldehyde, propionaldehyde, acetone, 2-butanone, and benzaldehyde, in samples of various dietary supplement dosages including tablets, capsules, pills, and drinks. All samples collected from South Korean markets were prepared. Formaldehyde was detected efficiently in the range 4.2 – 5066.7 μg/kg dietary supplement dosages weight and acetaldehyde in the range 8.8–43968.4 μg/kg dietary supplement dosages weight and propionaldehyde in the range 10.3 – 14240.6 μg/kg dietary supplement dosages weight in 40 samples. Concentrations of acetone, 2-butanone and benzaldehyde were 2.6–121.1, 5.5-8070.8 and 7.6–700.6 μg/kg dietary supplement dosages weight, respectively. From these results, it is represent that our development LC-MS/MS method is simple, accurate and reliable for monitoring carbonyl compounds in dietary supplements. Our result provides a simple and effective method for the determination of carbonyl compounds using LC-ESI-MS/MS. This method provides several advantages over the previous LC-MS methods, including shorter analysis times, the use of an IS for quantitation, and improvements in chromatographic conditions. The procedure was optimized for the detection of carbonyl compounds derivatized with FTSC. The application of LC-MS/MS could simplify sample preparation and derivatization, and allow accurate and reproducible quantification of carbonyl compounds in dietary supplement dosages at sub-ppb levels. This study was successfully determined six of carbonyl compounds, the developed LC-MS/MS procedure can be used for routine analysis to monitoring carbonyl compounds in various forms of dietary supplement dosages. To the best our known, this is the first report of a LC-ESI-MS/MS method optimized for FTSC derivatization applied to the analysis of carbonyl compounds. This is the first report of a LC-ESI-MS/MS method optimized for FTSC derivatization applied to the analysis of carbonyl compounds

Symposium-4-C

Laser desorption/ionization (LDI) mass spectrometry based on nanomaterials for biomedical applications

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In conventional MALDI-TOF mass spectrometry, analyte molecules are known to be ionized by mixing with organic matrix molecules. As the organic matrix molecules are ionized, they generate unreproducible mass peaks such that MALDI-TOF mass spectrometry is nearly impossible in the low mass-to-charge (*m/z*) range (< 1000). In this work, we present laser desorption/ionization (LDI) mass spectrometry based on solid-matrices for the detection of small biomolecules in the low *m/z* range by using MALDI-TOF mass spectrometry: (1) Top-down synthesized TiO_2 nanowires were synthesized as arrays using a modified hydrothermal process directly on the surface of a Ti plate; (2) The nylon nanoweb with TiO_2 particles was prepared by the simultaneously electrospinning a nylon nanoweb and electrospraying TiO_2 nanoparticles; (3) The parylene-matrix chip was fabricated by the deposition of nano-porous parylene-N thin film on a dried organic matrix array. The mass spectrometry of multiple analytes was demonstrated in the low molecular weight range using eight amino acids. Additionally, model were used as model analytes to test the feasibility of solid-matrix chips for MALDI-TOF mass spectrometry. The biomedical application of LDI mass spectrometry was demonstrated for (1) the detection of chemical and biological warfare agents, (2) the newborn metabolite analysis and (3) the antibiotics-resistant bacteria screening.

Symposium-4-D

Quality Characterization and Evaluation Using Mass Spectrometry in Biosimilar Development

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Biosimilar is a copy-version of biological medicinal product that is developed to commercialize when patent of original product expires. Biosimilar products are expected to increase patients' accessibility to expensive biological medicines by promoting competitions on a market. Despite of vast demands, developing biosimilar is much more challenging compared to small-chemical generic drugs because of the intrinsically heterogeneous properties of biologics. Biosimilars of monoclonal antibodies are even more difficult to develop than smaller sized cytokines (e.g. insulin, growth factors etc.) due to their size and complex post-translational modifications. Numbers of regulatory agencies including FDA and EMA have established necessary guidelines so that applicants can obtain approval for their biosimilar products without necessity of full clinical trials. These guidelines emphasize a "step-wise approach" for the development of biosimilar; detail evaluation of original products is first required to obtain information for reference product. And then, extensive physicochemical and biological characterization needs to be performed to demonstrate analytical similarity between biosimilar and original product. Mass spectrometry is one of the powerful tools to evaluate product quality and similarity during product development. Thus, mass-based quality data are required to review product quality by regulatory agencies in the process of drug approval. In this regard, various analytical methods using mass spectrometry are applied to demonstrate product similarity in terms of structre, PTM, product-related impurity and process related impurity.

Symposium-4-E

Developments of automated high-throughput sample preparation methods using glycan-specific affinity capturing for glycosylated proteome analysis

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Glycosylation is one of the most important post-translational modifications (PTM) of proteins and contains various biological significances. Carbohydrate-protein interactions are involved in many cellular events such as protein localization, protein-protein interaction, immune responses, cell division, tumor immunology and cell signaling. Profiling of glycoprotein is an essential starting point to investigate the cellular events. The preparation of glyco-proteome samples involves delicate target enrichment and purification steps. These cause difficult to process a large number of samples in reproducible manners.

In this study, we present three automated Glyco-Omics sample preparation workflows for a 96-well plate liquid handling robotic system. The protocols are based on the filter-aided capture and elution method. First, we have constructed a method to capture glycopeptides using ConA and WGA lectins with 30-kDa membrane filters. Subsequently, the extracted glycopeptides are desalted by C18 clean-up process. Secondly, we have developed a method to extract N-glycan and o-glycopeptide at the one batch experiment. Thirdly, using the SNA lectin and the filters was building a way to extract glycolipid. All of these processes were automated using a liquid handling and a vacuum system. These protocols are efficiently applied for biomarker discovery candidates by limited protein amount of variety of clinical samples, so it is likely to be widely used in diagnosing and treating diseases in the future.

Symposium-4-F

Analysis of Homogeneous and Heterogeneous Antibody-Drug Conjugates (ADCs) for Bioanalytical and Pharmacokinetics Analysis Platforms

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Antibody-drug conjugates (ADCs) are a class of biopharmaceutical drugs designed as a targeted therapy. ADCs are comprised of a cytotoxic drug covalently linked to a monoclonal antibody, forming a complex molecule containing characteristics of small-molecule drugs and large-molecule biologics. Due to their complexity, however, unique bioanalytical strategies are needed to separately identify, characterize and quantify the ADC species most relevant to safety and efficacy. Improvements in analytical technology have provided the tools to better characterize ADC products, giving ADC developers the information needed for process and formulation development, and for identifying the methods needed for stability testing. Here, we developed the bioanalytical and pharmacokinetics analysis platforms for homogeneous (LegoChem biosciences, Inc. ADC)/heterogeneous (ADCETRIS) antibody-drug conjugates (ADCs). To this end, we first performed the evaluation of physical and chemical stability of these ADCs; Aggregation analysis (stability testing), peptide mapping, glycosylation profiling and analysis of drug to antibody ratio (DAR) were performed. Second, the pharmacokinetics (PK) of a homogenous ADC is assessed through a combination of assays including total antibody and unconjugated drug quantitation (free toxin level) we developed analytical method; MRM for selection of specific analytes and absolute quantitation of ADC, were performed using the Triple Quad 6500 System. Our developed platform for ADCs characterization and pharmacokinetics (PK) will provide a better understanding of how ADC structure affects clinical outcomes such as efficacy and safety.

Symposium-5-A

<KEYNOTE SPEAKER>

Illuminating the Structural Diversity of the Lipidome: Ultraviolet Photodissociation Tandem Mass Spectrometry for Comprehensive Lipid Characterization

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Lipids play diverse structural and functional roles in the maintenance of cellular homeostasis, including as components of cellular membranes and membrane proteins, in energy storage, and as intra- and inter-cellular signalling molecules. Furthermore, aberrant lipid metabolism is known to be functionally associated with the onset and progression of certain metabolically linked diseases. The biological activities of these lipids are dependent on their structures. However, due to the limitations of conventional MS/MS ion activation strategies, there is a recognized need for improved methods for their detailed structural characterization, particularly for the multitude of isomeric lipids that may be present within complex lipidomes. Here, the utility of positive and negative ionization mode 193 nm or 213 nm UVPD-MS/MS and -MS^3, implemented in Orbitrap Q Exactive Plus or Orbitrap Fusion Lumos mass spectrometry platforms, respectively, have been explored for the detailed structural characterization of individual lipid species (including isomeric lipids) across a range of lipid categories, including fatty acids, glycerolipids, glycerophospholipids, sphingolipids and sterol esters. In addition to the product ions formed by conventional HCD, positive ionization mode UVPD is shown to yield unique pairs of structurally diagnostic product ions indicative of the presence and site(s) of unsaturation within mono- and poly-unsaturated alkyl chains, as well as sphingosine and plamalogen ether C=C double bonds. Additional unique UVPD product ions are also observed that enable improved characterization of the lipid backbone (e.g., sphingoid base, ester-, ether- and amide bond-linked alkyl chains) and headgroup identities. HCD-MS/MS followed by UVPD-MS^3 can be used effectively to assign sites of unsaturation in isomeric lipids where there is the possibility of ambiguity due to isomeric mixture complexity (e.g., TAG's), as well as to determine branching sites in fatty acid esters of hydroxy fatty acids. With activation timescales and dissociation efficiencies similar to those employed in conventional MS/MS strategies, we conclude that UVPD is a promising new tool in the arsenal of ion activation techniques, toward providing complete structural elucidation in automated, high-throughput lipid analysis workflows.

Keywords: Lipids, lipidomics, photodissociation, tandem mass spectrometry, structural characterization

Symposium-5-B

<KEYNOTE SPEAKER>

Integrated Omics Approach Centered on Mass Spestrometry-based Metabolomics to Decipher Mechanism Implicated in Human Diseases

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Due to the higher sensitivity and favorable structural identification ability of mass spectrometry (MS), MS-based metabolomics has shown great potential in disease study. Yet, integration with other omics datasets is necessary for a deep research. In this work, we combined MS-based metabolomics and transcriptomics to unravel the molecular mechanism underlying human disease.

LC-MS-based metabolomics and lipidomics analyses were performed on matched prostate cancer (PCa) tissues and adjacent noncancerous tissues, 20 of which were subjected to RNA-seq analysis. Centering on the findings at the metabolic level on differential metabolites and related metabolic pathways, we further combined the transcriptional data for the mechanism investigation.

LC-MS based metabolomics approach yielded 128 differential metabolites, including 13 carnitines and acylcarnitines, 68 lipids and fatty acids, and 47 organic acids and alkaloids. Using lipidomics approach, we defined 130 differential lipid species, most of which were dominantly elevated in tumor tissues, covering a multitude of lipid classes including PC, PE, PG, PI, Cer, DAG, CE and FFA, with 1.65–15.87 fold' increase. To trace the upstream variations of the metabolome, we analyzed the expressed gene levels of the differential metabolic species. The alteration of gene expression further confirmed the metabolic pathway dysregulation in prostate cancer. Moreover, we found impaired sphingosine-1-phosphate receptor 2 signaling, downstream of sphingosine, representing a loss of tumor suppressor gene and a potential key oncogenic pathway for therapeutic targeting.

On the other hand, one of the most important metabolic characteristics in PCa is an increased citrate oxidation because of the inability of the epithelial cells to accumulate zinc, but the corresponding metabolic reprogramming and potential mechanisms remain unelucidated. To unravel the molecular abnormalities in the TCA cycle and the potential regulatory networks underlying metabolic reprogramming in PCa we further used gas chromatography-mass spectrometry (GC-MS)-based metabolomics method and RNA sequencing to investigate the alterations of PCa in both metabolic and transcriptional levels among the matched PCa tissues and adjacent normal tissues (ANTs). Significant accumulation of metabolic intermediates and enrichment of genes in the tricarboxylic acid (TCA) cycle was observed in tumor tissues, indicating TCA cycle hyperactivation in PCa tissues. Additionally, the levels of fumarate and malate were correlated with the Gleason score, tumor stage and expression of genes encoding related enzymes and were highly related to the expression of genes involved in branched chain amino acid degradation. Our results also suggested that 2-ketoglutarate is replenished via MYC-regulated glutamine metabolism to fuel the TCA cycle in PCa.

Integrated omics provides a broad picture of the molecular network on prostate cancer and contributes to a better understanding of the mechanism. MS-based metabolomics shows a great potential in shedding light on the disease mechanism focusing on metabolic reprogramming. The challenges include metabolite coverage, metabolite identification and detection stability etc.

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Symposium-5-C

Revisiting the Metabolism and Bioactivation of Ketoconazole Using LC–MS-Based Metabolomics

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Although ketoconazole (KCZ) has been used worldwide for 30 years, its metabolic characteristics are poorly described. Moreover, the hepatotoxicity of KCZ limits its therapeutic use. In this study, we used liquid chromatography–mass spectrometry-based metabolomics to evaluate the metabolic profile of KCZ in mouse and human and identify the mechanisms underlying its hepatotoxicity. A total of 28 metabolites of KCZ, 11 of which were novel, were identified in this study. Newly identified metabolites were classified into three categories according to the metabolic positions of a piperazine ring, imidazole ring, and *N*-acetyl moiety. The metabolic characteristics of KCZ in human were comparable to those in mouse. Moreover, three cyanide adducts of KCZ were identified in mouse and human liver microsomal incubates as “flags” to trigger additional toxicity study. The oxidation of piperazine into iminium ion is suggested as a biotransformation responsible for bioactivation. In summary, the metabolic characteristics of KCZ, including reactive metabolites, were comprehensively understood using a metabolomics approach.

Symposium-5-D

Free Fatty Acids as biomarkers in Pulmonary Fibrosis

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Metabolome has drawn attention as molecular phenotypes underneath clinical symptoms or outcomes. Global metabolome profiling has great potential to find novel targets or disease mechanisms in various human diseases. Pathogenesis of idiopathic pulmonary fibrosis (IPF) has been suggested to be related to the dysregulation of metabolism. Thus, metabolomics approaches were used to find novel biomarkers for IPF pathogensis in this study. Global metabolic profiling was performed for the lung tissues of IPF patients. The amount of free fatty acids was found to be statistically different between normal and IPF tissues after metabolite identification. To validate the observations, free fatty acids in lung tissues were quantitated. Fatty acid methyl esters were analyzed with Agilent 7890/5975 GCMSD system, and HP-5 MS 30 m × 250 μm × 0.25 μm column (Agilent 19091S-433) in the lung tissues of controls and IPF patients. Human lung fibroblasts were treated with TGF- β1, one of the most known profibrotic cytokines in pulmonary fibrosis, and/or each fatty acid to evaluate the function of FFA. We found that free fatty acids play an important role in pulmonary fibrosis.

Symposium-5-E

Recent advances in steroid signatures to monitor endocrine diseases evaluated by GC-MS/MS

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Alteration of steroid metabolism is responsible for the development and prevention of endocrine diseases. To understand metabolic changes of steroids, 37 steroids, including 6 androgens, 2 estrogens, 13 progestins, 9 corticoids, and 7 sterols, were quantitatively analyzed using the supported liquid extraction (SLE) coupled to high-temperature gas chromatography-tandem mass spectrometry (HTGC-MS/MS). For the comprehensive determination of steroid hormones in body fluids, SLE purification was optimized and compared with the solid-phase extraction method as sample preparation procedures. The devised assay resulted in the increase of extraction efficiency with good chromatographic selectivity. The detection limits ranged from 0.1 to 2 ng/mL, except that for cholesterol (0.1 μg/mL), and the correlation coefficients for standard curves were higher than 0.99. The overall recoveries of 30 steroid hormones ranged from 62.1% to 104.3%, except those for 7 sterols (44.7% ~75.7%). The validated method was applied to the evaluation of the steroid levels in human saliva and serum samples under different pathophysiological conditions. This technique can be useful for monitoring altered steroid levels during the diagnosis in clinical practice.

Symposium-6-A

Chemical Fingerprints and their applications

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The primary aims of forensic chemical analyses are identification and comparison of various samples with the intention of establishing a link between samples from a crime scene to samples relating to a specific person or location (e.g., clandestine laboratory). With automated instrumentation widely available, highly specific spectroscopic and mass spectrometry based analytical techniques are now, in most modern forensic science laboratories, the most valuable tool used to achieve these analytical goals. Should chromatographic and spectroscopic data of two compounds correspond, it may be concluded that they are chemically indistinguishable. However, with increasing frequency an argument is brought forward by way of defence, asserting that samples that are chemically indistinguishable may be chemically identical but are not necessarily the same. Being the same is interpreted here as sharing a common sample history or sample provenance. chemical fingerprints with IRMS and ICP-MS hold the potential to resolve this argument by providing an additional set of independent variables (e.g., independent of other spectroscopic characteristics) and thus increasing the overall discriminatory power of the forensic analysis. Therefore, some cases and(or) on-going research would be introduced using chemical fingerprints.

Symposium-6-B

Development of Certified Reference Materials for Accurate Determination of Fluoroquinolone Antibiotics in Chicken Meat

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Certified reference materials (CRMs; KRISS CRM 108-03-003, 108-03-004) were developed for the accurate determination of fluoroquinolones (enrofloxacin and ciprofloxacin, respectively) in chicken meat. Two groups of chickens were cured with feeds containing enrofloxacin and ciprofloxacin, respectively. After slaughter, the thigh and breast meats were combined for the respective groups and the meat was freeze-dried, pulverized, sieved, and V-mixed. The final bulk material was bottled in 10 g portions. For certification of the CRMs, isotope dilution-liquid chromatography/tandem mass spectrometry was used. The certified values of the CRMs were (19.06 ± 0.86) mg/kg for enrofloxacin and (1.095 ± 0.038) mg/kg for ciprofloxacin. The stabilities of the CRMs were monitored at −70 °C for 12 months, at−20 °C for 2 months, and at room temperature for 1 month. Both CRM candidates were stable during the monitoring period for each temperature.

Keywords: Certified reference material, Fluoroquinolones, Chicken meat, ID-LC/MS/MS

Symposium -6-C

Simultaneous and Rapid Analysis of 500 Pesticide Multiresidues in Crops Using GC-MS/MS and LC-MS/MS

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Given that wide range of pesticides can be used in agricultural environmental, a rapid and reliable analytical method for pesticide residues is essential to ensure food safety and human health. The challenge for pesticide residue analysis has been to analyze as many pesticides as possible, providing a fast, easy, simple and reliable results. This study was aimed to develop a rapid, simple, and high-throughput screening method for the analysis of five hundreds of pesticides using gas and liquid chromatography-triple quadrupole mass spectrometry (LC-MS/MS and GC-MS/MS) in representative crops (brown rice, orange, and spinach). Multiple reaction monitoring transition parameters (e.g., collision-induced dissociation voltages, precursor and product ions) in MS/MS were carefully optimized to achieve the best selectivity and sensitivity. In GC-MS/MS analysis (360 compounds), a short (20 m) and microbore (0.18 mm i.d.) column was employed, resulting in better signal-to-noise ratio with reduced analysis time (25 min) compare with the conventional analytical column. The effects of the priming injection were investigated, indicating a priming injection after a liner change is essential to achieve higher sensitivity and precision. In LC-MS/MS analysis (310 compounds), injection volume and mobile phase were optimized to improve the analytical performance. The QuEChERS methodology, has been considered as the “golden standard” in the pesticide residue analysis were modified by comparing the extraction solvents and various cleanup absorbents to cover the wide range of GC-amenable and LC-amenable pesticides. The optimized method was validated with recovery tests considering the validation parameters including accuracy, precision, limit of quantitation, linearity, and matrix effects. The method was successfully applied to monitoring of pesticide residues in real sample analysis.

Symposium-6-D

Analysis of functional nutrients in human milk from three Asian countries

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Human milk is fundamental nutrient essential to the newborns and infants. From the mother milk, infants can obtained every chemical molecules that necessitate early stage of their life. Some of nutrients serve as energy molecules as well as building blocks for their body. This energy nutrient are featured as primary structure-based chemical molecules such as amino acid, mono- or disaccharides and triglycerides. The importance of energy nutrient is the composition and the amounts described as concentration or calorie. Another form nutrient that found in the milk is the functional nutrient. Functional nutrient is not served as an energy materials nor building block, it is essential to maintain the proper functionalities of metabolic activity itself. It includes the vitamins and minerals, those of which were referred as micronutrient traditionally. Functional macronutrients are the same molecules as proteins, lipid, or carbohydrates, however, the structural integrity and accompanying functionality are more important. For example, IgG or lactoferrin is proteins present in human milk, those were primarily used as enzymes or antibodies as intact molecule rather than as amino acid units. Among carbohydrates in milk, human milk oligosaccharides (HMOs) are the functional nutrient that is not used infant but manipulate the intestinal microbiota which are able to influence the infant health. Since the functional nutrients impact on the infant health as direct or indirect regulatory materials, the importance of composition and the distribution across the people are beyond the doubts. Here, we collect the human milk samples from Korea, China and Vietnam mothers, the comprehensively analyze the functional and metabolic nutrients to acquire the reference lines for the differences and commonalities between peoples.

Symposium-6-E

Risk Prevention and Management of Pesticides Residues in the Food Industry

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Food safety is one of the most sensitive and important issues both domestically and internationally, because food can easily provide hazardous compounds to human bodies. Therefore, we need to research how to minimize intentional pollutants and how to manufacture safe food from farm to table. In addition, a comprehensive food safety assurance policy should be implemented so that it can be safely provided to our table through various necessary processes, as well as being hygienically cooked and consumed. In these days, another important thing is new hazardous compounds and unintentionally occurring compounds during process, so many companies have been working to find new pesticides or substances that are at risk.

In Korea, government has been providing safer agricultural products to consumers by legally setting the maximum residue limit (MRL) of residual pesticides. Initiation of positive list system (PLS) for food ingredients and materials will be an opportunity to look back on the current food safety system such as several technologies of agriculture products, food processed product distribution system and food analysis. However, it seems to have difficulties in managing a large number of pesticides that are used in various parts around the world. Based on the helpful and nonconformity information of pesticides provided globally, it is necessary to enlarge the list of pesticide analysis items in the form of creating and managing a list of pesticides that are not suitable for each country and each crop.

Symposium-6-E

Discrimination of Geographical Origins of Rice and Ginseng Using a Mass Spectrometer-Based Electronic Nose

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The objective of this study was to discriminate the cultivar, growing region, and geographical origin of rice (Oryza sativa) using a mass spectrometry-based electronic nose (MS E-nose).

The inside-needle dynamic extraction (INDEX) system was used to concentrate the samples for MS E-nose, following which the ion fragment data obtained were used to perform discriminant function analysis. Discriminant functions 1 and 2 readily separated all 16 cultivars of rice samples. It was also confirmed that MS E-nose could distinguish the region in which rice cv. Chucheong and Koshihikari were grown, likely due to variation in environmental factors, such as soil and climate. Finally, it was confirmed that MS E-nose could be used to detect the geographical origin of rice, discrimination of Korean rice from Japanese rice. Therefore, this simple and rapid technique is of value for discriminating the cultivar, growing region, and geographical origin of rice.

The geographical origin of ginseng and ginseng products were studied using a mass spectrometry based electronic nose. The treated ginseng and ginseng product were analyzed, and discriminant function analysis (DFA) was used for discriminating ~~of~~ geographical origins. The DFA plots indicated a significant separation of domestic and Chinese. These developed analytical methods using MS E-Nose can be useful to determine the geographical origin of ginseng and ginseng products in origin test.

<KEYNOTE SPEAKER>

Real-Time Monitoring of Molecular Products in Thin-Film Fast Pyrolysis of Glucose-based Carbohydrates

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Fast pyrolysis produces high yields of condensable vapors (bio-oils) which can be upgraded into drop-in fuels or commodity chemicals. Fundamental understanding of fast pyrolysis is very limited despite three decades of research, mostly owing to the complexity involved in the pyrolysis process. The kinetics of biomass pyrolysis has mostly been studied with global lump-sum models which ignore the chemical reactions of each molecular compound, leading to inconsistent kinetic parameters between measurements and no information on the pryolysis product distribution.

Here, we report an analytical platform to monitor each pyrolysis molecular product in virtually real-time with 0.1 second temporal resolution by directly attaching a drop tube microfurnace with a time-of-flight mass sepctrometer (TOF MS) via dopant-assisted atmospheric pressure chemical ionization (dAPCI). This instrumentation allows to monitor pyrolysis process with a very short reactor residence time, ~0.2 s, by pyrolyzing a thin-film of materials spotted outside of the sample cup and tracking soft-ionized each molecular product with high-resolution TOF MS. Combined with thin-film pyrolysis for isothermal kinetics conditions, we monitored the fast pyrolysis of a series of small carbohydrates (glucose, cellobiose, cellotriose, and cellotetraose). Additionally, fast pyrolysis of thin-film and powder of α-cyclodextrin and cellulose were studied to gain a better understanding of the size effect on reaction kinetics.

Small carbohydrates are completely pyrolyzed within one second and as short as one-half second for glucose pyrolysis. This is much faster than predicted by theoretical modeling by the Broadebelt group (>2 s). The shortcoming of the theoretical model is largely attributed to 1) the imperfection of the proposed reaction mechanisms (e.g., missing reactions) and 2) incorrect reaction parameters. The latter is especially significant because many of the reaction parameters were obtained by fitting to experimental data from pyrolysis-GC-MS analysis of 200-500 μg of materials. Such large amounts of powder piled inside the sample cup leads to the significant sample dimension of ~0.5 mm and result in non-isothermal kinetics, while isothermal kinetics are inherently assumed in the model.

Furthermore, we could find many pyrolysis products that are not identified in conventional pyrolysis-GC-MS study, because either they are thermally unstable in typical GC-MS condition or not present in NIST EI-MS library. For example, glyceraldehyde ($C_3H_6O_3$) is thermally unstable at high temperatures and not present in the NIST EI-MS library. However, thermally unstable pyrolysis products can be still detected in our instrumentation as long as they can survive for 0.2 s inside the reactor. In our glucose pyrolysis, $C_3H_6O_3$ is the highest yield product and could be explained as mostly coming from glyceraldehyde before they further break into smaller products. Individual time profiles could be extracted and examined for each molecular product, and the differences could be explained in regards to reaction mechanisms. Intermdeidate product ($C_8H_{14}O_7$) that is not previously found in any of the Py-GC-MS studies was detected with significant abundance in the pyrolysis of cellobiose or larger carbohydrates, which gave us a deep insight in the pyrolysis reaction mechansim induced by glycosidic bond cleavage.

Unlike other small carbohydrates, a surprising time delay of one second is observed for the thin-film pyrolysis of cellulose and α-cyclodextrin, and attributed to the phase transition to molten phase. The product yield distribution in the pyrolysis of various carbohydrates was compared with previous work, and the origin of the differences will be discussed in regards to the reactor residence time and unstable intermediates.

Symposium-7-B

Rapid, real-time and simultaneous quantification of volatile organic compounds with Selected Ion Flow Tube Mass Spectrometery (SIFT-MS)

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Volatile organic compounds (VOCs) are representative air pollutants due to their detrimental effects on human health and their role in formation of secondary organic aerosols. Atmospheric concentrations of VOCs can vary dramatically in time and space under the influence of mixing events driven by meteorogical processes. And assessments and monitoring programs of VOCs using periodic grab sampling like Tedlar bags, canisters, and sorbent traps provide limited information, often with delay times of days or weeks. We developed mobile laboratory system equipped with selected ion flow tube mass spectrometry (SIFT-MS) to effectively cope with environmental emergencies like oil and hazardous materials spill accidents. In such cases, top priorities are rapid, real-time and simultaneous quantification of various contaminants including VOCs. SIFT-MS is an emerging analytical technique for the real-time quantification of VOCs in air. It relies on chemical ionization of the VOCs molecules in air introduced into helium carrier gas using H_3O^+, NO^+, and $O_2^{+\cdot}$ precursor ions. It is reported that absolute concentrations of VOCs can be determined by SIFT-MS down to ppb levels, obviating sample collection and calibration. Overall performances of mobile laboratory were tested: 1) analytical integrity of SIFT-MS, 2) stationary and mobile measurement capability. Firstly, real-time monitoring method of 60 VOCs in the ambient air was developed using TO-15/17 standard gas mixture. Calibration curves, method detection limit, and quantitation reproducibility of the target compounds were tested, which produced similar results with previously reported values. Secondly, representative pollution sources of VOCs including petrochemical plants, industrial complex, major harbor, power plant, and urban area were selected to test stationary and mobile measurement capability. In the petrochemical plants, the major emission substances, BTEX (benzine, toulene, ethylbenzene and xylenes) were measured for 24 hours. The average concentration of BTEX was 3.54±1.31 ppbv, which was two times higher than those in rural area (1.70±1.33 ppbv). Similarly total VOCs (sum of 60 VOCs) were also measured at harbor, industrial complex, and power plant. One hour average concentrations of total VOCs were in the following order: harbor (129±4.34 ppbv), power plant (121±7.05 ppbv), and industrial complex (96.0±10.7 ppbv). Mobile measurements of BTEX were also tested on road while moving along the main road of Geoje Island. Spatial distribution of BTEX on road well matched with traffic volume, where benzene and toluene were found to be the major pollutants. It is expected that mobile lab system with SIFT-MS will be a versatile monitoring platform for environmental emergencies and atmospheric pollution.

Symposium-7-C

Comparing discrimination capabilities of fluorescence spectroscopy versus FT-ICR-MS for sources and hydrophobicity of sediment organic matter

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Characterizing the chemical and molecular composition of sediment organic matter (SeOM) provides critical information for a complete picture of global carbon and nutrient cycles, and helps to track the sources and the fate of organic carbon in aquatic environments. In this study, we examined fluorescence properties and molecular composition of the alkaline extractable organic matter (AEOM) of sediments in a coastal lake (Lake Sihwa) and its surrounding creeks (rural, urban, wetland, and industrial areas). Five fluorescence-based indices and 20 molecular parameters were selected from fluorescence spectroscopy and Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), respectively, and utilized to discriminate the AEOM among five different sources as well as two chemical composition of hydrophobic acid (HoA) and hydrophilic (Hi) fractions. Ordination based on Bray Curtis dissimilarity matrices showed that the fluorescence-based indices distinguished among urban, lake, and the other three sources, while the molecular parameters from FT-ICR-MS performed better in discriminating among the sources of rural, wetland, and industrial areas. Irrespective of the sources, the two different chemical fractions were statistically distinguished by their relative distributions of UVA-humic like fluorescent component and carbohydrate molecular group. However, a rigorous test based on percent dissimilarities indicated no superior capability of either of the two tools in discriminating the sources or their two chemical fractions, which might be attributed to the inherent structural heterogeneity of SeOM and the limited analytical window of FT-ICR-MS for relatively large molecular sized molecules.

Symposium-7-D

Ultra-High Resolution FT-ICR Mass Spectrometry for Analaysis of Fine Aerosol ($PM_{2.5}$)-derived Organic Substances

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Airborne particulate matter consisting of ionic species, salts, heavy metals and carbonaceous material is one of the most serious environmental pollutants owing to its impacts on the environment and human health. Although elemental and organic carbon compounds are known to be major components of aerosols, information on the elemental composition of particulate matter remains limited because of the broad range of compounds involved and the limits of analytical instruments. In this talk, an ultra-high resolution 15 Tesla Fourier transform ion cyclotron resonance (15T FT-ICR) mass spectrometry that has recently been used to successfully identify the chemical compositions of extremenly complicated samples (i.e. crude oils, soil and aerosol-derived organic substances) will be introduced. The comprehensive analysis of $PM_{2.5}$-derived organic compounds by 15T FT-ICR MS would allow us to better understand the chemical and structural features of the aerosol-carried harmful compounds.

Symposium-7-E

Applications and Results of Ambient Aerosol Measurement using High Resolution Time of Flight Aerosol Mass Spectrometry

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Aerosols play important roles in adverse health effects, indirect and direct forcing of Earth's climate, and visibility degradation. Long-range transport processed aerosol are also often dominant sources of aerosol pollution in Korea. In order to increase understanding of the formation of particulate matter and the chemical characteristics of aerosol in general, High Resolution Time of Flight Aerosol Mass Spectrometer (HR-ToF-AMS) was deployed in series of field experiments with either 6 - 10 minute or 10 sec time resolution. This included the special study in supersite, Beong-Yeong Island, as the regional background station and the composition of aerosols in oceanic regions as a part of the SHIPPO (Ship-borne Pole-to-Pole Observations on-board the Korean icebreaker R/V *ARAON*), and Aircraft-based aerosol measurement of Megacity Air Pollution Studies-Seoul (MAPS-Seoul) in May, 2015 and Korea U.S. Air Quality (KORUS-AQ) in June 2016.

The chemical composition of aerosol was dominated by carbonaceous and sulfate during many periods of the studies. Increasing sulfate and organic concentrations were associated with changes in air transport patterns to the site, Beong-Yeong Island. Overall, our results reveal the several different mechanisms of organic aerosol formation and identified new (or small) particle formation and growth events using powerful new tool of HR-ToF-AMS.

HR-ToF-AMS was deployed on aircraft platforms onboard King Air (Hanseo University) and DC-8 (NASA) aircrafts during MAPS-Seoul and KORUS-AQ campaigns. We characterized aerosol chemical properties and mass concentrations of sulfate, nitrate, ammonium and organics in polluted air plumes and investigate the spatial and vertical distribution of the species. The results of studies show that organics is predominant in Aerosol and a significant fraction of the organics is oxygenated organic aerosol (OOA) at the high altitude. The results of those studies can provide the details on the width, depth and spatial distribution of the pollutant plume and aerosol, which are valuable for modeling input parameters for modeling aerosol behavior.

This presentation will provide a detail principle and operation of HR-ToF-AMS. The measurement by HR-ToF-AMS provides insight into particle size distributions and the chemical compositions of non-refractory fine particle at Korea EPA supersite, Beong-Yeong Island and examine secondary aerosol formation over the ocean and the marine boundary layer and Megacity

Symposium-8-A

<KEYNOTE SPEAKER>

Glycomic and Glycoproteomic Mass Spectrometry Approaches

Lance Wells*, Peng Zhao, Osman Sheikh, Stephanie Stalnkaer, Jeremy Praissman, Meng Fang, Brent Weatherly, Seokho Yu, Kelley Moremen, Geert-Jan Boons, Richard Steet

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Glycomic and glycoproteomic approaches have lagged behind that of proteomics. Here we present several quantitative approaches for glycomics that have been developed and/or applied to biological samples. Our developed isotopic-detection of amino sugars with glutamine (IDAWG) method will be described along with our recent advancement in making this a dynamic method to determine half-life and remodelling of glycans. A detailed description of our selective exo-enzymatic labeling (SEEL) will be provided along with its application to defining the cell surface glycoproteome of cells. Finally, we will discuss briefly the application of various site-mapping strategies to determine the stoichiometry and heterogeneity of N-linked glycosylation using the HIV-1 GP120 protein as a test case.

Symposium-8-B

Ultraplexed MS1-based accurate protein quantification

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Isotopic labeling-based protein quantification has several advantages such as accurate quantity ratios and reduced technical bias over other approaches. However, conventional isotopic labeling schemes (e.g., SILAC) have a limited multiplexity (≤ 3-plex), mainly due to isotope overlap and retention time shift (RT shift) between labeled ions. Previous efforts to increase multiplexity either require expensive/unavailable resources or lack dedicated analysis algorithms. Also, currently adopted discovery-proteomics approaches (including isotopic labeling-based approaches) are known to have high LLOQ (lower limit of the quantification) resulting in narrow linear dynamic range.

Here we present EPIQ (Epic Protein Integrative Quantification), a model-based reconstruction method for n-plexed isotopic labeling-based quantification achieving low LLOQ and wide linear dynamic range. In the analysis of HeLa sample labeled by in-house-designed reductive di-ethylation 6-plex labeling, EPIQ showed accurate and sensitive quantification results. We also show EPIQ outperforms MaxQuant, the state-of-the-art quantification tool, especially for low abundance peptides. We anticipate that EPIQ could not only be widely adopted for diverse biological applications but expedite the development of further chemical/metabolic isotopic labeling schemes.

Symposium-8-C

Multiplexed parallel reaction monitoring assays for protein tyrosine kinases

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Protein tyrosine kinases (PTKs) play key roles in cellular signal transduction, cell cycle regulation, cell division, and cell differentiation. In this study, we have developed a parallel reaction monitoring (PRM)-based assay for quantitative profiling of 83 PTKs. The assay detects 308 proteotypic peptides from 54 receptor tyrosine kinases and 29 nonreceptor tyrosine kinases in a single run. We implemented the assay in lung cancer cell lines with either susceptibility (11-18) or acquired resistance (11-18R) to the epidermal growth factor receptor tyrosine kinase inhibitor erlotinib. Immunoblot analyses and shotgun proteomics data were highly consistent with PRM data. We applied micro-scale basic reverse phase liquid chromatographic (bRPLC) fractionation method for targeted quantitation. Micro-bRPLC fractionation of cell proteomes increased sensitivity by an average of 4.5-fold in targeted quantitation using PRM for 3 representative PTKs (EGFR, PGFRA, and BMX), which are present at low abundance in 11-18 and 11-18R cells. Multiplexed PRM assays provide a targeted, systems-level profiling approach to evaluate cancer-related proteotypes and adaptations

Symposium-8-D

MS based Glycoproteome Analysis Using IQ-GPA and Its Applications

Jin Young Kim, Gun Wook Park, Heeyoun Hwang, Ju Yeon Lee, Hyun Kyoung Lee, Eun Sun Ji, Kwang Hoe Kim, Hoi Keun Jeong, Ki Na Yun, Young-Mook Kang, and Jong Shin Yoo

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Protein glycosylation, one of the most prevalent posttranslational modifications in proteins, plays important roles in biological systems via various processes, such as adhesion, signaling through cellular recognition, and response to abnormal biological states. However, due to the complexity and heterogeneity of glycoprotein, current glycoprotein analyses focus mainly on either the identification of glycosites or the released glycans. We have developed MS based high-throughput method for intact N-glycopeptides analysis, named IQ-GPA. It can automatically identify and quantify the N-glycopeptides including glycan compositions and amino acid sequences. The efficiency of IQ-GPA was demonstrated by the analysis of standard α1-acid glycoprotein and benchmark glycoprotein mixture. In total, 165 site-specific N-glycopeptides representative of all N-glycosylation sites were identified from AGP 1 and AGP 2 isoforms. Finally, IQ-GPA was applied for the various analyses of *N*-glycoproteins present in cell, tissue, and blood from human and mouse. The results show how useful IQ-GPA to automatically identify and quantify N-glycoproteins at the proteome level is.

This presentation is supported by the Bio-Synergy Research Project (grant number: NRF-2014M3A9C4066461) of the Ministry of Science, ICT and Future Planning through the National Research Foundation

Symposium-8-E

Integrative Multi-Omics of Th1 Differentiation

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T-cells are a major type of lymphocyte that play an essential role in cell-mediated immunity and thus are considered as the master regulators of immune defense. Similar to most differentiation processes it is controlled by a limited set of master transcription factors (TFs), which control the differentiation at early time-points. However, TFs are in general poor targets such that it is important to identify downstream targets. Mass spectrometry (MS)-based proteomic analysis has been a pivotal tool in biomedical research. Recent advance in biochemical enrichment of phosphorylated proteins and peptides combined with high resolution MS will allow large-scale proteomics experiments (Kim et al. Proteomics. 2012; Kim et al. Molecular and Cellular Proteomics. 2014.). Combined with transcriptomics data, multi-omics analysis allow to identify new drugs and to repurpose existing ones by analyzing a validated multi-layered model for the early protein signaling network that regulates the master transcription factors (TFs) of T-cell differentiation. Here, we will isolate desired number of T cells first and subjected to Th1 differentiation upon treatment of ligand cocktail. Activated cells will be collected during the early time course of differentiation as specified such as 0 min, 60 mins, 120 mins, 6 hours, 24 hours, and 5 days. Subsequently phosphoproteome analysis will be carried out by employing a quantitative LC-MS/MS using high resolution Orbitrap mass spectrometry. MS data will further be analyzed prior to modelling. Next, the mathematical model for the regulation of the master TFs in T-cell differentiation, and link this model to TF regulatory networks will be derived. The model will allow for computational predictions of the genome-wide effect of drugs.

KSMS

2017 한국질량분석학회 여름정기학술대회 및 총회

POSTER PRESENTATION

포스터 발표 및 우수포스터상 안내

■ **포스터 게시 및 철거**

- 게시: 24일(목), 08:00 ~ 10:00 까지
- 철거: 25일(금), 12:00 ~ 이후

- 포스터 발표자는 아래의 포스터 번호 및 배치도를 참고하여 포스터를 게시하고, 24일(목) 10:50~ 11:50까지 포스터 앞에 대기하여 질문에 응해야 합니다.

- 포스터 발표자 순서: 홀수번호 10:50~11:20 / 짝수번호 11:20~11:50

■ **우수포스터 상**

- 포스터 발표 회원중 심사를 거쳐 15명을 선정하여 우수포스터상을 수여합니다.
  ※ Brief Oral Presentation 발표자는 우수포스터 상의 우선권이 주어짐.

- 시상: 2017년 8월 25일 (금), 폐회식
- 부상: 상장 및 상금 5 만원

■ **분야별 포스터 번호**

분야	포스터번호
Fundamental Instrumentation	001 ~ 012
Life & Informatics	013 ~ 029
Mass Spectrometry in Elemental Analysis	030 ~ 055
Medical/Pharmaceutical Science	056 ~ 113
Food Environment	114 ~ 139
General	140 ~ 184

1. Fundamental Instrumentation : P001 ~ P011

P-001

MATLAB-based Software Development for Screening Illegal Drugs and Analogues Identification Using LC-MS/MS Data

Inae Jang, Insu Song, Jungmin Lee, Yunha Ju and Han Bin Oh*

Dept of Chemistry, Sogang University, Seoul 04107, Korea

P-002

Rapid Classification of Edible Oils using MATLAB-based Statistical Analysis Software

Minhee Son, Han Bin Oh*

Dept of Chemistry, Sogang University, Seoul 04107, Korea

P-003

Protein Sequence Analysis by TEMPO-assisted Free Radical Initiated Peptide Sequencing (FRIPS) Mass Spectrometry

Jae-ung Lee and Han Bin Oh*

Dept of Chemistry, Sogang University, Seoul 04107, Korea

P-004

Efficient Enrichment of Phosphopeptides on Digital Microfuidic Chip Using TiO2-magnetic Bead.

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

Dept of Chemistry, Sogang University, Seoul, 04107, Korea

P-005

TEMPO-assisted Free Radical Initiated Peptide Sequencing (FRIPS) Mass Spectrometry Using MALDI-TOF/TOF

In Su Song[1], Sang Yun Han[2], Sangwon Cha[3], and Han Bin Oh[1*]

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P-006

On-line hydrogen/deuterium exchange of gas-phase molecules using gas chromatography-electrospray ionization/mass spectrometry

Eun Sook Jeong[1], Eunju Cha[1], Ho Jun Kim[1], Oh-Seung Kwon[1], Sangwon Cha[2], Sunghwan Kim[3], Hanbin Oh[4], Jaeick Lee[1,*]

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P-007

A new configuration of time-of-flight mass spectrometer for simultaneous measurements of primary ions and fragments of a selected ion

Bongyoon Yi[1,2], Seung Yong Kim[1], Wanseop Jeong[1,2], Myoung Yeo[1], Byeongwon Kang[2], Hyun Sik Kim[1,*] and Mo Yang[1]

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[2]Department of Physics, Chungbuk National University, Cheongju 28644, Republic of Korea

P-008

Nanosecond pulse of electron beam for a field-portable time-of-flight mass spectrometer

Wanseop Jeong[1, 2], Seung Yong Kim[1], Myoung Yeo[1], Bongyoon Yi[1, 2], Jae Yeong Eo[1], Byeongwon Kang[2], Hyun Sik Kim[1, *] and Mo Yang[1]

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P-009

The noble method of quantitative analysis of organic by-products using APC

Hyeon Jeong Eom*

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P-010

Good agreement observed between theoretical prediction and experiment data on ionization efficiency of polycyclic aromatic hydrocarbons by positive mode atmospheric pressure photoionization mass spectrometry.

Seulgidaun Lee[1], Arif Ahmed[1], Ji Won Ha[2] and Sunghwan Kim[1*]

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P-011

Development of inert-DART-MS system for analysis of air- or moisture-sensitive compounds

Young Hee Lim, Yeon Hwa Lee, Yong Jin Bae, Yeu-Young Youn, Hye Sung Cho

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P-012

Nanoparicles and CW laser-based efficient desorption for high resolution MS imaging of mouse brain tissue slices

Jae Young Kim[1*], Eun Seok Seo[1], Mi Hyang Shin[1], Hyunmin Kim[2], Ji-Won Park[3], Dong Kwon Lim[4], and Dae Won Moon[1]

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2. Life & Informatics : PO13~ PO29

P-013

Determination of ethnic differences in human saliva proteome by the construction and the characterization of the Korean whole saliva proteome

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

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P-014

Systematic integrative analysis of chemical-induced signal transduction in unicellular microalgae, *Chlamydomonas reinhardtii*

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P-015

Quantitative proteomic analysis of colon cancer cell line in two-dimensional and three-dimensional cell culture

Young Eun Kim[1*], Hyojin Jeon[2], Kwangrok Kim[2], Dukjin Kang[1]

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P-016

Profiling of a wide range of neurochemicals in human urine by ultra performance liquid chromatography-tandem mass spectrometry combined with *in situ* selective derivatization

Wonwoong Lee, Keon Hee Ko, Na Hyun Park, Jongki Hong *

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P-017

Development of an on-line proteolysis and glycopeptide enrichment method using enzyme immobilized thermo-sensitive porous polymer membrane enzyme reactor (μPPMER) and nanoflow liquid chromatography-tandem mass spectrometry

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P-018

Phospholipid quantification and enhancement of cardiolipin profiling based on isotope-labeled methylation by nUPLC-ESI-MS/MS

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P-019

Comprehensive proteomics of 2D-/3D-cultured adipocyte cell and its co-cultured with macrophage using a nLC-ESI-MS/MS

Sun Young Lee[1,2], Kwonseong Kim[2], Jongki Hong[1], Sung Bum Park[3], Ki Young Kim[3] , Dukjin Kang[2]

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P-020

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

Jae Hyun Lee, Joon Seon Yang, MyeongHee Moon*

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P-021

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

San Ha Kim [1], Joon Seon Yang[2], Myeong Hee Moon[1,*]

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P-022

Proteome analysis of Macaca fascicularis for Drug addiction model

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P-023

Quantitation of glycans in yeast using metabolic isotope labeling with isotopic glucose by mass spectrometry

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P-024

Quantitative analysis of *n*-linked glycan in *oryza sativa* using metabolic labeling with isotopic glucose by mass spectrometry

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P-025

Urine metabolic signature in human pulmonary tuberculosis disease

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P-026

Effect of tryptophan supplementation on endogenous metabolism and balance of neurotransmitters

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P-027

Intact glycopeptide analysis of targeted serum haptoglobin for gastric cancer biomarker discovery

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P-028

Plasma metabolomics for discrimination of graves' disease using GC-TOF-MS and LC-MS

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P-029

Discovery of potential metabolic biomarkers for discrimination of subtypes of Guillian-barre syndrome

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3. Mass Spectrometry in Elemental Analysis : PO30 ~ PO55

P-030

Development and validation of an analytical procedure for the total mercury in oyster and tuna using isotope-dilution inductively coupled plasma mass spectrometry

Hwijin Kim[1,2], Jong Wha Lee[1], Youngran Lim[1], Euijin Hwang[1], Yong-Hyeon Yim[1], Sung Woo Heo[1], Hyung Sik Min[1], Myung Chul Lim[1], Kyoung-Seok Lee[1*]

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P-031

Metabolic profiling for discrimination between Angelica gigas and other Angelica species using HPLC-QTOF/MS

Guijae Yoo, Youngse OH, SeonJu Park, Jun Hyung Park, Hee Jae Kwak and Seung Hyun Kim*

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P-032

HPLC-QTOF/MS based chemical profiling of the burs of Castanea creanata Sieb.

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P-033

Characterization and quantification of short chain fatty acids in biological samples using GC-MS

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P-034

Absolute and site-specific quantification of phosphopeptides using multiple reaction monitoring (MRM): It's potential to develop a quantitative platform

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P-035

Accurate measurement of chlorine in human serum based on validated sample preparation method with isotope-dilution mass spectrometry

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P-036

A study on analytical methods for the determination of the arsenic species in rice

Seong Hun Son, Won Bae Lee, and Sang Ho Nam*

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P-037

The experimental autoimmune myocarditis in rat activates the autophagy and apoptosis

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P-038

Probiotics-induced amelioration of obesity related lipid metabolism in high fat diet induced obese rat model

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P-039

Multiplex Proteins and Lipids ToF-SIMS Imaging Assisted with Metal Oxide Nanoparticles

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P-040

Evaluation of a set of calibrants for more accurate measurement of collision cross section (ccs) of polycyclic aromatic hydrocarbon compounds

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

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P-041

Development of lipid extraction method using super absorbent polymers for mass spectrometry

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

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P-042

A sandwich-type HBsAg immunoassay using ICP-MS with metal-doped nanoparticles

Chan-Mi Kim[1], Eun-Ji Kim[2], and H. B. Lim*

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P-043

Optimized chemical separation of Nd, Sm with LN resin in environmental samples for nuclear forensics purpose by using ICP-MS

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

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P-044

Isotopic ratio analysis of individual uranium particle using MC-ICP-MS

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P-045

Identification of binding sites between HuNoV and Concanavalin A using hydrogen/deuterium exchange mass spectrometry

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P-046

Pb-interference correction on uranium isotope analysis using secondary ion mass spectrometry (SIMS)

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P-047

Improvement of uranium bulk analysis in environmental samples with high thorium contents by using MC-ICP-MS

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P-048

Screening of functional metabolites with antiviral activity using systematic metabolomics.

Chang-Wan Lee[1*], Yu Jin Oh[1], Moon-Hee Sung[1], and Do Yup Lee[1]

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P-049

Optimization of copper sample shape in glow discharge mass spectrometer

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P-050

Determination of EDCs in surface water from Asan lake in Korea by season

Sungmin Kim*, Boyoung Kim, Hyojong Park, Jeoungsun Lee, Soyoung Park, Younglim Kho

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P-051

Level of phthalate metabolites in urine from students in Korea

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P-052

Analysis of plant metabolites via TOF-SIMS spectroscopy mode

Ji Yeong Sung[1], Sumin Lee[1,2] and Jong Sung Jin[1,*]

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P-053

Image analysis of grafted hydrophobic functional group onto paper using TOF-SIMS

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P-054

Application of Two-Color Three-Photon Scheme on the Resonance Laser Excitation of Uranium for Sputtered Neutral Mass Spectrometry

Jinkyu Park, Taehee Kim, Chi-Gyu Lee, Sang Ho Lim, Sun-Ho Han

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P-055

Quantification of high purity gallium metal by optimized condition of glow discahrge mass spectrometer using copper pin and flat samples

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4. Medical/Pharmaceutical Science
: PO56 ~ P113

P-056

Comparative proteomics analysis to the anti-obesity effect of taeumjowui-tang in the livers of Type 2 diabetic mice.

Yoon-sun Yi[1]*, Sun Joo Kim[1], Ha Young Lee[1,2], Sung Ho Yun[1], Sang-Yeop Lee[1], Chi-Won Choi[1], Jin Young Kim[1], Gun-Hwa Kim[1], Seung Il Kim[1,2], Edmond Changkyun Park[1,2]

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(grant number: NRF-2014M3A9C4066461)

P-057

Proteome analysis of anti-obesity effect of extracted *platycondon grandifloras* root in the livers of Type 2 diabetic mice

Sung Ho Yun[1]*, Hayoung Lee[1,2]*, Sang-Yeop Lee[1], Gun-Hwa Kim[1,2], Jin Young Kim[1], Seung Il Kim[1,2], Edmond Changkyun Park[1,2]

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P-058

Effects of storage conditions on the protein stability in human growth hormone

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P-059

Comparative proteomic analysis of human follicular fluid during the natural cycle and stimulated cycle undergoing an in vitro fertilization program

You-Rim Lee[1], Ae Eun Seok[1], Jiyeong Lee[2], Sora Mun[1], Arum Park[1], Byung Heun Cha[2], Yunseok Yang[3], Hee-Gyoo Kang[2]

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P-060

Theranostic System for Hypoxia Mediated Drug Delivery by Rhodamine-Derived Azobenzene Mustards

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P-061

Comparative Proteomic Analysis of Human Follicular Fluid : Younger versus Older Women

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P-062

A Preliminary Study for determination of neurosteroids by liquid chromatography-electrospray tandem mass spectrometry

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P-063

Characterization of C_{18} ceramides with metal ions using paper spray ionization mass spectrometry

Shavkatjon Azizov[1], Jae-Min Lim[1], Yong-Ill Lee[1*]

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P-064

Systems-wide Analysis of Protein Expression in Formalin-fixed Paraffin-embedded Rare histological Types of Breast

Hyeyoon Kim[1,&], Hyeyun Kim[1,&], Hyunsuk Shin[1], Ki Soon Dan[1], Han Suk Ryu[2,*], And Dohyun Han[1,*]

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P-065

Method validation and Application of 164 Toxicological Drugs in Whole Blood and Urine using LLE and UPLC-ESI-tandem MS (QQQ and Q-TOF)

Choong Sik Lee* and Phil Sang Ahn

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P-066

Establishment of measurement standards for flavor compounds in Kimchi

Jeesoo Han, Hong Hee Lee, Byungjoo Kim*, Song-Yee Baek, Sunyoung Lee

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P-067

Targeted quantitation of proteins for discriminating obese from normal-weight adolescents by liquid chromatography-mass spectrometry

Hyunsuk Shin[1], Kisoon Dan[1], Sang Hoon Song[2], and Dohyun Han[1]

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P-068

Application of extracted common ion chromatogram and neutral loss scan for rapid screening of sulfonamide in supplements by UHPLC-Q/TOF-MS

Nam-Yong Ki, Na-Hyun Park, Wonwoong Lee, Jisu Hur, Keon-Hee Ko, Youna Kim, Jongki Hong*

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P-069

Simultaneous determination of imperatorin and its metabolite xanthotoxol by LC–MS/MS and its application to pharmacokinetic studies

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P-070

Screening and confirmation of 64 PDE-5 inhibitor counterfeit drugs in dietary supplements based on extracted common ion chromatograms using gas chromatography tandem mass spectrometry

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P-071

Comparability and Similarity Assessment of Primary Structure for Antibody Biologics

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P-072

Clinical application of multi hormones in human serum by liquid tandem mass spectrometry

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P-073

Simultaneous determination of mixture of biopharmaceuticals by a liquid chromatography-quadrupole time-of-flight mass spectrometric method in rat plasma following cassette-dosing

Min-Ho Park*, Jin-Ju Byeon, Seok-Ho Shin, Nahye Kim, Yuri Park, Byeong ill Lee, Jangmi Choi, Yeonjae Kang and Young G. Shin

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P-074

Development of a parylene-matrix chip for small molecule analysis with MALDI-TOF MS

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P-075

Rapid and sensitive carbapenemase assay using LDI-MS based on a parylene-matrix chip

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P-076

Newborn screening by MALDI-ToF mass spectrometry using parylene-matrix chip

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P-077

Detection of small molecules and amino acid using MALDI-ToF mass spectrometry with TiO_2 nanowire chips

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P-078

Simultaneous quantification of sterols and fatty acids in human saliva samples using high-temperature gas chromatography-tandem mass spectrometry

Ju-Yeon Moon, Tae Yeon Kong, Hyun-Jun Jang, Ju-Hyun Kim, Won-Gu Choi, Hye Suk Lee

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P-079

Assessment of cerebrospinal fluid concentration or plasma free concentration as a surrogate measurement for brain free concentration

Jangmi Choi[1], Nahye Kim[1], Yeonjae Kang[1], Jin-Ju Byeon[1], Min-Ho Park[1], Seok-Ho Shin[1], Byeong ill Lee[1], Yuri Park[1], Young G. Shin*[,1]

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P-080

Quantification of a novel aldehyde dehydrogenase inhibitor in rat using liquid chromatography-quadrupole time-of-flight mass spectrometric method.

Nahye Kim[1], Yuri Park[1], Byeong ill Lee[1], Min-Ho Park[1], Seok-Ho Shin[1], Jin-Ju Byeon[1], Jangmi Choi[1], Yeonjae Kang[1], Inkyu Hwang[1], Young G. Shin*[,1]

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P-081

Specific and sensitive Liquid Chromatography – Electro Spray Ionization – Triple Time of Flight / Mass Spectrometry assay for the quantification and application of Fabry disease biomarker – Globotriaosylceramide (GB3)

Seok-Ho Shin, Min-Ho Park, Jin-Ju Byeon, Yuri Park, Byeong ill Lee, Jangmi Choi, Nahye Kim, Yeonjae Kang and Young G. Shin*

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P-082

Qualification and application of a liquid chromatography-quadrupole time-of-flight mass spectrometric method for the determination of adalimumab in rat plasma

Yuri Park[1], Nahye Kim[1], Jangmi Choi[1], Minho Park[1], Byung ill Lee[1], Seokho Shin[1], Jinju Byeon[1], Yeonjae Kang[1] and Young G. Shin[1]

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P-083

A single liquid chromatography-quadrupole time-of-flight mass spectrometric method platform for the quantification of antibody-drug conjugates

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P-084

Comparison of tricin concentration in different parts of *Phragmites communis*

Dae Wook Kim, Seung-Young Lee, Buyng Su Hwang, Sang-Chul Jeong*

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P-085

Novel metabolomic markers in acute liver transplantation rejection

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P-086

Quantification and application of a liquid chromatography–tandem mass spectrometric method for the determination of WKYMVm peptide in rat using solid phase extraction

Byeong ill Lee[1]*, Min-Ho Park[1], Soon chul Heo[2], Yuri Park[1], Seok ho Shin[1], Jin ju Byeon[1], Jangmi Choi[1], Nahye Kim[1], Yeonjae Kang[1], Jae ho Kim[2], Young G. Shin[1]

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P-087

Simultaneous quantification of the four coumarins including one active metabolite in humans by UHPLC-MS/MS: Application to pharmacokinetics

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Development and validation of a quantification method for free amino acids in human plasma to develop the certified reference material using liquid chromatography-tandem mass spectrometry

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Quantitative proteomics of a human neuronal cell culture model of Alzheimer's disease

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Global N-glycoproteome analysis in the course of human neural stem cell differentiation

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Feasiblity of desorption electrospray inoization (desi)-q-tof system as a new imaging system for evaluation of the distribution of indocyanine green in sentinel lymph nodes

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High-sensitivity, high-throughput quantitation of catecholamines in plasma by automatable derivatization and SPE coupled to LC-MS/MS for clinical research

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Simultaneous determination and identification in individual herbs and Bojungikgi-tang(mixture) by UHPLC/Q-Orbitrap & MS/MS for NDIN submission

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Lipidomics Analysis of Serum in Traumatic Injury Patients with Blood Stasis

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Genetically Modified Resveratrol-enriched Rice Attenuates UVB-ROS Induced Skin Aging via Downregulation of Inflammatory, Apoptosis and MMP1 Mediated Aging Cascades

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Quantitative analysis of ethanol in micro volume blood samples by GC-MS headspace detection

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Sensitive UPLC Method with Tandem Mass Detection for Analysis of Genotoxic Impurities of Imatinib Mesylate Drug

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Lipid quantification-based cancer diagnosis by using nanostructure-assisted laser desorption ionization mass spectrometry

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Label-free quantitative strategy for non-human sialic acid using MRM-MS

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I knew you were trouble: expanding LC methods to include difficult GC compounds using a novel ionization technique

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MALDI-TOF MS Characterization of Poly(ethylene glycol)-conjugated Octapeptides Fractionated Drop-by-drop from Reversed-phase HPLC

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Data independent top-down characterization of proteins for biotherapeutic applications

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Optimization of SONAR elevated energy ramps applied to different molecular classes

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Liquid chromatography-tandem mass spectrometry (LC-MS/MS) based metabolic profiling of steroids and prostaglandins in pattern baldness

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Investigation of exercise effects using non-targeted metabolomics and targeted polyamine profiling by liquid chromatography-mass spectrometry (LC-MS) in athlete's urine

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Application of LC-MS/MS method for simultaneous determination of tramadol and its metabolites in human plasma

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Automated robotic platform to enrich native glycans using liquid handling system

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Specific ion chromatograms for rapid screening of steroids in dietary supplements by GC-MS/MS combined with selective derivatization

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TMT-Based quantitative proteomics in adipose and liver tissue of high-fat diet induced mice

Ki Na Yun[1,3], Eun Sun Ji[1], Gun Wook Park[1], Sung Ho Yun[2], Sang-Yeop Lee[2], Seung Il Kim[2], Ju Yeon Lee[1], Jong Shin Yoo[1], Han Bin Oh[3], Jin Young Kim[1]

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(grant number: NRF-2014M3A9C4066461)

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Method validation for the determination of urea in serum by IDMS and proficiency testings

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Quantitative profiling of adrenal and hybrid steroids using a polarity switching LC-MS/MS

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Metabolic signatures of polyamines and cholesterols using GC-triple quadrupole-mass spectrometry

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Determination of dermal absorption rate of propylidene phthalide, a cosmetic ingredient, using LC/MS/MS

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A Gas-phase Host-guest system for Identifying Diverse Types of Monosaccharide Derivative Isomers

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Non-targeted analysis of soybean recombinant inbred lines by LC-MS/MS

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Development simultaneous analytical method for determination of volatile alcohols in drinking water using TMS derivatization

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Optimization of sample preparation and analytical condition for simultaneous multi-residue analysis of phenols, parabens, phthalates, PAHs, VOCs, cotinine by LC-MS

Minho Yang[1], Eun Sook Jeong[2], Hojun Jung[1], Yong Min Cho[1], Eunju Cha[2], Sang Moon Han[2,3], Seunghwa Lee[2,4], Sangwon Cha[5], Sang Beom Han[6], Jaeick Lee[2], Hosub Im[1,*]

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Autosampler Based Online GC-MS System: SPME and Purge-Trap technique for Online Water Quality Monitoring

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In-depth characterization and comparative profiling of ethanol-extracts of propolis by ultra-high resolution FT-ICR mass spectrometry

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Determination of N-nitrosamines in Kimchi by HR-ESI-UPLC-Q-Orbitrap-MS

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Fat-Soluble Vitamin Analysis by online SFE-SFC-MS/MS

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Characterization of weathered oil by paper spray ionization and estimation of the oxidation degree of spilled oils depending on the chemical class distribution

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Screening metabolites responsible for distinct soybean types and bioactivities evaluated by correlation analysis

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Profiling for the volatile organic compounds in fermented coffees using HS-SPME and Pyrolysis-GC/MS

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Residual behaviour of insecticide chlorfenapyr on strawberry using QuEChERS with gas chromatography mass spectrometry

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Chemical composition of the essential oils from four kinds *Chrysanthemum indicum*

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Evaluation of Ultra-high Resolution Mass Spectrometry as a Tool for Stable Carbon Isotope Ratio Analysis of Oils at the Molecular Level

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Determination of perfluorooctanoic acid (PFOA) extractable from the frying pan in fatty acids by LC/MS/MS

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Comparative analysis of functional components in Asian milk; Korean, Chinese, and Vietnamese

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LiveID™: A new software approach for statistical modeling and real-time recognition for use in direct analysis work flows

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Serum biomarker and treatment mechanism of Allium Hookeri on hyperlipidemia using UPLC/ESI-Q-TOF mass spectrometry

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

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Simultaneous determination of preservatives and sweeteners in kimchi using LC-ESI-MS/MS

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Characterization of polysaccharides extracted from red ginseng by MALDI-TOF MS

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A research of metabolic perturbations of domestic soybeans for characterizing and discriminating regional specificity

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Development of Sensitive and Selective Methods for Identification of Marine Toxins by Liquid Chromatography Tandem Mass Spectrometry

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Which Chemicals are Generated with Higher Temperature Coffee Roasting?:Molecular Level Analysis of Coffee Extracts by Using Ultrahigh Resolution Mass Spectrometry

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Molecular characterization of soil organic matter in the foreland of Midtre Lovénbreen glacier in Svalbard using ultra-high resolution FT-ICR mass spectrometry

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Determination of fenpyroximate from honey by LC-MS/MS

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Identification of prostate cancer specific signature in cell lines based on proteomic analysis

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Improvement of rheumatoid arthritis (RA) pre-screening accuracy through liquid chromatography tandem-mass spectrometry

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Biomarker Discovery of Rheumatoid Factor-Correlated Proteins for Rheumatoid Arthritis

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Effects of acetonitrile amounts on bovine serum albumin and myoglobin tryptic digestion in gentle mixing or microwave

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Derivatization of myoglobin after microwave-assisted acid hydrolysis

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Optimized condition in MALDI-TOF MS analysis of N-glycans

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Comparison of Desorption Enhancement Methods in the Low Temperature Plasma Ionization Mass Spectrometry for Detecting Fatty Acids in Drosophila

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Lipids profiling of *Drosophila melanogaster* heads using electrospray ionization mass spectrometry (ESI-MS)

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Optimization of paper spray ionization for sensitive protein analysis

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Investigation of various liquid chromatography mass spectrometry (LC/MS) methods for comprehensive ganglioside profiling

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The analysis of discoloration of thermally conductive tape

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A Study of Mechanism for Impurity Generation in Liquid Crystal

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Glycomics-based Forensic Platform for the Identification of Human Saliva

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Fragmented monoclonal antibody drug peptide mapping by IdeS proteolytic enzyme

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Competitive Homo- and Hetero- Self-assembly of Amyloid-β 1-42 and 1-40 in the Early Stage of Fibrillation

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In vivo Study of Sulfur Mustard Exposure by LC-MS/MS

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Human serum albumin and amyloid-βcomplex characterized by mass spectrometry and ion mobility spectrometry

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Investigating alpha-synuclein aggregation mediated by calcium ions at a molecular level

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Estimation of Elemental Compositions for Additives in Polymers Using Newly Developed EI/CI Ion Source without Venting MS

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Validation of triple quadrupole GC-MS/MS for the analysis of dioxins (PCDD/Fs) in soil

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Analysis of tocopherol in spinach using isotope dilution liquid chromatography mass spectrometry

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Profiling of fragmentation pathway for thiamethoxam

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Analysis of polycyclic aromatic hydrocarbons in olive oil using isotope dilution-gas chromatography mass spectrometry

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The Comparison of Volatile Organic Compounds Present in Human's Foot Odor Using SPME-GC/MS

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Establishing an analysis method of anticancer drugs to study cellular uptake and efficiency of combination therapy

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Development of relative quantification method for lipidome by using ^2H_2O partial metabolic labeling

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The characterization of volatile organic compounds present in the headspace of decomposing animal and human remains

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Direct identification of polymer additives in manufacturing plastics without sample preparation using pyrolysis gas chromatography mass spectrometry

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Mass analysis of neuropeptides in salty environment using hydrophilic ring-shaped anchors

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Trifluoroacetylation of ethanol amines using MBTFA for GC-MS analysis

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Structure elucidation of alkoxyamine (Flamestab NOR 116) by MALDI-TOF mass spectrometry

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LC-MS/MS analysis of fucosylated N-glycoproteins in human plasma of liver cancer

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Development of liquid chromatography mass spectrometry based on Boc derivatization for analysis of amino compounds

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Comprehensive lipid profiling of tissue in breast cancer mouse reveals novel biomarkers using MALDI imaging and UPLC/MS

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Analysis of albumin adduct in rat plasma exposed to nerve agent GB using LC-MS/MS

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Fabrication of carbon nanotube membranes for single-molecule mass spectrometry

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Development of a structural characterization method of lignin oligomers using pseudo-LC-MS3 analysis

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Screening of Skin Lightening Products for the Corticosteroid Clobetasol Propionate using Direct Analysis in Real Time (DART) and Mass Detection

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Quantitative determination of urinary hydrophilic metabolites for non-targeted metabolomic approach by gas chromatography-mass spectrometry

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Simultaneous monitoring of environmental chemicals by gas chromatography-mass spectrometry in drinking water

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LC/MS based quantitative strategy to determine o-glycan expression in galnt13 ko mouse brain

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Environmental behavior of water and sediment of benzophenone-based ultraviolet screening agents

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Chemical derivatization strategies on analysis of 3-keto-4-ene adrenal steroids using aryl hydrazides and LC-MS

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Comparative solid-phase extraction methods in GC-MS-based steroidal cytochrome P450 assay

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P-184 **Effect of ethanol on Freeze Vacuum Drying sample preparation in MALDI-MS** Jangsu Lee, Jihyun Paek, Yeoseon Kim, Dabin Lee, Sooyeon Chae, Jeongkwon Kim* *Department of Chemistry, Chungnam National University, Daejeon 34134, Republic of Korea* *E-mail:marufirst@naver.com*	