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Others

The Korean Federation of Science and Technology Societies (KOFST)
Gyeongnam Convention & Visitors Bureau (GNCVB)

KSMS

2018년 한국질량분석학회 여름정기학술대회 및 총회
일시: 2018년 8월 22일(수) ~ 24일(금)
장소: 창원, 창원컨벤션센터(CECO) 3F

목차

"이 발표논문집은 정부재원(과학기술진흥기금 및 복권기금)으로 한국과학기술단체총연합회의 지원을 받아 발간되었음."

"This work was supported by the Korean Federation of Science and Technology Societies(KOFST) Grant funded by the Korean Government."

조직위원회

<회장>

임용현 (한국표준과학연구원)

<조직위원>

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김민식 (경희대학교)
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김성환 (경북대학교)
김영환 (한국기초과학지원연구원)
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김정권 (충남대학교)
김태영 (광주과학기술원)
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이재익 (한국과학기술연구원)
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최만호 (한국과학기술연구원)
최용석 (단국대학교)
한상윤 (가천대학교)

안내 사항

2018년 한국질량분석학회 여름정기학술대회 및 총회에 참가하신 회원 여러분 환영합니다

■ **현장등록**

8월22일(수), 12:00 ~ 23(목), 17:00

■ **Plenary Sessions**

Plenary Lecture: 23일(목), 10:00

■ **Special Sessions**

Special Lecture: 24일(금), 11:10

■ **Short Course**

22일(수), 13:00 ~ 17:10
이름표를 꼭 패용해 주시기 바랍니다.

1. Introduction to MS
2. Techniques in LC-MS & GC-MS
3. MS-based Applications

■ **Symposium Sessions**

23일(목)
SYM1 (12:50 ~ 14:50, 컨벤션홀III)
SYM2 (12:50 ~ 14:50, 회의실301)
SYM3 (12:50 ~ 14:50, 회의실302)
SYM4 (15:00 ~ 17:00, 컨벤션홀III)
SYM5 (15:00 ~ 17:00, 회의실301)
SYM6 (15:00 ~ 17:00, 회의실302)

24일(금)
SYM7 (08:50 ~ 10:50, 컨벤션홀III)
SYM8 (08:50 ~ 10:50, 컨벤션홀II)

■ **기기전시**

22일(수) ~ 24(금),
창원, 창원컨벤션센터 3F 로비 부스전시장소

■ **포스터게시 및 철거**

게시: 23일(목), 10:00 까지
철거: 23일(목), 19:00 이후

■ **Poster Session**

포스터 발표자는 23일(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**

23일(목), 19:00 ~ 20:30

창원, 창원컨벤션센터(CECO) 3F / **컨벤션홀I+II**

■ **공지사항**

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

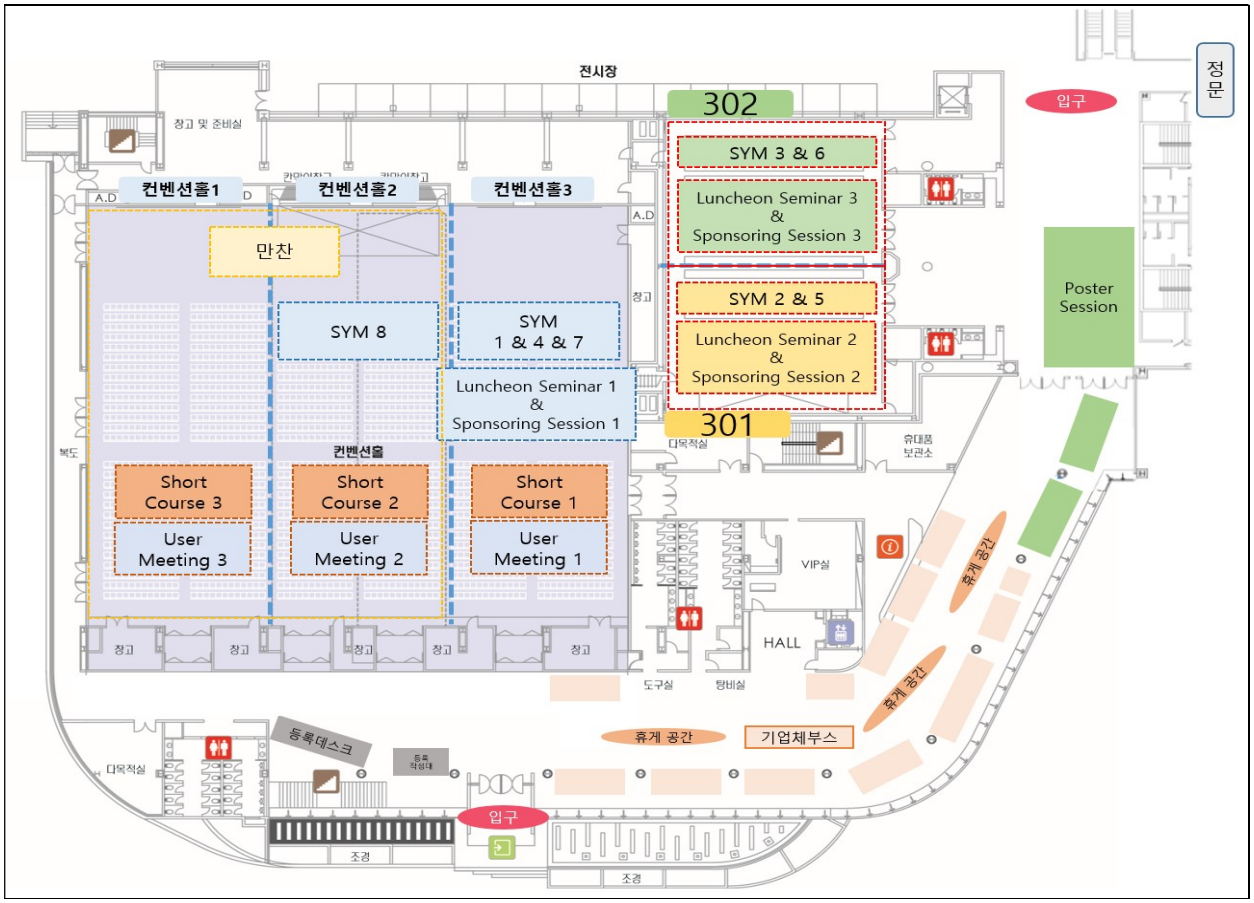
》 행사기간내 이름표를 꼭 패용해 주시기 바랍니다.

》 창원컨벤션센터 모든 건물은 금연구역입니다.

》 세션 중에는 핸드폰을 진동 혹은 무음으로 해 주십시오.

》 세션 중에는 발표가 방해되지 않도록 사진촬영은 자제하여 주십시오

행사장 안내



▶행사장 안내

Convention Hall Ⅲ	Short Course 1
Convention Hall Ⅱ	Short Course 2
Convention Hall Ⅰ	Short Course 2
Convention Hall Ⅲ	Symposium 1, 4, 7
Conference Room 301	Symposium 2, 5
Conference Room 302	Symposium 3, 6
Convention Hall Ⅱ	Symposium 8

Convention Hall Ⅲ	Brief Oral Presentation-1
Conference Room 301	Brief Oral Presentation-1
Convention Hall Ⅲ	Plenary Lecture
Convention Hall Ⅲ	Special Lecture

Convention Hall Ⅲ	User Meeting-1
Convention Hall Ⅱ	User Meeting-2
Convention Hall Ⅰ	User Meeting-3
Convention Hall Ⅲ	Luncheon Seminar I Sponsoring Session I
Conference Room 301	Luncheon Seminar II Sponsoring Session II
Conference Room 302	Luncheon Seminar III Sponsoring Session III

3F Lobby	Poster Session

행사장 안내

▶전시부스 안내

1
Agilent Technologies Korea

2
Thermo Fisher Scientific Korea

3
SCIEX KOREA

4
Dong-il SHIMADZU Corp.

5
Waters Korea

6
Bruker Korea Co., Ltd./SCINCO Co., LTD./
Euro Science Co., Ltd

15
Merck Korea

16
Goojung Chromatech Inc.

14
ASTA Inc.

7
Euro Science Co., Ltd

8
ACT Technology

9
APM Engineering Co., Ltd.

10
PerkinElmer

11
JEOL KOREA Ltd.

12
Scion Instruments Korea Co., Ltd.

13
LECO Korea Co., Ltd

프로그램

August 22 (Wednesday)

TIME	P R O G R A M		
12:00 ~	Registration		
SHORT COURSE (Organizer: 한상윤(가천대학교) & 박종호(한국원자력연구원))			
	Introduction to MS (Room: 컨벤션홀Ⅲ)	**Techniques in LC-MS & GC-MS** (Room: 컨벤션홀Ⅱ)	**MS-based Applications** (Room: 컨벤션홀Ⅰ)
13:00 ~ 14:15 (75min)	Introduction to MS 김정권(충남대학교)	Practical Aspects of Chromatography-MS 이재익(한국과학기술연구원)	MS-based Metabolomics 이도엽(국민대학교)
Coffee Break			
14:30 ~ 15:45 (75min)	Ionization Methods in MS 김성환(경북대학교)	Practical Separation Techniques 정문철(Waters Corp.)	MS-based Proteomics 김민식(경희대학교)
Coffee Break			
16:00 ~ 17:15 (75min)	Mass Analyzers in MS 박종호(한국원자력연구원)	Tandem MS Techniques 김태영(광주과학기술원)	Interpretation of MS spectra 오한빈(서강대학교)
Coffee Break			
17:20 ~ 18:40 (80min)	**User Meeting-1** (Sponsored by Agilent Technologies Korea) (Room: 컨벤션홀Ⅲ)	**User Meeting-2** (Sponsored by Thermo Fisher Scientific Korea) (Room: 컨벤션홀Ⅱ)	**User Meeting-3** (Sponsored by Waters Korea) (Room: 컨벤션홀Ⅰ)

August 23 (Thursday)

TIME	PROGRAM		
08:50 ~ 09:50 (60min)	**Brief Oral Presentation of Selected Posters-1** (Organizer & Chair: 장경순(한국기초과학지원연구원) & 김민식(경희대학교)) (Room: 컨벤션홀Ⅲ)	**Brief Oral Presentation of Selected Posters-2** (Organizer & Chair: 장경순(한국기초과학지원연구원) & 김민식(경희대학교)) (Room: 대회의실 301)	
10:00 ~ 10:50 (50min)	**Plenary Lecture** Prof. Kenzo Hiraoka (Clean Energy Research Center, University of Yamanashi) (Organizer & Chair: 임용현(KSMS 회장)) (Room: 컨벤션홀Ⅲ)		
SYMPOSIUM			
10:50 ~ 11:50 (60min)	**POSTER SESSION** (Organizer & Chair: 장경순(한국기초과학지원연구원) & 김민식(경희대학교)) (Poster Session - 3F 로비)		
11:50 ~ 12:40 (50min)	**Luncheon Seminar I** (Sponsored by Bruker Korea Co., Ltd) (Room: 컨벤션홀Ⅲ)	**Luncheon Seminar II** (Sponsored by Agilent Technologies Korea) (Room: 대회의실 301)	**Luncheon Seminar Ⅲ** (Sponsored by Waters Korea) (Room: 대회의실 302)
SYMPOSIUM			
12:55 ~ 14:55 (120min)	**SYM1: <Special Session Ⅰ>** Mass Spectrometry in Korean Society for Laboratory Medicine (Organizer & Chair: 김재석(한림대학교) & 최만호(한국과학기술연구원)) (Room: 컨벤션홀Ⅲ)	**SYM2: MS Fundamentals & Elemental Analysis** Keynote Speaker: Ph.D. Fumitaka Esaka (Research Group for Safeguards Analytical Chemistry, Japan Atomic Energy Agency (JAEA)) (Organizer & Chair: 박종호(한국원자력연구원) & 황희진(극지연구소)) (Room: 대회의실 301)	**SYM3: Food & Agriculture** (Organizer & Chair: 이도엽(국민대학교) & 이혜영(동의대학교)) (Room: 대회의실 302)
SYMPOSIUM			
15:10 ~ 17:10 (120min)	**SYM4: Pharmaceutical MS** Keynote Speaker: Prof. Troy D. Wood (Department of Chemistry, State University of New York at Buffalo) (Organizer & Chair: 최용석(단국대학교) & 신소영(원광대학교)) (Room: 컨벤션홀Ⅲ)	**SYM5: MS for Metabolomics** (Organizer & Chair: 김태영(광주과학기술원) & 안현주(충남대학교 분석과학기술대학원)) (Room: 대회의실 301)	**SYM6: <Special SessionⅡ>** 환경질량분석 특별세션: 미세먼지 문제 해결을 위한 질량분석학의 응용 Keynote Speaker: Ph.D. 배귀남 (한국과학기술연구원) (Organizer & Chair: 김성환(경북대학교) & 배귀남(한국과학기술연구원)) (Room: 대회의실 302)

17:20 ~ 17:50 (30min)	**'2018 KSMS General Meeting'** (Room: 대회의실 301)		
18:00 ~ 18:50 (50min)	**Sponsoring Session I** (Sponsored by Thermo Fisher Scientific Korea) (Room: 컨벤션홀Ⅲ)	**Sponsoring Session II** (Sponsored by Dong-il SHIMADZU Corp.) (Room: 대회의실 301)	**Sponsoring Session Ⅲ** (Sponsored by SCIEX Korea) (Room: 대회의실 302)
19:00 ~ 20:30 (90min)	**Conference Banquet** (Organizer: 강덕진 (KSMS 총무이사)) (Room: 컨벤션홀Ⅰ+Ⅱ)		

August 24 (Friday)

TIME	P R O G R A M	
08:50 ~ 10:50 (120min)	**SYM7: New Technologies for MS** Keynote Speaker: Prof. Jonathan Amster (Department of Chemistry, University of Georgia) (Organizer & Chair: 오한빈(서강대학교) & 정가영(성균관대학교)) (Room: 컨벤션홀Ⅲ)	**SYM8: MS for Protein Analysis** Guest Speaker: SungKyu Robin Park (박성규) (The Scripps Research Institute Integrated Proteomics Applications, Inc) (Organizer & Chair: 조 건(한국기초과학지원연구원) & 임재민(창원대학교)) (Room: 컨벤션홀Ⅱ)
11:10 ~ 11:50 (40min)	**Special Lecture** 송규석(한국원자력연구원) (Organizer: 임용현(KSMS 회장)) (Room: 컨벤션홀Ⅲ)	
11:50 ~ 12:30 (40min)	**Poster Award & Closing Remarks** (Room: 컨벤션홀Ⅲ)	

세부프로그램

Wednesday Afternoon, August 22

SHORT COURSE
13:00 - 17:15

Introduction to MS (Convention Hall Ⅲ)

13:00 - 14:15	**Introduction to MS** 김정권 (충남대학교)
14:30 - 15:45	**Ionization Methods in MS** 김성환 (경북대학교)
16:00 - 17:15	**Mass Analyzers in MS** 박종호 (한국원자력연구원)

Techniques in LC-MS & GC-MS (Convention Hall Ⅱ)

13:00 - 14:15	**Practical Aspects of Chromatography-MS** 이재익 (한국과학기술연구원)
14:30 - 15:45	**Practical Separation Techniques** 정문철 (Waters Corp.)
16:00 - 17:15	**Tandem MS Techniques** 김태영 (광주과학기술원)

MS-based Applications (Convention Hall Ⅰ)

13:00 - 14:15	**MS-based Metabolomics** 이도엽 (국민대학교)
14:30 - 15:45	**MS-based Proteomics** 김민식 (경희대학교)
16:00 - 17:15	**Interpretation of MS Spectra** 오한빈 (서강대학교)

Thursday Morning / Afternoon, August 23

BRIEF ORAL PRESENTATION OF SELECTED POSTERS - 1

8:50 – 09:50

Session 1 - Convention Hall Ⅲ

Organizer & Chair: 장경순 (한국기초과학지원연구원)

08:50–08:54 Energy-resolved collision-induced dissociation study of Na+-bound G-quartets with mixed ligands, [Na(Guanine)n(9-methylguanine)m]+
최윤경 (가천대학교)

08:54–08:58 Proteomic analysis of cervicovaginal fluid for early detection of preterm birth by 2D-nLC-ESI-MS/MS
김권성 (서강대학교 / 한국표준과학연구원)

08:58–09:02 Profiles of oxidized phospholipids in exosome from oxidatively stressed cells by flow field-flow fractionation and nUHPLC-ESI-MS/MS
양준선 (연세대학교)

09:02–09:06 Quantitative proteomics of 2D-/3D-cultured adipocyte cells and its co-cultured with macrophages using a nanoLC-ESI-MS/MS
이선영 (경희대학교 / 한국표준과학연구원)

09:06–09:10 Spatial distribution of siloxanes in coastal sediment and identification of procedural contamination sources in GC/MS analysis
이단비 (울산과학기술원)

09:10–09:14 Validation and application of analytical tools for stable carbon isotope analysis of crude oils in molecular level using ultra-high resolution mass spectrometry
손승우 (경북대학교)

09:14–09:18 Parallel reaction monitoring of fucosylated glycopeptides of alpha-fetoprotein in human serum for early hepatocellular carcinoma by LC-MS/MS with immunoprecipitation
김광회 (한국기초과학지원연구원)

09:18–09:22 Detection of Neu5Gc in human serum via MRM-MS
고재경 (충남대학교 분석과학기술대학원)

09:22–09:26 Newborn screening by MALDI-ToF mass spectrometry using parylene-matrix chip
노주윤 (연세대학교)

09:26–09:30 Determination of the geographical origins of various propolis samples via UPLC combined with high-resolution FT-ICR mass spectrometry
김초현 (한국기초과학지원연구원)

09:30–09:34 Analysis of Polycyclic Aromatic Hydrocarbons in Olive Oil using Isotope Dilution-Gas Chromatography/Mass Spectrometry
주현정 (한국표준과학연구원)

09:34–09:38 Simultaneous determination of five urushiol analogues in lacquer tree extract by using LC-MRM and QuEChERS with EDTA
이효천 (단국대학교)

09:38–09:42 Mass spectrometric study on the source of error in quantification of fatty acids
박혜진 (광주과학기술원)

09:42–09:46 Study on analysis method of polyol in Polyurethane foam by Matrix-assisted laser desorption/ionization-Time of flight (MALDI-TOF)
유영석 (한국기초과학지원연구원)

Thursday Morning / Afternoon, August 23

BRIEF ORAL PRESENTATION OF SELECTED POSTERS - 2

8:50 – 09:50

Session 2 - Conference Room 301

Organizer & Chair: 김민식 (경희대학교)

08:50–08:54 Anomaly in collision-induced dissociation of proton-bound hoogsteen base pairs of cytosine and guanine by proton transfer
박정주 (가천대학교)

08:54–08:58 Effect of aging on lipid alteration in serum, kidney, and heart from mice by nUHPLC-ESI-MS/MS
엄정용 (연세대학교)

08:58–09:02 Metabolic signitures of adrenal steroids in serum and saliva measured by polarity switching LC-MS
이채린 (한국과학기술연구원)

09:02–09:06 Cross-validation of sulfur-based and amino acid-based quantification methods for the development of insulin reference material
김휘진 (과학기술연합대학원대학교/한국표준과학연구원)

09:06–09:10 Computer language (scripting) for automated profiling in airborne particulate matter with GC×GC-TOFMS
이호영 (울산과학기술원)

09:10–09:14 Comparison of organic mixtures from particulate matters collected in Korea and China by using GCxGC/high resolution mass spectrometry
박문희 (한국기초과학지원연구원)

09:14–09:18 Characterization of site-specific O-glycopeptides in fibroin heavy chain from silkworm cocoon using high resolution LC-MS/MS
이현경 (한국기초과학지원연구원)

09:18–09:22 Synergistic antibacterial activity of phenolic compound-antibiotic combination and their quantitative determination by LC-QTOF-MS
강정우 (농림축산검역본부)

09:22–09:26 Global absolute quantitation of human whole saliva proteins using nLC-Q-IMS-TOF with MS^E
김동윤 (단국대학교)

09:26–09:30 Validation of tocopherol analysis in leafy vegetables using Standard addition-isotope dilution liquid chromatography mass spectrometry method (SA-IDMS-LC/MS)
성민경 (한국표준과학연구원)

09:30–09:34 Primary and secondary metabolic profiles according to regional characteristics of Glycine max in Korea
이은미 (국민대학교)

09:34–09:38 MALDI-MS analysis of small molecules using N-doped carbon dots as matrix
이다빈 (충남대학교)

09:38–09:42 Production of high purity gallium metal for compound semiconductor and trace elements quantification
양재열 (충남대학교)

Thursday Morning / Afternoon, August 23

PLENARY LECTURE

Convention Hall Ⅲ

Organizer & Chair: 회장 임용현 (한국표준과학연구원)

10:00 – 10:50

10:00-10:50 **Probe Electrospray Ionization (PESI)**

Prof. Kenzo Hiraoka (Clean Energy Research Center, University of Yamanashi)

POSTER SESSION

3F 로비홀

Organizer & Chair: 장경순 (한국기초과학지원연구원) & 김민식 (경희대학교)

10:50 – 11:50

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

KEYNOTE SPEAKER (SYM-2, SYM-4, SYM-5, SYM-7)

GUEST SPEAKER (SYM-8)

Thursday Afternoon, August 23

SYM-2: MS Fundamentals & Elemental Analysis (Conference Room 301)

12:55-13:25 **Isotope Ratio Analysis of Individual Particles containing Uranium and/or Plutonium with Inorganic Mass Spectrometry**

Ph.D. Fumitaka Esaka

(Research Group for Safeguards Analytical Chemistry, Japan Atomic Energy Agency (JAEA))

SYM-4: Pharmaceutical MS (Convention Hall Ⅲ)

15:10-15:40 **The Hunt for Autism Biomarkers**

Prof. Troy D. Wood (Department of Chemistry, State University of New York at Buffalo)

SYM-5: <Special Session Ⅱ>

환경질량분석 특별세션: 미세먼지 문제 해결을 위한 질량분석학의 응용 (Conference Room 302)

15:10-15:40 **미세먼지 국가전략프로젝트 사업단 연구현황**

Ph.D. 배귀남 (한국과학기술연구원)

Thursday Morning, August 24

SYM-7: New Technologies for MS (Convention Hall Ⅲ)

10:10-10:40 **Expanding the Repertoire of Ion Activation Methods for Glycosaminoglycans**

Prof. Jonathan Amster (Department of Chemistry, University of Georgia)

SYM-8: MS for Protein Analysis (Convention Hall Ⅱ)

08:50-09:20 **Overview of Proteomic Data Analysis**

SungKyu Robin Park (박성규)

(The Scripps Research Institute Integrated Proteomics Applications, Inc)

SYMPOSIUM 1 & 2 & 3

12:55 – 14:55

SYM-1: <Special Session Ⅰ> (Convention Hall Ⅲ)

Mass Spectrometry in Korean Society for Laboratory Medicine

Organizer & Chair: 김재석 (한림대학교) & 최만호 (한국과학기술연구원)

12:55-13:15	**Introduction of clinical laboratory testing using mass spectrometry** 윤여민 (건국대학교병원)
13:15-13:35	**Drug Abuse Screening Test Using LC-MS/MS** 이용화 (순천향대학교 부천병원)
13:35-13:55	**Newborn screening test for lysosomal storage disease using MS/MS** 이경훈 (분당서울대학교병원)
13:55-14:15	**Screening for Steroid Profiling in Dried Blood Spots by Liquid Chromatography-Tandem Mass Spectrometry** 박형두 (성균관의대 삼성서울병원)
14:15-14:35	**Microbial Identification using Mass Spectrometry** 신정환 (인제대학교 부산백병원)

SYM-2: MS Fundamentals & Elemental Analysis (Conference Room 301)

Organizer & Chair: 박종호 (한국원자력연구원) & 황희진 (극지연구소)

12:55-13:25	**Isotope Ratio Analysis of Individual Particles containing Uranium and/or Plutonium with Inorganic Mass Spectrometry** Ph.D. Fumitaka Esaka (Research Group for Safeguards Analytical Chemistry, Japan Atomic Energy Agency (JAEA)) : Keynote Speaker
13:25-13:45	**Experimental Evaluation of the Detection Methods of TIMS for Isotopic Analysis of Ultra-trace Level Uranium** 박종호 (한국원자력연구원)
13:45-14:05	**The analysis of halogen elements in snow from Antarctica** 강정호 (극지연구소)
14:05-14:25	**금속 안정동위원소의 해양환경 연구 적용** 나공태 (한국해양과학기술원)
14:25-14:45	**Proton Transfer Reactions in Collision-induced Dissociation of Proton-bound Nucleic Acid Bases** 한상윤 (가천대학교)

SYM-3: Food & Agriculture (Conference Room 302)

Organizer & Chair: 이도엽 (국민대학교) & 이혜영 (동의대학교)

12:55-13:15	**Next generation proteomics for agriculture and food science** 김선태 (부산대학교)
13:15-13:35	**Comprehensive Anlaysis of Glycolipids in Milks** 김재한 (충남대학교)
13:35-13:55	**Urinary change of neurochemicals and endogenous metabolites with tryptophan supplementation in the rat** 박현미 (한국과학기술연구원)
13:55-14:15	**Non-targeted analysis in the recombinant inbred line derived from the cross between a wild and a cultivated soybean** 심희정 (안전성평가연구소)
14:15-14:35	**Metabolomics as a Tool for the Comprehensive Understanding of Korean Fermented Food** 이장은 (한국식품연구원)
14:35-14:55	**Rapid and Simultaneous Analysis of 360 Pesticides in Brown Rice, Spinach, Orange, and Potato Using Microbore GC-MS/MS** 문준관 (한경대학교)

SYMPOSIUM 4 & 5 & 6
15:10 – 17:10

SYM-4: Pharmaceutical MS (Convention Hall Ⅲ)

Organizer & Chair: 최용석 (단국대학교) & 신소영 (원광대학교)

15:10-15:40	**The Hunt for Autism Biomarkers** Prof. Troy D. Wood (Department of Chemistry, State University of New York at Buffalo) : Keynote Speaker
15:40-16:00	**Diagnostic biomarker development for methicillin-*resistant Staphylococcus aureus* based on multi-directed proteomics** 김경곤 (서울아산병원/울산의대)
16:00-16:20	**Rapid Detection of Antimicrobial Resistance by MALDI-TOF MS** 박형순 ((주) 아스타/㈜노스퀘스트 (ASTA/NosQuest)
16:20-16:40	**Aberrant Glycosylation is Associated with Gastric Cancer and Precancerous Diseases** 김운용 ((주)글라이칸)
16:40-17:00	**Korean Whole Saliva Proteome: Identification, Characterization, and Quantitation** 최용석 (단국대학교)

SYM-5: MS for Metabolomics (Conference Room 301)

Organizer & Chair: 김태영 (광주과학기술원) & 안현주 (충남대학교 분석과학기술대학원)

15:10-15:30 **Comparative Lipidomics of 5-Fluorouracil Sensitive and Resistant Colorectal Cancer Cells**
김광표 (경희대학교)

15:30-15:50 **LC/MS/MS Assay for Immunogenicity Screening in a Therapeutic Glycoprotein: Identification and Characterization of Non-human Glycan Epitope**
안현주 (충남대학교 분석과학기술대학원)

15:50-16:10 **Metabolic heavy water labeling for lipidomics**
김태영 (광주과학기술원)

16:10-16:30 **Metabolomic Analysis in Plasma of Mouse Model with Asthma by Mass Spectrometry and Pattern Recognition**
백만정 (순천대학교)

16:30-16:50 **Extending a substrate range of *Saccharomyces cerevisiae* using metabolomics-guided strain engineering**
김수린 (경북대학교)

SYM-6: <Special SessionⅡ>

환경질량분석 특별세션: 미세먼지 문제 해결을 위한 질량분석학의 응용 (Conference Room 302)

Organizer & Chair: 김성환 (경북대학교) & 배귀남 (한국과학기술연구원)

15:10-15:40 **미세먼지 국가전략프로젝트 사업단 연구현황**
Ph.D. 배귀남 (한국과학기술연구원)
: Keynote Speaker

15:40-16:00 **Mechanistic Studies of Secondary Aerosol Formation Using Mass Spectrometry**
임용빈 (한국과학기술연구원)

16:00-16:20 **초고분해능 질량분석기를 이용한 이차유기에어로졸 특성 규명**
임호진 (경북대학교)

16:20-16:40 **초미세먼지 유기지표성분 특성 및 기여량 분석**
배민석 (목포대학교)

16:40-17:00 **Deciphering Chemical Information of Aerosol-derived Organic Substances Using Ultra-High Resolution FT-ICR Mass Spectrometry**
장경순 (한국기초과학지원연구원)

17:00-17:20 **Characteristics of fine particle contamination in Ulsan, Korea: influence of local pollution and long-range transport**
최성득 (울산과학기술원)

Fridy Morning, August 24

SYMPOSIUM 7 & 8

08:50 – 10:50

SYM-7: New Technologies for MS (Convention Hall Ⅲ)

Organizer & Chair: 오한빈 (서강대학교) & 정가영 (성균관대학교)

08:50-09:10	**Targeted and Non-targeted Metabolomics Approach to Comprehensive Understanding of the Effects of Brewing Conditions on Green Tea Infusions** 이정미 (성균관대학교)
09:10-09:30	**Surface labeling mass spectrometry for GPCR singaling analysis** 정가영 (성균관대학교)
09:30-09:50	**Photoisomerization in the Gas Phase Studied by Laser Spectroscopy and Tandem Ion Mobility Mass Spectrometer** 최창민 (한국기초과학지원연구원)
09:50-10:10	**Electrospray Ionization Mass Spectrometry Coupled With Gas Chromatography** 이재익 (한국과학기술연구원)
10:10-10:40	**Expanding the Repertoire of Ion Activation Methods for Glycosaminoglycans** Prof. Jonathan Amster (Department of Chemistry, University of Georgia) : Keynote Speaker

SYM-8: MS for Protein Analysis (Convention Hall Ⅱ)

Organizer & Chair: 조 건 (한국기초과학지원연구원) & 임재민 (창원대학교)

08:50-09:20	**Overview of Proteomic Data Analysis** SungKyu Robin Park (박성규) (The Scripps Research Institute Integrated Proteomics Applications, Inc) : Guest Speaker
09:20-09:40	**Secondary structural analysis of peptides and proteins using ion mobility-mass spectrometry combined with gas-phase infrared spectroscopy** 서종철 (포항공과대학교)
09:40-10:00	**Molecular insights of amyloid fibrillation and inter-fibrillar aggregations of α-synuclein associated with hard divalent metal cations** 한종윤 (고려대학교 ~~화학과~~)
10:00-10:20	**Mass spectrometry for Biomedical Research** 김민식 (경희대학교)
10:20-10:40	**Comprehensive RNA-interactome profiling in multicellular samples using formaldehyde-crosslinking** 김종서 (서울대학교)

SPECIAL LECTURE

영수홀 A+B

Organizer & Chair: 임용현 (한국표준과학연구원)

11:10-11:50 **Development of Ultra-trace Analysis Techniques of Nuclear Materials in Environmental Sample Analysis and Nuclear Forensics**

Ph.D. 송규석 (한국원자력연구원(KAERI) / 전임회장)

KSMS

2018 한국질량분석학회 여름정기학술대회 및 총회

BRIEF ORAL PRESENTATION

Brief Oral 1-1

[P-009]

Energy-resolved Collision-induced Dissociation Study of Na^+-bound G-quartets with Mixed Ligands, $[Na(Guanine)_n(9\text{-methylguanine})_m]^+$

Yoon Kyung Choi,† Sang Yun Han*

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Collision-induced dissociation (CID) of square-planar Na^+-bound complexes of G-quartets with mixed ligands of guanine (G) and 9-methylguanine (9mG), $[Na{\cdot}G_n{\cdot}9mG_m]^+$ (n = 0 - 4, m = 0 - 4; $n + m = 4$) were investigated using tandem mass spectrometry. The mass spectrum of $[Na{\cdot}G_n{\cdot}9mG_m]^+$ produced by electrospray ionization (ESI) exhibited pronounced generation of mixed clusters of Na^+-bound monomers, dimers, and G-quartets, wherein Na^+-bound trimers were essentially missing. Similarly, CID of G-quartets hardly produced fragments of Na^+-bound trimers from the square-planar complexes. Those suggest that a great stability is gained by forming a complete hydrogen bonding network in G-quartets, which agrees well with a large predicted stepwise enthalpy of formation by complexation with the fourth ligand to be as large as 55 kcal/mol. The stability gained by hydrogen bonding between G moieties in G-quartets further suggests that Na^+-bound dimeric fragments may be formed from neighboring, hydrogen-bonded ligands; which in other words suggests preferential neutral loss of hydrogen-bonded G dimers in CID. It further allowed to address the stereochemistry of G-quartets, of which population for *cis*- and *trans*-conformers of $[Na{\cdot}G_2{\cdot}9mG_2]^+$ can be assessed to be 50:50 in the gas phase. The observed ratio of 50:50 agrees well that the G-quartets were likely to be formed in the solution and produced according to thermochemical stability rather than in the course of electrospray ionization via kinetic trapping.

Brief Oral 1-2

[P-016]

Proteomic Analysis of Cervicovaginal Fluid for Early Detection of Preterm Birth by 2D-nLC-ESI-MS/MS

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

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

Preterm birth (PTB) before 37 weeks of pregnancy is one of major causes of poor pregnancy outcome, resulting in perinatal mortality and neonatal morbidity. Despite medical advances, PTB has continuously increased over the last two years and the development of biomarker(s) for early detection of PTB has not been matured. In this study, we performed shotgun proteomic analysis of the cervicovaginal fluid (CVF) samples that delivered at preterm and term so as to unveil the protein biomarkers using isobaric tags for relative and absolute quantitation (iTRAQ) coupled with two dimension-nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (2D-nLC-ESI-MS/MS). We compared the CVF proteome of individual PTB and control using pooled control CVF as a spike-in reference standard. We identified 1294 CVF proteins, of which 605 were newly identified proteins. Of 990 proteins quantified in both PTB and control, 154 proteins were significantly up/down-regulated in PTB compared to control. Differently expressed proteins were subjected to Gene Ontology (GO) analysis. These promising results could lead to improved understanding of PTB etiology and discovery of biomarkers for PTB.

Brief Oral 1-3

[P-012]

Profiles of oxidized phospholipids in exosome from oxidatively stressed cells by flow field-flow fractionation and nUHPLC-ESI-MS/MS

Joon Seon Yang and Myeong Hee Moon*

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

Oxidative stress is caused by excessive production of reactive oxygen species (ROS), which include oxygen derived radical species such as superoxide anion ($O_2^{\cdot-}$) and hydroxyl radical($^{\cdot}OH$) as well as hydrogen peroxide (H_2O_2). Although ROS participates in some physiological roles (e.g. signaling, host defence), high levels of ROS not only induces cellular impairment by altering DNA, RNA, proteins and lipids but is also involved with a number of diseases like cardiovascular disease (CVD) or cancer.

Exosomes are nano-sized extracellular vesicles secreted from cells. When oxidative stress is given to cells, it has been reported that exosome transports some protective RNA against oxidative stress or transfer stress signals to recipient cells. However, physiological roles or changes of lipids in exosome during oxidative stress conditions have not yet been studied.

In this study, oxidative stress was induced to human embryonic kidney cell 293 (HEK293) by treating with H_2O_2 for 72 hours. Exosome from control and oxidatively stressed conditions were analyzed by flow field-flow fractionation, which separates samples according to their sizes. Moreover, comparison of lipidomic alteration, including oxidized phospholipids in cell and exosome was conducted by nUHPLC-ESI-MS/MS.

Brief Oral 1-4

[P-038]

Quantitative proteomics of 2D-/3D-cultured adipocyte cells and its co-cultured with macrophages using a nanoLC-ESI-MS/MS

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

[3]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, P.O. Box 107, Yuseong-gu, Daejeon 305-600, Republic of Korea*

Adipocytes in human body play a role in regulating the fat storage and energy homeostasis. Excessive accumulation of adipocytes can 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 *in vitro* 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 4052 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 involving in glucose and fatty acid metabolisms, such as glucose transporter member 4, fatty acid binding protein, and acetyl-CoA carboxylase, were up-regulated, compared to that of 2D cultured-ones. Consequentially, 3D *in vitro* model offers to the alternative of 2D *in vitro* and *in vivo* models for the assessment of new medical products associated with metabolic disorder.

Brief Oral 1-5

[P-052]

Spatial distribution of siloxanes in coastal sediment and identification of procedural contamination sources in GC/MS analysis

Danbi Lee*, Sung-Deuk Choi

School of Urban and Environmental Engineering, Ulsan National Institute of Science and Technology (UNIST), 50 UNIST-gil, Ulsan, 44919, Korea

Cyclic and linear siloxanes have been used as chemical additives in consumer and industrial products. However, several studies have reported potential toxicity of siloxanes, especially estrogen mimicry, reproductive, and liver damage in laboratory animals. Therefore, the occurrence of siloxanes in various environmental matrices can lead to negative effects on the ecosystem. The analytical determination of these compounds have been challenging because procedural contamination is highly affected during gas chromatography mass spectrometry (GC/MS) analysis. Therefore, this study was aimed to minimize the sources of background contamination of siloxanes during GC/MS analysis and analyze siloxane compounds, including 6 cyclic siloxanes (octamethylcyclotetrasiloxane–octadecamethylcyclononasiloxane) and 13 linear siloxanes (octamethyltrisiloxane–dotriacontamethyl pentadecasiloxane) in coastal sediments collected from southeastern industrial bays in Korea. The results identified that high level of cyclic siloxanes contamination was derived from the use of GC column and silicone septum of GC/MS ($\sum_6$ cVMS: 73.4±21.0 ng) or vial (38.9 ng). In particular, not only analysis, but the pretreatment process also significantly induced the contaminations. The use of silicone tube, during the concentration process, showed high levels of background contamination of $\sum_6$ cVMSs (73.4±5.8 ng). We analyzed $\sum_{19}$ Siloxanes in coastal sediments from the four industrial bays including Gwangyang, Jinhae, Busan, and Ulsan Bay. Almost all sediments had detectable levels of siloxanes and the total mean concentrations of the sites are higher than other countries. The distribution of siloxanes varied widely among the sampling sites, and compositional profiles of siloxanes were strongly affected by industrial activities in each bay. As a further study, risk assessment of siloxanes in the sediment will be carried out.

Brief Oral 1-6

[P-056]

Validation and application of analytical tools for stable carbon isotope analysis of crude oils in molecular level using ultra-high resolution mass spectrometry

Seungwoo Son[1], Donghwi Kim[1], Sunghwan Kim[1*]

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

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

Brief Oral 1-7

[P-050]

Parallel reaction monitoring of fucosylated glycopeptides of alpha-fetoprotein in human serum for early hepatocellular carcinoma by LC-MS/MS with immunoprecipitation

Kwang Hoe Kim[1, 2], Soo-Youn Lee[3], Heeyoun Hwang[2], Ju Yeon Lee[1], Eun Sun Ji[1], Hyun Joo An[2], Jin Young Kim[1,*] and Jong Shin Yoo[1, 2,*]

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We introduced direct analysis of fucosylated glycopeptides of α-fetoprotein (AFP) by parallel reaction monitoring (PRM) mass spectrometry (MS) combined with immunoprecipitation. α-fetoprotein (AFP) is a widely used serological marker that has been associated with hepatocellular carcinoma (HCC). In this study, we directly monitored fucosylated glycopeptides in AFP to provide a more accurate diagnosis of HCC. Because AFP is present at low concentrations in human serum, a more sensitive approach is required. In this study, two analytical methods were assessed to overcome sensitivity issues. First, LC-PRM MS combined with immunoprecipitation was performed to analyze AFP glycopeptides. Second, sialic acid was removed using a α-2,3,6,8 neuraminidase to improve the analytical sensitivity of target glycopeptides. The treatment of neuraminidase to glycopeptides for desialylation was useful to improve MS detection limit (LOD < 2 ng/mL) and to obtain reliable signal (CV < 20%) of target glycopeptides in AFP from sub μL serum. Finally, relative percentage of fucosylated AFP (AFP-fuc%) out of total glycosylated one was applied to compare sera with HCC, liver disease and healthy subjects. AFP-fuc% showed an area under the ROC curve (AUC = 0.949, p value < 0.0001) to discriminate between HCC and liver disease patients. These results suggest that our approach to target individual fucosylated glycopeptides using PRM provides an assay useful for the diagnosis of HCC.

Brief Oral 1-8

[P-073]

Detection of Neu5Gc in Human Serum via MRM-MS

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

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Sialic acid expressed as an outer terminal unit on a glycan plays immunological and physiological roles such as immunological processes, hormonal response, and signal transmission. Unlike other mammalian, human cannot biosynthesize N-Glycolylneuraminic acid (Neu5Gc) due to irreversible mutation on gene CMAH. Exogenous Neu5Gc can be an immunogenic antigen in human cells and it is also reported to be found in a high level of concentration in human cancers, suggesting that immunogenic Neu5Gc is a cancer-associated glycan. Therefore, the determination of Neu5Gc from human fluids and tissue is highly important in clinical research. In this study, for the first time, we developed an analytical method using mass spectrometry to selectively identify and quantify Neu5Gc in human serum. Briefly, sialic acids were liberated from human serum by chemical hydrolysis and further enriched using solid phase extraction with a PGC cartridge. The Neu5Gc was chromatographically separated on a PGC column, then analyzed by MRM-MS. The limits of detection/ quantitation (LOD/ LOQ) for Neu5Gc and the linearity between Neu5Gc concentration and MS signal for quantitation were examined. The concentration of Neu5Gc from human serum was determined at low pico mole levels with high reproducibility (CV<6%). This result could be used for newly updated data of human serum, and moreover it is expected to be applied as a valuable reference for clinical research.

Brief Oral 1-9

[P-063]

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

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Newborn screening for phenylketonuria (PKU), homocystinuria (HCU), and maple syrup urine disease (MSUD) have been generally diagnosed by various detection methods including Guthrie test (substituting bacterial inhibition assay), HPLC, and LC-MS/MS. MALDI-ToF mass spectrometry could be utilized to quantify the biomarkers of the metabolic diseases by easy sample preparation and simultaneous detection.

In this work, parylene-matrix chip was developed for the qualitative and quantitative analysis of biomarkers (amino acids) using MALDI-ToF mass spectrometry by reducing the organic matrix-related noise at low mass-to-charge ratio range ($m/z<500$). [1] Parylene-N thin film was deposited on dried organic matrix (CHCA) spots with the thickness of 50~80 nm. Methanol extraction was conducted for easy and rapid sample preparation of serum sample before the mass spectrometric analysis precipitating proteins in human serum. Calibration curves were obtained by analyzing amino acids in water and serum. They showed good linearity ($R^2 > 0.98$) and the LODs were ranging from 9.0 to 22.9 μg/mL.

From these results, MALDI-ToF MS using parylene-matrix chip could be applied to the quantitative detection of amino acids for the screening of neonatal metabolic disorders with less background noise at low mass-to-charge ratio range.

Brief Oral 1-10

[P-095]

Determination of the geographical origins of various propolis samples via UPLC combined with high-resolution FT-ICR mass spectrometry

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Propolis, the resinous substance collected by honey bees (*Apis mellifera*) from buds and resins of various plant species, is widely used in folk medicine because of its beneficial effects on various symptoms. Because the compositional diversity of propolis depends on the habitats of the plant sources, propolis samples from different origins exhibit different characteristics or biological activities. In this study, the ethanol-extracted propolis (EEP) from various propolis raw materials originating from different countries (*i.e.*, Argentina, Brazil, China and Korea) were analyzed using high-resolution 15 T Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry coupled with a reverse-phase ultra-performance liquid chromatography (RP-UPLC) system to determine the geographical origins of the propolis and the origin-specific key compounds. Based on approximately 8,000 molecular features extracted from UPLC/FT-ICR MS datasets, a partial least squares-discriminant analysis (PLS-DA) plot showed distinct separations among propolis samples from four different origins, whereas plots constructed from the UPLC analysis datasets did not. According to the variable importance in projection (VIP) scores (VIP ≥ 4.0) and fold change values (≥2 or ≤ −2), key propolis components contributing to the discrimination of Korean propolis from Brazilian and Chinese propolis were identified. This analysis revealed the characteristic features of the different propolis samples, and these results can be used to determine the geographical origins and to assess the quality of the commercial products.

Brief Oral 1-11

[P-097]

Analysis of Polycyclic Aromatic Hydrocarbons in Olive Oil using Isotope Dilution-Gas Chromatography/Mass Spectrometry

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Polycyclic aromatic hydrocarbons (PAHs) composed of two or more benzene ring structures have a long residence time and carcinogenic effects in humans. A major route of human exposure to PAHs is intake of fatty foods like edible oil. The edible oil can be contaminated by trace PAHs occurred during food preparation processes, such as frying, grilling, or smoking. Thus, several countries set regulations to maximum residue level in edible oil. In South Korea, the maximum residue limit of benzo(a)pyrene is below 2 μg/kg in edible oils.

The aim of this study is developing the analysis method using isotope dilution(ID)-GC/MS as a higher-order reference method for the accurate measurement of four PAHs (Benzo(a)antracene, Chrysene, Benzo(b)fluoranthene, Benzo(a)pyrene) in olive oil. Sample preparation procedure includes liquid-liquid extraction (LLE) and solid phase extraction (SPE). To optimize the sample clean-up process, we tested the clean-up performance of various cartridges for SPE such as florisil, C_{18}, silica, EZ-POP-NP dual-layer, and NH_2 cartridges. In addition, we compared the results when using deuterium and ^{13}C labeled isotopic analogues as internal standards. PAHs were quantitated by SIM mode in GC-MS (Agilent 7890 GC/Jeol JMS 800D-UF MS). The ID-GC/MS method was validated by accuracy, repeatability, reproducibility, LODs, LOQs, assessment of uncertainty, and comparison with other reference method. The developed ID-GC/MS method can also be applied to other edible oils.

Brief Oral 1-12

[P-099]

Simultaneous determination of five urushiol analogues in lacquer tree extract by using LC-MRM and QuEChERS with EDTA

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Lacquer tree (*Rhus verniciflua*), known to have not only biological activities such as anti-oxidation, anti-cancer, anti-inflammation but also urushiol group allergens, is used as food material in South Korea. Thus, for its safe use as food material, the appropriate removal of urushiols prior to its use. However, its present regulatory test in Korean Food Code has limitations including miss-targeting and too high limit of quantitation. Therefore, here, an LC-MRM method to quantitate four urushiol compounds (urushiols I, II, III, and V) and laccol in lacquer tree extract, the most widely-used type of lacquer tree food material, simultaneously was developed. For extraction and purification of the targets from samples, QuEChERS with EDTA was employed, and the developed method was successfully validated in the aspects of specificity, linearity (r^2>0.990), accuracy (recovery: 84.83-102.95%), precision (relative standard deviation: 1.18-8.71%) and sensitivity (the limit of quantitation: 5 ng/g). Finally, the validated method was applied to the monitoring of the targets in 33 lacquer tree extract goods purchased from internet food markets. The present method could contribute to the establishment of the suitable regulatory system for the safe use of lacquer tree as food material in the future.

Brief Oral 1-13

[P-116]

Mass spectrometric study on the source of error in quantification of fatty acids

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Identification and quantification of fatty acids are important in fields of lipidomics and metabolomics. Although exogenous fatty acid contaminants, which leads to inaccurate quantification, have been neglected in lipidome analyses, unexpected contamination can be occurred from plasticware and glassware during the sample preparation. Therefore, quantitative measurement of the contaminants is necessary for reducing an error associated with accurate determination of the amount of endogenous fatty acids in biological samples.

Fatty acid contaminants were investigated with respect to different types of sample containing tubes, extraction solvents, and sample preparation. The contaminants were analyzed by high-performance liquid chromatography electrospray ionization quadrupole time-of-flight mass spectrometry in technical triplicate. The target molecules were palmitic acid and stearic acid that account for the largest portion of the contaminants. As a result, among sample containing tubes, glassware washed using methanol revealed the minimum contamination of fatty acids. By evaluation of different types of extraction solvents, chloroform showed the least contamination. Also, the amount of contaminants generated in the sonication step was about 57 times higher than that in the pipetting step, which is expected to be the most abundant source of the contamination.

Brief Oral 1-14

[P-124]

Study on analysis method of polyol in Polyurethane foam by Matrix-assisted laser desorption/ionization-Time of flight (MALDI-TOF)

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Polyurethane foam is used to various industrial field with other material due to outstanding insulation. It has much different form such as soft form, hard form, coating, special adhesives, sealant and elastomer. Polyurethane could be obtained by reaction between polyol and diisocyanate or polymeric isocyanate in existence of additives and catalyst. The various types of polyurethane could be made according to many kinds of polyol and diisocyanates. Thus, it is important to research physical and chemical property of polyol in polyurethane foam.

Recently, modern analytical methods (ex. GPC, NMR, GC) were used to analyze polyol. In this research, MALDI-TOF (Matrix-assisted laser desorption/ionization-Time of flight) method was applied for MS and MS/MS analysis to obtain m/z (mass to charge ratio) value and structure information of various polyor.

From MS results, we got MS spectrum and m/z values of various polyols according to acid and alcohol types. Also, we could confirm structure information of polyols from fragment pattern results.

Brief Oral 2-1

[P-010]

Anomaly in Collision-induced Dissociation of Proton-bound Hoogsteen Base Pairs of Cytosine and Guanine by Proton Transfer

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We report the anomalous collision-induced dissociation (CID) behavior of the proton-bound Hoogsteen base pairs of Cytosine (C), 1-methylcytosine (1-MeC), and 5-methylcytosine (5-MeC) with Guanine (G) as a common base partner, $(C:G:H)^+$, $(1\text{-}MeC:G:H)^+$, and $(5\text{-}MeC:G:H)^+$. In the results, in contrast to the other base pairs, CID of $C:H^+\cdots G$ exhibited more abundant production of $C:H^+$, the fragment protonated on the moiety with a smaller proton affinity, than $G:H^+$. This appeared to contradict general prediction based on the kinetic method. However, further theoretical exploration of potential energy surfaces found that there can be facile proton transfers in the proton-bound Hoogsteen base pairs during the CID process, which makes the process accessible to an additional product state of O-protonated C for $C:H^+$ fragments. The presence of an additional dissociation channel, which in other words corresponds to 2-fold degeneracy in the transition state leading to $C:H^+$ fragments, effectively doubles the apparent reaction rate for production of $C:H^+$. In this way, the process gives rise to the anomaly, the observed pronounced formation of $C:H^+$ in the CID of the proton-bound Hoogsteen base pair, $C:H^+\cdots G$.

Brief Oral 2-2

[P-013]

Effect of aging on lipid alteration in serum, kidney, and heart from mice by nUHPLC-ESI-MS/MS

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Lipids are not only the sources of energy production and basic building blocks of cell membrane, but also the important signaling molecules in intercellular communications. All living organisms are inevitable from aging which induces gradual reduction of lipid-regulated cellular metabolism. This is because lipid alteration in aging subjects can cause problems in cellular metabolism, leading to age-related diseases, such as cardiovascular disease, neurodegenerative disease, and diabetes mellitus. Although a number of studies have been conducted to elucidate the relationship between age-related diseases and lipids, only few studies have compared lipid changes with aging effect. In this study, lipid profiles in serum, kidney, and heart from C57BL/6 aging mice were examined. Uniformly raised 4 and 25-month-old mice were analyzed by nanoflow ultrahigh pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). More than 350 lipid species were identified in each sample types and 163 in serum, 210 in kidney, and 202 in heart were quantified. From quantification, most lipid species showing significant changes (> 1.5 fold and $p < 0.01$) were found to be down-regulated by aging, and lipid alteration in serum was more distinct than those in tissues (kidney and heart).

Brief Oral 2-3

[P-018]

Metabolic signitures of adrenal steroids in serum and saliva measured by polarity switching LC-MS

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Adrenal steroids are generated in adrenal glands and metabolized by various enzymes, such as hydroxylases and reductases. Profiling analysis of adrenal steroids in serum and saliva was therefore established to evaluate their metabolic functions in adrenal diseases. All steroids were separated through an 1.9 μm particle C18 column (50 × 2.1 mm) at a flow rate of 250 μL/min and quantitatively measured by the high-speed polarity switching LC-MS in MRM modes. In method validation, the linearity (r^2) was higher than 0.992 within 0.1 and 500 ng/mL dynamic range, while precision (%CV) and accuracy (%bias) were 1.1 ~ 9.8% and 85.9 ~ 112.1%, respectively. The levels of salivary steroids were compared with those of serum, and a comparison between saliva sampling techniques was also investigated. This validated assay was successfully applied to patients with Cushing's syndrome and the results from saliva were comparable to those from serum. Therefore, the present LC-MS method could be an useful tool for monitoring diseases, including Cushing's syndrome.

Brief Oral 2-4

[P-042]

Cross-validation of sulfur-based and amino acid-based quantification methods for the development of insulin reference material

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Protein analysis is an essential means in clinical laboratories, pharmaceutical industries, and basic biological and medical research. In the establishement of a highter order analytical method for protein quantification, multiple stages of reduced protein such as petide, amino acid (AA), and element can be analyzed and deduce the quantity of original protein. In this study, an element (sulfur)-based reductive approach for protein quantification has been applied to determine mass fraction of insulin in a pure protein certified reference material (CRM). The absolute protein quantification using sulfur measurements was based on the isotope-dilution inductively coupled plasma mass spectrometry (ICP-MS) using enriched ^{34}S isotope as an internal standard to achieve the highest accuracy. Pressurized microwave-assisted acid digestion with concentrated nitric acid was utilized for sample digestion. Then, the mass fraction of sulfur in the candidate CRM was obtained from the isotope ratios of ^{32}S over ^{34}S which were measured by ICP-MS. In addition, the size-exclusion and reversed-phase LC methods were used with ICP-MS to characterize and quantify sulfur-containing impurities. The quantification result obtained with the present method based on sulfur analysis was in excellent agreement with the result determined via a well-established protein quantification method based on AA analysis. In the AA-based analysis, conventional acid hydrolysis combined with an ID LC-MS/MS method was used.

Brief Oral 2-5

[P-054]

Automated screening of organic pollutants in airborne particulate matter using GC×GC-TOFMS

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Comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry (GC×GC-TOFMS) has been applied to analyze complex samples such as airborne particulate matter (PM). PM samples contain thousands of compounds with unresolved carbonaceous matter (UCM), but they belong to many chemical groups such as polycyclic aromatic hydrocarbons (PAHs) and persistent organic pollutants (POPs). GC×GC is a powerful separation technology that can recognize individual chemical compounds and groups. Especially, computer-based tools with mass spectra can be applied for identification and classification of chemical compounds and groups. In this study, an automated screening method was developed based on chromatographic information on PAHs and POPs in airborne PM using GC×GC-TOFMS. First, basic search criteria of peaks and rule of classification were optimized with a special software, LECO ChromaTOF, and applied to $PM_{2.5}$ samples. Secondly, the script was written for automated classification based on fragmentation patterns, retention time, and mass spectra transformation. Finally, the efficiencies of classification methods were compared, and various $PM_{2.5}$ samples were evaluated with automated profiling. This method will be used for quick identification of persistent chemicals in PM collected during episode days.

Brief Oral 2-6

[P-040]

Comparison of organic mixtures from particulate matters collected in Korea and China by using GCxGC/high resolution mass spectrometry

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In Korea and neighboring China, airbone particulate matter ($PM_{2.5}$) is very serious environment problems, having primary organic pollutants directly released from emission sources and secondary organic pollutants generated from atmosphere chemical reaction. Thus, the complex organic compounds extracted from $PM_{2.5}$ collected day after day during one month in each country were analyzed to compare their identifications, relative quantities and emission sources. Samples of $PM_{2.5}$ were simultaneously collected day after day for 28 days (4-31 January 2018) in Gwangju and Beijing using a high volume air sampler. The two days of extracts were combined, filtered and concentrated under N_2 gas. Comprehensive two-dimensional gas chromatography/high resolution time-of-flight mass spectrometry (GCxGC/HRMS) was utilized to analyze the organic extracts. Approximately, 460 compounds were separated on the polar and sequencial nonpolar GC columns and identified based on the mass spectral data from NIST and Wiley libraries, and exact mass accuracy (<1 ppm) of molecular ion from high resolution data, including alkanes, carboxylic acids, hopanes, PAHs, substituted aromatics and steranes, so on. A variety of PAHs were identified in Beijing samples such as benzo[ghi]fluoranthene, benzo[a]anthracene, acepyrene, pyrene and benzo[A]yrene. Their concentrations in Beijing were more 49 to 3 times according to PAHs compounds than those in Gwangju for 16/17 days $PM_{2.5}$. Thus, it is anticipated that the issues between two countries related about the emission sources will be discussed, based on these objective results obtained for PM2.5 collected in Korea and China.

Brief Oral 2-7

[P-053]

Characterization of site-specific O-glycopeptides in fibroin heavy chain from silkworm cocoon using high resolution LC-MS/MS

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Silk fibroin, the structural protein of silkworm cocoon produced from bombyx mori has been reported to improve cognition function and immune system in healthy humans. Several silk proteins are known as glycoproteins but, fibroin protein is not yet known. Glycosylation is one of common post-translational modifications in a protein, which play a key role such as protein folding and protein-protein interaction. Therefore, characterization of glycosylation in fibroin protein is necessary in order to extend our understanding of its bioactivities. Fibroin protein is composed of highly repeating amino acid units of [G-A-G-A-G-S]n, and glycosylation is present at low concentration, which is difficult to analyze. So, we used HILIC enrichment and high resolution LC-MS/MS to effectively extract and identify the site-specific O-glycopeptides from nonspecific enzyme digestion of fibroin protein. A total 34 O-glycopeptides, 31 O-glycosylation sites, and 9 different O-glycans were identified from fibroin heavy chain. Most of the identified O-glycosylation sites were found at serine. Their exact O-glycosylation sites were identified by EThcD MS/MS spectra. We first report that O-glycosylation occurs in fibroin heavy chain with evidence of specific glycopeptide fragment ions in LC-MS/MS spectra. In conclusion, this new discovery of glycosylation through effective analytical method will contribute to understanding the biological systems of silkworm.

Brief Oral 2-8

[P-074]

Synergistic antibacterial activity of phenolic compound-antibiotic combination and their quantitative determination by LC-QTOF-MS

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Bacteria have a remarkable ability to acquire resistance against antibiotics by several mechanisms. New strategies are needed to block the development of resistance and to prolong the life of traditional antibiotics. Thus, we intended to increase the efficacy of commercially available antibiotics by combining with opportunistic phenolic compounds. Ten commercial antibiotics and 5 phenolic compounds were used against *Salmonella* Typhimurium, *Escherichia coli* and *Staphylococcus aureus* to evaluate the antibacterial combination effect. Finally, LC-QTOF-MS was used to quantify individual compounds from mixtures of antibacterial agents. Phenolic compounds demonstrated good antimicrobial activity varied with minimum inhibitory concentration depending on compounds and strains. Fractional inhibitory concentration (FIC) index of 40 sets of combination against *S.* Typhimurium, *E. coli* and *S. aureus* ranged from 0.281 to 1.016. Three combinations were selected for further investigation depending on the critically important antibiotics list of World Health Organization and the FIC index of our study. Inhibition rates of *S.* Typhimurium in presence of Gallic Acid+Ceftiofur, *E. coli* in presence of Hamamelitannin+Erythromycin, and Gallic Acid+Ampicillin demonstrated improved efficacy compared to the efficacy of those antimicrobials alone. The effect of those three combinations on the cell morphology of *S.* Typhimurium and *E. coli* were evaluated and found that those antimicrobial combinations have no effect on cell morphology. All of the three combinations showed different degrees of biofilm inhibition potential. Among them Hamamelitannin+Erythromycin combination demonstrated better inhibition potential of *E. coli* biofilm. Viability of biofilm of *S.* Typhimurium in presence of Gallic Acid+Ceftiofur, and *E. coli* in presence of Hamamelitannin+Erythromycin, and Gallic Acid+Ampicillin demonstrated improved efficacy compared to the efficacy of those antimicrobials alone. All of these five compounds were successfully quantified by LC-QTOF-MS from different compound mixtures. Based on the result of this study, it is concluded that the therapy of these combinations can be more effective than the conventional antibiotics in controlling *S.* Typhimurium and *E. coli* associated infections. Further investigations are recommended to determine the safety profile and combination antimicrobial effect in *in vivo* system.

Keywords: Combination therapy, critically important antibiotics, gallic acid, hamamelitannin, biofilm.

Brief Oral 2-9

[P-086]

Global absolute quantitation of human whole saliva proteins using nLC-Q-IMS-TOF with MS^E

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Saliva has potential to be widely used for the discovery of biomarkers due to its many good characteristics such as communication with blood and non-invasive nature during the sampling. However, its applications are still limited in comparison with other biological fluids such as blood. Thus, here, to expand the applications of saliva to the biomarker research, global absolute quantitation of proteins in human whole saliva (WS) by nLC-Q-IMS-TOF with MS^E was carried out. WS samples were obtained from 22 healthy Korean volunteers (11 male and 11 female) and pooled for its analyses which produced quantitative information of 93 proteins, ranging from 5.89×10^1 ng/mL (immunoglobulin heavy chain) to 1.59×10^4 ng/mL (α-amylase 1). For the validation of this study, human serum albumin in the sample was quantitated by ELISA and its result was compared with that from the nLC-Q-IMS-TOF study. As a result, there was no significant difference between two results ($1.18 \times 10^4 \pm 0.03 \times 10^4$ ng/mL from nLC-Q-IMS-TOF vs. $1.23 \times 10^4 \pm 0.07 \times 10^4$ ng/mL from ELISA, n=3, p=0.309). Since the present study is the first global absolute quantitation of proteins in human whole saliva, the resulting information can be used as the first level reference for the future human salivary protein biomarker research as well as its quantitative applications.

Brief Oral 2-10

[P-096]

Validation of tocopherol analysis in leafy vegetables using Standard addition-isotope dilution liquid chromatography mass spectrometry method (SA-IDMS-LC/MS)

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Tocopherol is an antioxidant that prevents damage to cell membranes and tissues. Primary method for analysis of tocopherol in infant formula was previously developed using standard addition-isotope dilution liquid chromatography/mass spectrometry (SA-ID LC/MS) for development of infant formula certified reference material (CRM). The aim of this study is to validate the SA-ID LS/MS method to characterize the property values of α, γ-tocopherols in spinach flour and kimchi cabbage flour CRMs.

The sample was treated with saponification and conducted liquid-liquid extraction with hexane. The separation was carried out isocratic condition with 100% methanol (10 mmol/L ammonium acetate) and Cadenza C_{18} (3 μm, 4.6 mm x 250 mm) column. Mass spectrometry analysis was conducted in the negative mode of electrospray ionization and selected reaction monitoring mode was applied.

The measurement results were agreed within their uncertainties between ID LC/MS and SA-ID LC/MS methods using deuterium labeled isotope. Also, α-tocopherol-[^{13}C] was applied on ID LC/MS in order to examine bias from using deuterium labeled isotope during SA-ID LC/MS analysis. Results of repeatability and reproducibility supported that the method is able to apply to certify the spinach flour and kimchi cabbage flour CRMs. Also, the homogeneity and stability were examined in both CRMs. SA-ID LC/MS was applied to similar type of vegetables such as kale, broccoli, leaf beet and lettuce.

Brief Oral 2-11

[P-101]

Primary and secondary metabolic profiles according to regional characteristics of *Glycine max* in Korea

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Glycine max is one of the most important crops which contain a lot of nutrients such as carbohydrates, proteins, and flavonoids. The nutritional quality and metabolic characteristics of soybean is determined by a range of environmental factors (e.g. climate and soil). Thus, the metabolic investigation may be essentially valuable.

In this study, we conducted non-targeted metabolomic analysis by using GC-TOF MS and LC-Orbitrap MS. A total of 210 metabolites were structurally identified, further employed for statistical analysis, which fairly covered a range of chemical entity, thus allowed comprehensive metabolic phenotyping.

The resultant profiles integrative of primary and secondary metabolites were differentiated by multivariate statistical model according to 7 representative cultivation regions in Korea. The metabolic cluster relocated with five metabolites (malonylgenistin, malonyldaidzin, N-acetylornithine, allysine, tryptophan) showed outstanding discrimination power for the profiles of all seven regions, which was determined by ROC analysis.

The subsequent interrogation on covarianced structures of the metabolome revealed region-specific metabolic features that systematically isolated list of metabolites and linked it to different region of the soybean cultivation. Our result suggested metabolite analysis can be applied to authentic methodology that identifies origin of agricultural products, and also provide nutritional information according to cultivation region.

Brief Oral 2-12

[P-104]

MALDI-MS analysis of small molecules using N-doped carbon dots as matrix

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Matrix-assisted laser desorption/ionization (MALDI) is simple and useful soft ionization method. The matrix helps ionize analytes, where organic matrices such as 2,5-dihydroxybenzoic acid and sinapic acid are commonly used. Organic matrices are effective for large molecule analysis such as proteins and peptides. Due to strong background interferences from intrinsic matrix-related ion in the low mass region, organic matrices are not suitable for small molecule analysis in MALDI-mass spectrometry (MS). To overcome the limitation, various alternative matrices such as nanomaterials and porous silicon, carbon-based materials and metal oxides are being studied.

In this study, N-doped carbon dot (N-CD) was selected as an alternative matrix for analysis of small molecules. To synthesize N-CDs, a solution containing 1 g citric acid, 1 g urea, and 10 mL distilled water was heated in 800 W microwave for 4 min. Characterization of N-CDs was performed by Fourier-transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), UV-Vis absorption (UV-Vis), photoluminescence spectroscopy (PL), and X-ray diffraction (XRD). Glucose, sucrose, amino acids, and nilotinib were successfully analyzed using the synthesized N-CDs as matrix in MALDI analysis

Brief Oral 2-13

[P-114]

Production of high purity gallium metal for compound semiconductor and trace elements quantification

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Gallium is used as an essential raw material for the production of high-purity III-V compound semiconductors or semi-insulators such as gallium arsenide (GaAs). Particularly, semi-insulator(GaAs) requires high purity of 8N or higher, and gallium metal used as a raw material must have a high purity of 8N or more, and a method of analysis of high purity gallium is necessary.

In this study, we quantitatively analyzed gallium crystallized at high purity using Czochralski(CZ) method. Three types of CRM selected to calculate relative sensitivity factors (RSF) for quantifying impurity elements in high purity gallium. CRM has an aluminum matrix containing gallium contents of 175, 100 and 330 ppmw, respectively. The calculated RSF for the aluminum matrix CRM was 2.65, 2.36 and 2.34, respectively. The average RSF was 2.45 and the relative standard deviation (RSD) was about 7%. Using this standard sample, for the 17 elements of Al, Ga, Mg, Si, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Ag, Cd, Sn, Pb and Bi, Quantitative analysis is possible. Finally, in the analysis of gallium crystallized by the CZ method, four kinds of impurity elements were detected as Al, Si, Cr, and Fe, and all of the other elements were below the detection limit. The quantitative analysis in GD-MS was calculated by multiplying the ion beam ratio (IBR) by RSF. The IBR of Al, Si, Cr and Fe were 5.12, 2.84, 3.09, 1.57 ppbw respectively. The RSF of Al, Si, Cr, and Fe calculated using CRM were 0.41, 0.43, 0.58, and 0.30. Therefore, the quantitative analysis for the final four elements can be expressed as (2.10, 1.22, 1.79, 0.47) ppbw, and the total amount of impurity elements is 5.58 ppbw and the final purity of gallium is about 99.9999994% (8N).

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2018 한국질량분석학회 여름정기학술대회 및 총회

PLENARY LECTURE

Plenary Lecture

Probe Electrospray Ionization (PESI)

Kenzo Hiraoka

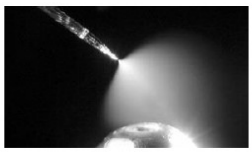
Clean Energy Research Center, University of Yamanashi

PESI and Related Techniques: ESI is one of the most typical desorption/ionization method. To mimic FD, we developed probe electrospray ionization (PESI) in which a sharp solid metal needles was used as a sampling probe [1]. The needle was driven down and up by using a linear motor actuator. At the lowest position, the needle captured pL~nL liquid samples. At the highest position, a high voltage was applied to generate electrospray. PESI can be applicable directly to various biological samples such as cancer tissues. The cancerous/non-cancerous tissues (kidney, liver, etc.) can be clearly distinguished by PESI. The merit of PESI is its less invasiveness. Imaging MS for mouse brain tissue was also performed.

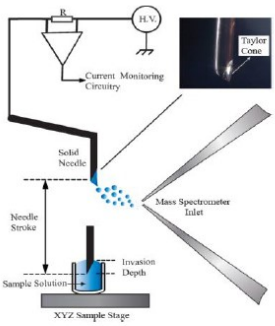
PESI is applicable only to wet samples. For the application of PESI to dry samples, dipping PESI(dPESI) and sheath-flow PESI(sfPESI) were developed[2]. In dPESI, dry sample captured at the needle tip was dipped in a pure solvent making the sample wet. In sf-PESI, solvent was preloaded in a gel loading tip in which a fine metal needle was inserted. sf-PESI was suited for remote sampling MS. To examine the inductive ionization, a glass capillary inserted with a fine metal needle was investigated. To our surprise, stable electrospray was generated from the tip of the glass capillary.

Minimize the Suppression Effect: In PESI, dPESI and sfPESI, *sequential* and *exhaustive* electrospray took place depending on the surface active values of analyte ions. As a result, the suppression effect that is inherent to capillary-based ESI can be largely moderated in PESI. This unique nature is based on the fact that excess charges are continuously supplied to the liquid droplet trapped on the needle tip by electrochemical reactions taking place at the interface between the metal electrode and the liquid sample.

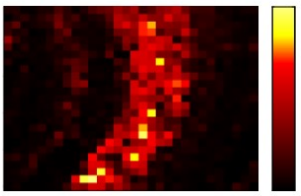
Future Prospects: Remote sampling and proximity ionization are the key factors for the next generation MS. In this respect, the coupling of sf-PESI with a robotic system is underway.



Electrospray



Probe electrospray(PESI)

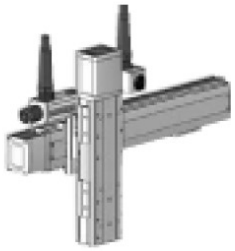


Imaging MS by PESI

Dipping PESI

Sheath-flow PESI
with a touch sensor

Glass PESI



Robotic MS

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[2]D. T. Usmanov et al., *RCM*, 2018, 32, 407-413.

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2018 한국질량분석학회 여름정기학술대회 및 총회

SPECIAL LECTURE

Special Lecture

Development of Ultra-trace Analysis Techniques of Nuclear Materials in Environmental Sample Analysis and Nuclear Forensics

Kyuseok Song, Jong-Ho Park, Chi-Gyu Lee, Sang Ho Lim, Sun-Ho Han, Jinkyu Park

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The ultra-trace analysis techniques of nuclear material in environmental samples and nuclear forensics are important in nuclear safeguards and nuclear security. Environmental sample analysis has been an important measure in nuclear safeguards since it can provide evidences about the existence of the unreported nuclear activities and verify the reported activities. Meanwhile, nuclear forensics can provide evidences regarding the illicit trafficking of the nuclear materials as well as radioactive materials. KAERI has been pursuing ultra-trace analysis techniques for nuclear materials in regards to the nuclear safeguards as well as nuclear security. During the establishment of the techniques, a new clean facility has been established (CLASS) and many new analytical techniques have been developed during the last decade. As a result, KAERI become a member of network of analytical laboratories (NWALs) for environmental sample analysis since 2012. In addition, development of nuclear forensics techniques has been also initiated at KAERI in a small step. In this presentation, development progress of the ultra-trace analytical technique in KAERI has been summarized. Some key points of the developed techniques and important applications are also introduced.

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SYMPOSIUM

Symposium-1-A

Introduction of clinical laboratory testing using mass spectrometry

Yeo-Min Yun

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최근 들어 질량분석기 검사장비를 사용하여 다량 검체에 대한 고속분석이 가능해짐으로써 의료기관 임상검사실에서 신생아선별검사, 대사이상 검사, 약물남용선별 및 약물농도검사, 호르몬 검사, 미생물 동정 검사 등 다양한 질환의 진단 및 치료 경과 관찰을 위하여 활발히 시행되고 있다. 현재 임상검사실에서 사용되고 있는 질량분석기로는 GC-MS, ICP-MS, LC-MS/MS, MALDI-TOF 등이 있다.

GC-MS 및 ICP-MS는 비교적 오래 전부터 임상검사실에서 유기산 및 중금속 검사에 주로 사용되었고, 최근 검체 전처리가 간단하고 고속분석이 가능한 LC-MS/MS 검사법이 검사실에 도입되면서 신생아선별검사 및 대사이상 질환 검사를 비롯하여 각종 약물 농도 검사, 비타민 및 스테로이드 호르몬 농도 검사 등 다양한 검사항목에 질량분석기를 사용하고 있다. 아직 고가의 검사장비와 숙련된 검사인력이 필요하고 검사수행 전체 과정(검사처방 정보 인식, 검체 전처리, 정도관리 수행, 검사 결과 검증 및 전송 등)의 자동화가 기존의 다른 검사장비에 비하여 부족한 부분이 있어 많은 임상검사실에서 사용하기에는 어려움이 있지만, 다양한 검사항목에 대하여 동시 측정이 가능하고, 면역측정법(immunoassay) 등에 비하여 검사 대상 물질에 대한 특이도가 높다는 장점 때문에 기존 검사항목에 대한 검사방법을 LC-MS/MS 검사법으로 변경하거나 신규 검사항목 세팅 시 LC-MS/MS 검사법을 사용하는 검사실이 증가하고 있는 추세이다. 또한 최근 미생물 균 동정 및 유전자변이 분석 방법으로 MALDI-TOF 검사법이 도입되면서 감염성 질환 진단 및 치료를 위한 미생물 균 동정 검사에 MALDI-TOF 검사법을 사용하는 검사실이 증가되고 있다.

본 강의에서는 국내 임상검사실에서 질량분석기의 이용 현황과 향후 전망에 대해 알아보도록 하겠다.

Symposium-1-B

Drug Abuse Screening Test Using LC-MS/MS

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근래 치료 약물이나 중독성 약물에 대한 오남용 사례가 증가함에 따라 이들을 신속히 선별할 수 있는 오남용 약물 선별검사의 중요성 역시 증가하고 있다. 진단의학검사실에서는 오남용약물 선별검사를 주로 급성 약물 중독 여부를 신속히 확인하거나 채용 신체 검사시 오남용약물의 상습 투여 여부를 확인하기 위해 시행하고 있다.

검체로 모발, 혈액이나 타액 등이 가능하나 주로 소변이 이용된다. 검체 채취가 용이하고 소변에서 약물이 검출될 수 있는 기간이 비교적 길기 때문이다. 그러나 검사의 목적에 따라 소변 검체는 위변조 조작이 가능하기 때문에 실제 검사가 이루어지기 전에 검체 채취와 운반시 검체의 무결성 여부를 확인하기 위해 소변의 pH, 비중, 크레아티닌, 아질산염과 온도 측정이 권고되고 있다. 식약처에서 발행한 의료기관 등의 마약류 검사 가이드라인에 따르면 검체의 변조 및 희석을 방지하기 위해 전용 채취 시설에서 검체 채취 및 전달 과정의 연속성을 유지하기 위한 일련의 절차를 따르도록 하고 있다. 또한 선별검사로서 갖추어야 할 분석적 성능이 검증되어야 하며, 주요 약물에 대한 검출 기준(cut-off)을 아래와 같이 제시하고 있다.

오남용 약물	검출 기준 (cut-off, ng/mL)
Amphetamine, methamphetamine	500
Cannabis metabolites (THC)	50
Cocaine metabolites (benzoylecgonine)	300
Opiates (morphine)	300

선별검사 방법으로서 현장에서 신속하고 간편하게 이용할 수 있는 면역크로마토그래피 정성검사법이 주로 이용되고 있으나, 측정 약물수가 적고 육안 판독으로 인해 판정이 다소 주관적일 수 있다는 점이 단점으로 지적되고 있다. 근래에는 임상검사실에서 광범위 오남용 약물을 더욱 민감하고 특이도 높게 검출해낼 수 있는 질량분석법을 사용하는 예가 증가하고 있다. 질량분석법 중에서도 LC-MS/MS가 다른 GC-MS법이나 LC-UV법에 비해 많이 이용되는데 훨씬 다양한 오남용 약물을 짧은 시간내에 검출해낼수 있다는 장점이 있기 때문이다. 질량분석법을 이용한 오남용약물 선별검사를 시행함에 있어서 본 검사법이 검사의 목적에 부합하는지 검토해 보고, 검출 대상에 대사체를 포함한 주요 오남용 약물들이 모두 포함되어 있는지, 관련 지침에서 제시하는 cut-off 기준을 충족하는지와 정확한 판독이 가능한지 여부 등을 꼼꼼히 살펴 보아야 할 것이다.

본 연제에서는 임상검사실에서 이용되고 있는 다양한 오남용약물 선별검사법들을 비교해보고 LC-MS/MS 검사법의 도입과 사용 경험을 공유함으로써 본 검사법의 임상적 활용 방안에 대해 생각해보고자 한다.

Symposium-1-C

Newborn screening test for lysosomal storage disease using MS/MS

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리소좀축적병(lysosomal storage disease, LSD)는 리소좀에 있는 여러 효소들 중 하나 또는 그 이상의 효소 결핍으로 인하여 리소좀 내에서 분해되지 못하고 축적되어 임상적인 증상을 일으키는 질환입니다. 리소좀축적병의 유병율은 1:100,000(크라베병), 1:57,000(고셔병), 1:80,000~1:117,000(파브리병), 1:14,000~1:138,000(폼페병), 1:88,000(헐러병), 1:250,000[니만-픽병(A/B)] 등으로 질병, 인종 등에 따라서 다양하게 나타나고 있습니다 [1-4].

현재 효소활성도검사와 유전자 돌연변이 분석검사가 리소좀축적병을 진단할 수 있는 검사방법입니다. 효소활성도검사는 형광물질을 이용한 방법이 주로 이용되어 왔으나 최근 크로마토그래피 탠덤질량분석기를 이용하여 보다 빠르고, 정확하게 측정할 수 있는 방법이 개발되고 있습니다. 더 적은 검체를 사용하여 측정이 가능한 크로마토그래피 탠덤질량분석기 방법은 혈액여과지 검체에서 각 효소의 기질과 산물의 농도를 동시에 측정할 수 있으며 기존방법보다 특이도가 높아서 진단에 도움이 된다는 연구가 발표되었습니다 [5]. 그리고 대만에서는 신생아의 혈액여과지 검체를 이용하여 국가적으로 리소좀축적병에 대한 신생아 선별검사를 시행하고 있습니다 [6].

우리나라에서는 2017년 7월 20일 보건복지부 고시 제2017-130호에서 리소좀축적병 선별검사 [정밀분광/질량분석]에 대한 신의료기술의 안정성 유효성 평가결과가 고시되었습니다 [7]. 구제적으로 고시 내용에서는 리소좀 축적병 중에서 크라베병, 고셔병, 파브리병, 폼페병, 헐러병, 니만-픽병(A/B)의 선별이 사용목적이며, 환자의 말초혈액을 이용하여 질량분석법으로 위의 언급된 질병과 관련있는 효소의 활성도를 측정하는 검사방법으로 나와 있습니다.

이 연제에서는 크로마토그래피 탠덤질량분석기를 이용한 리소좀축적병 검사에 대한 기본적인 방법과 그 방법을 이용하여 측정한 경험에 대하여 공유하려고 합니다.

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Symposium-1-D

Screening for Steroid Profiling in Dried Blood Spots by Liquid Chromatography-Tandem Mass Spectrometry

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Congenital adrenal hyperplasia (CAH), the most common adrenal gland disorder in infants and children, is a group of autosomal recessive disorders, in particular 21-hydroxylase deficiency, which is the cause of about 95% of CAH cases. In most newborn screening programs worldwide, the detection of CAH is currently implemented, and the standard test parameter is 17 -hydroxyprogesterone. Although immunoassays to evaluate 17 -hydroxyprogesterone are easy to handle, rapid, and highly sensitive, they have shown questionable reliability because of a lack of specificity and matrix effects. While inclusion of extraction steps improve immunoassay specificity, all interfering molecules cannot be completely eliminated, and several publications state low specificity due to cross-reactivity of antibodies with steroids other than 17 -hydroxyprogesterone such as steroid sulfates, 17 -hydroxypregnenolone, and 17 -hydroxypregnenolone sulfate. So, conventional screening for CAH using immunoassays for 17 -hydroxyprogesterone generates a large number of false-positive results. A specific liquid chromatography–tandem mass spectrometry (LC–MS/MS) method with simultaneous detection of multiple steroids has been introduced to minimize unnecessary follow-up. We developed and validated an LC-MS/MS method to simultaneously determine blood concentrations of nine steroids in dried blood spot (DBS) samples; cortisol, 17-hydroxyprogesterone, 11-deoxycortisol, 21-deoxycortisol, androstenedione, corticosterone, 11-deoxycorticosterone, testosterone, and progesterone. A total of 1146 DBS samples from 272 premature and 874 full-term neonates were used to establish reference intervals. Fourteen additional samples from anonymized neonates and children were tested to validate the clinical applicability of the method. Accuracy, precision, matrix effects, and extraction recovery were satisfactory for all of the steroids at three concentrations. Values of intra- and inter-day precision coefficients of variance and recovery were 2.52-12.26%, 3.53-17.12%, and 61.7-74.2%, respectively. The linearity range was 1.0-144.0 ng/mL for cortisol, 1.0-12.50 ng/mL for 21-deoxycortisol, and 0.25-12.50 ng/mL for the other steroids (R^2>0.99). The reference intervals were in agreement with previous reports. Finally, the analysis of samples from 21-hydroxylase defective patients demonstrated the potential usefulness of multiplexed steroid profiling for diagnosis and/or monitoring of CAH. This LC–MS/MS method provides appropriate analytical performance and can be successfully applied to the analysis of nine steroids in DBS for diagnosis of steroid metabolic disorders including CAH.

Symposium-1-E

Microbial Identification using Mass Spectrometry

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Microbial detection and identification is essential to diagnose infectious diseases and a primary duty of the clinical laboratory. For a long time, biochemical testing was the mainstay of bacterial identification. Among several ionization methods, ESI and MALDI have been used for organism detection and identification. Quadrupole and time-of-flight mass analyzers also have been employed. Two principal mass spectrometry types, MALDI TOF and ESI-MS, have been introduced. The introduction of MALDI-TOF MS has brought about tremendous changes in practice, and today, the technique is used routinely for the identification of both bacteria and fungi. It is effective for most organisms, including gram-positive and gram-negative bacteria, both cocci and bacilli, as well as for anaerobic bacteria and mycobacteria. There are two main commercial instruments: the VITEK MS and the MALDI Biotyper. The MALDI-TOF MS method has several attractive features such as rapid reporting of results, a larger database of organisms for comparison, and no effect of gram staining or any specific biochemical testing. Ibis T5000, the prototype instrument for PCR-ESI-MS, was advanced as the PLEX-ID. This technique uses multiplex PCR or RT-PCR techniques based on broad-range amplification. With this method, we can detect pathogens directly in clinical specimens. We also can identify resistance genes and virulence factors. The method has the potential to reveal genetic evidence of undiscovered pathogens, as well as genetic changes. Today, I will talk about the successful adoption of MALDI-TOF MS in clinical microbiology laboratories and the unfulfilled needs that require further work.

Symposium-2-A

<KEYNOTE SPEAKER>

Isotope Ratio Analysis of Individual Particles containing Uranium and/or Plutonium with Inorganic Mass Spectrometry

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Isotope ratio analysis of uranium and/or plutonium in environmental samples taken at nuclear facilities is performed with inorganic mass spectrometry to find out undeclared nuclear activities. We have developed techniques using secondary ion mass spectrometry (SIMS) and fission track-thermal ionization mass spectrometry (FT-TIMS) for individual uranium particle analysis. Consequently, we analyze environmental samples by using these techniques as one of the IAEA Network of Analytical Laboratories (NWALs). In SIMS analysis, uranium particles in the sample are identified with energy dispersive X-ray analysis, manipulated and transferred onto a planchet under a scanning electron microscope. Since this manipulation allows us to perform SIMS analysis without any molecular ion interferences, isotope ratios of uranium in individual particles are accurately determined. Recently, we have just started to utilize large geometry-SIMS (LG-SIMS) for more precise measurements. In this presentation, the role of TIMS and inductively-coupled plasma mass spectrometry (ICP-MS) for individual particle analysis will also be presented.

A portion of this study is being performed under the auspices of the Nuclear Regulation Authority, Japan.

Symposium-2-B

Experimental Evaluation of the Detection Methods of TIMS for Isotopic Analysis of Ultra-trace Level Uranium

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Detection methods of TIMS (thermal ionization mass spectrometry) were experimentally evaluated by analysis of 1 ng, 100 pg, 30 pg, 5 pg, and 1 pg of a uranium(U) standard material(U030). Accuracy, precision, and measurement uncertainty were the criterion to evaluation the analytical performance. Isotopic analysis by TIMS for the 10 replicated U with relatively high amounts(1 ng and 100 pg) showed no significant improvement in analytical performance irrespective of the detection method adopted. On the other hand, slight improvement in accuracy and precision for the analysis of 30 pg U was observed when the multi-dynamic and static detection methods were adopted. The static detection method offers the greatest accuracy and precision, and the smallest measurement uncertainty for TIMS measurements of 5 pg and 1 pg of uranium, which correspond the amount level of uranium contained in individual particles of environmental interest, due to the greater detection sensitivity of ion counters than faraday cups, the elimination of ion signal drift, and the large number of valid data sets in a measurement. Isotopic analysis of uranium microparticles of sizes 1 μm or less agreed well with the certified values, thus verifying the applicability of the static detection method to particle analysis of environmental samples required for nuclear safeguards.

Symposium-2-C

The analysis of halogen elements in snow from Antarctica

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Halogen elements in the polar regions participate in key atmospheric reactions including the formation of cloud concentration nuclei and ozone depletion events. We have developed a simple and accurate method for the measurement of bromine (Br) and iodine (I) at the picogram-per-gram levels in Antarctic snow by Inductively Coupled Plasma Sector Field Mass Spectrometry (ICP-SFMS; Element2, ThermoFischer, Bremen, Germany) equipped with a cyclonic Peltier-cooled spray chamber. Particularly attention must be given to the cleaning process for the strong memory effect of Br and I. In addition, we have controlled the blank levels of sodium providing the Si coating on the cones. Detection limits for I and Br were 5 and 50 pg g^{-1} with an uncertainty of less than 5%. The method was evaluated using certified reference materials, groundwater reference materials with low and high halogen contents.

Symposium-2-D

금속 안정동위원소의 해양환경 연구 적용

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금속 안정동위원소는 해양에서의 생지화학적 순환 규명 혹은 오염원 추적에 널리 사용되고 있다. 국내에서도 다검출기 유도결합플라즈마 질량분석기(MC-ICP-MS)가 보급되고 있으나, 다양한 미량원소의 동위원소비를 분석하기 위한 분석법이 부족한 실정이다. 정확도 및 정밀도 높은 동위원소 자료 생산을 위해서는 다양한 방해물질을 제거하는 화학적 분리가 필요하며, 연구하고자 하는 시료 특성에 맞는 분리기법/분석법 개발이 필수적이다. 특히 해양시료의 경우, 염분의 존재로 인하여 기존에 정립되어 있던 방법을 적용하기 어려운 실정이다. 본 연구는 Cu, Fe, Zn 안정동위원소를 분석하기 위하여 음이온 교환수지를 사용한 복합분리기법 정립 및 단·장기 안정성 테스트의 중요성에 다루고 있으며, 실제 한국해양과학기술원에서 연구하고 있는 다양한 환경연구에 대한 소개를 다루고 있다.

Symposium-2-E

Proton Transfer Reactions in Collision-induced Dissociation of Proton-bound Nucleic Acid Bases

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Protonation of nucleic acid bases has been known to cause certain alternations in DNA structures, which may affect related biological processes. In this subject, proton-bound dimers of nucleic acid bases including cytosine (C) and guanine (G) have been important model systems to study base-pairing interactions using mass spectrometry. In particular, IRMPD (infrared multiple photon dissociation) and ER-CID (energy-resolved collision-induced dissociation) experiments have played important and complementary roles in elucidating structures and energies of proton-bound dimers of nucleic acid bases. In addition, a combined approach with quantum chemical calculations offered further insight into dissociation dynamics as well. In this presentation, a variety of proton-bound dimers of $C{\cdot}C^+$ and $C{\cdot}G^+$ explored by quantum chemical calculations are introduced, which displays key information on base-pairing, where multiple hydrogen bonding including an ionic hydrogen bond are deeply involved in the pairing interactions. In addition, IRMPD spectroscopy and ER-CID experiments of the proton-bound dimers of CC^+ and CG^+ are discussed, which demonstrates the role of proton transfer in the course of dissociation process, determining the fate of energized complexes. Finally, the facile proton transfer in dissociation successfully accounts for the known “anomaly” found in CID and IRMPD of proton-bound Hoogsteen base pair of $C{\cdot}G^+$ as well.

Symposium-3-A

Next generation proteomics for agriculture and food science.

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Proteomics technology aims to map the protein landscapes of biological samples, and it can be applied to a variety of samples including cells and tissues. Because the proteins are the main functional molecules in the cells, their levels reflect much more accurately the cellular phenotype and the regulatory processes within them than gene levels, mutations, and even mRNA levels. With the advancement in the technology, it is possible now to obtain comprehensive views of the biological systems and to study large proteome overview. Here, we discuss the technological advancements in mass spectrometry–based proteomics called as next generation proteomics, which allow analysis of tissue samples for agriculture and food science, leading to the large-scale plant proteomics studies. Furthermore, we discuss the technological developments in plant proteomics studies, which provide the basis for biological clues to understanding protein function. So far, using an in-house developed method for protein isolation, combined with the Q-Exactive Hybrid Quadrupole-Orbitrap Mass Spectrometer, more than 5000 proteins were identified in plant tissues as a case study. The acquired MS data to quantify protein abundance were analyzed with MaxQuant (ver. 1.5.3.30). As a case study, we like to introduce soybean proteomics studies.

Phytohormones are central to plant growth and development. Despite the advancement in our knowledge of hormone signaling, downstream targets, and their interactions upon hormones action remain largely fragmented, especially at the protein and metabolite levels. With an aim to get new insight into the effects of two hormones, ethylene (ET) and abscisic acid (ABA), this study utilizes an integrated proteomics and metabolomics approach to investigate their individual and combined (ABA+ET) signaling in soybean leaves. Targeting low-abundance proteins, our previously established protamine sulfate precipitation method was applied, followed by label-free quantification of identified proteins. A total of 4129 unique protein groups including 1083 differentially modulated in one (individual) or other (combined) treatments were discerned. Functional annotation of the identified proteins showed an increased abundance of proteins related to the flavonoid and isoflavonoid biosynthesis and MAPK signaling pathway in response to ET treatment. HPLC analysis showed an accumulation of isoflavones (genistin, daidzein, and genistein) upon ET treatment, in agreement with the proteomics results. A metabolome analysis assigned 79 metabolites and further confirmed the accumulation of flavonoids and isoflavonoids in response to ET. A potential cross-talk between ET and MAPK signaling, leading to the accumulation of flavonoids and isoflavonoids in soybean leaves is suggested.

Symposium-3-B

Comprehensive Anlaysis of Glycolipids in Milks

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Gangliosides are glycolipid that consist of glycans attached on a ceramide lipid. Gangliosides are found in mammalian fluids, cell membrane and tissues such as nerve system. As a functional lipid, milk ganglioside plays an important biological role such as the development of immune system and infant brain, and the recognition ligand for the pathogen bindings. Analysis of ganglioside in milk sample is extremely difficult due to the complexity and diversity of fatty acids and glycans, and the hindrance of selective isolation from huge amount of neutral lipids. In this study, we optimized method that is ganglioside extraction from milk sample. We analyzed the edible mammalian milks from cow, procine, white goat, block goat, bore goat, human and cheese wheys. After addition of internal standard for the recovery calculation, glycolipids were extracted by the methanol/chloroform/water mixture and purifided by SPE. UPLC/Q-TOF has been used to profile gangliosides using the bio-synthetic library based identification. Absolute quantity of each profiled ganglioside was estimated by the MRM using UPLC/QQQ.

Symposium-3-C

Urinary change of neurochemicals and endogenous metabolites with tryptophan supplementation in the rat

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Tryptophan is an essential amino acid, the source of which is dietary only. It plays an important role as a precursor of various substances involved in diverse biological functions as well as in protein synthesis. The aim of this study is to investigate the effects of tryptophan supplementation based on the combination of untargeted and targeted urinary metabolomic profiling in rat experimental model. Rats received daily oral administration of either tryptophan (125mg/kg body weight, n=10) or vehicle (control group, n=10) for 4 weeks. Urine was collected for 6 hours at 2nd and 4th week after tryptophan supplementation. Untargeted metabolomics approach using UPLC-ESI-QTOF-MS has been performed and multivariate statistical analysis demonstrated clear discrimination between control and tryptophan supplementation group. Tryptophan metabolism-related metabolites showed strong predictive component for the group classification. In the case of targeted metabolomics, 32 metabolites related to tryptophan, serotonin, tyrosine, and GABA metabolism pathway, which are considered as neurochemicals, were quantified using UPLC-QTRAP tandem mass. Our results showed that tryptophan supplementation influenced diverse neurochemicals and endogenous metabolites. Moreover, this study indicates that MS-based metabolomics can be a powerful tool to elucidate the interaction between nutrients and metabolic pathways including neurochemicals in nutritional research.

Symposium-3-D

Non-targeted analysis in the recombinant inbred line derived from the cross between a wild and a cultivated soybean

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Cunsumption of soybean has been steadily increased in the world, generating a significant economic impact to farmers around the world. In Korea, soybean is one of the main crops along with rice, wheat, barley and potato and widely consumed as a bean curd, a fermented paste, a sauce and oil. As interest in health has increased, so does the demand for soybean varieties containing bioactive metabolites. This study aimed at investigating the metabolite differences among recombinant inbred line (RIL) populations derived from a cross between a common cultivar, Hwang-Geum (Glycine max cv. HG) and a wild type IT182932 (Glycine soja) in Korea. Non-targeted analysis of seed metabolites was performed to identify meaningful compounds in 88 RIL populations by ultra-performance liquid chromatography (UPLC) coupled to quadrupole time-of-flight mass spectrometry (QToF/MS) which enabled high throughput analysis with excellent mass accuracy and resolution. Features were picked and aligned by XCMS package using R. The representative features of HG and IT182932 were selected based on their fold change and significance level (*p*-value). Some of these peaks were identified by matching their precursor and fragment ions to those of commercial standards or on-line databases. Pearson's correlation analysis and quantitative trait locus (QTL) mapping were performed to investigate metabolite-metabolite correlations and to identify genomic loci, respectively. The metabolites participating in the same biosynthetic pathway showed high correlations and similar QTL results. This study may potentially provide a basis for metabolic engineering and breeding of soybeans.

Symposium-3-E

Metabolomics as a Tool for the Comprehensive Understanding of Korean Fermented Food

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Metabolomic approaches are actively used to investigate the metabolite profile of various types of food, including fermented foods. Fermented food products contain diverse metabolites derived from raw materials and fermentative microorganisms. Fermentative metabolites are possibly an overall result of the activity of the microorganisms and the effect of enzymes produced during fermentation. Therefore, it is important to identify the metabolites in fermented food as well as the fermentative microorganisms to understand how they affect the quality and characteristics of the fermented food. Nevertheless, the correlation between the metabolite profile and the quality as well as functionality of fermented food has not yet been elucidated clearly, especially in traditional Korean fermented foods. Therefore, a comprehensive metabolomics study of the metabolite profile and ingredients of traditional Korean food can facilitate the identification of quality markers and help understand their production. In this study, a combination of metabolomic and metagenomic approaches was used to generate the comprehensive metabolite and microbial profiles of traditional Korean food. Different analytical techniques such as GC-MS and CE-TOF-MS in combination with multivariate analyses were used to obtain the metabolomic profiles of each fermented food. In addition, microbial communities were monitored to identify a correlation between metabolites and microbes. The metabolomic profiles of traditional Korean fermented food products generated in this study will be useful to identify the correlation between their metabolite content and their health functionality and quality; these data may also be applied to product development. Furthermore, the results of this study will be crucial in forming a basis for further research to scientifically establish the values of traditional foods.

Symposium-3-F

Rapid and Simultaneous Analysis of 360 Pesticides in Brown Rice, Spinach, Orange, and Potato Using Microbore GC-MS/MS

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A multiresidue method for the simultaneous and rapid analysis of 360 pesticides in representative agricultural produce (brown rice, orange, spinach, and potato) was developed using a modified QuEChERS procedure combined with gas chromatography−tandem mass spectrometry (GC-MS/MS). Selected reaction monitoring transition parameters (e.g., collision energy, precursor and product ions) in MS/MS were optimized to achieve the best selectivity and sensitivity for a wide range of GC-amenable pesticides. A short (20 m) microbore (0.18 mm i.d.) column resulted in better signal-to-noise ratio with reduced

analysis time than a conventional narrowbore column (30 m × 0.25 mm i.d.). The priming injection dramatically increased peak areas by masking effect on a new GC liner. The limit of quantitation was <0.01 mg/kg, and the correlation coefficients (r2) of matrix-matched standards were >0.99 within the range of 0.0025−0.1 mg/kg. Acetonitrile with 0.1% formic acid without additional buffer salts was used for pesticide extraction, whereas only primary−secondary amine (PSA) was used for dispersive solid phase extraction (dSPE) cleanup, to achieve good recoveries for most of the target analytes. The recoveries ranged from 70 to 120% with relative standard deviations of ≤20% at 0.01 and 0.05 mg/kg spiking levels (n = 6) in all samples, indicating acceptable accuracy and precision of the method.

Symposium-4-A

<KEYNOTE SPEAKER>

The Hunt for Autism Biomarkers

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Autism spectrum disorders (ASD) growing incidence in the United States and Korea has become a major medical concern which has substantial educational and economic impact. Over a decade ago, our group began to search for evidence related to the opioid excess theory of autism; this hypothesis was that exogenous foods, such as dairy and wheat, when digested produced peptides with opiate-like effects that might influence behavior. While we established such peptides could exist in blood, more interesting was the marked difference in the abundance of a substance in urines between children with ASD and controls. This substance was identified as stercobilin, and was depleted in ASD urines (~33% of controls). With a target identified, effort along two lines to produce standards for quantitative assessment by ESI-MS was achieved, leading to deuterated and 18O isotopologues. Recent work in our group shows that stercobilin, and its closely-related metabolite stercobilinogen, are depleted in the fecal matter of a mouse-model of autism. Indeed, a $p < 0.001$ has now been achieved for stercobilin (45% depletion in subjects), while a $p = 0.07$ has been achieved for stercobilinogen (38% depletion in subjects). The implications of our work with relation to diagnostic tests and microbiome studies of ASD subjects will be discussed.

Symposium-4-B

Diagnostic biomarker development for methicillin-*resistant Staphylococcus aureus* based on multi-directed proteomics

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A gram-positive causing skin, respiratory infection, *Staphylococcus aureus* can get multi- resistance to beta-lactam antibiotics (methicillin, dicloxacillin, nafcillin, oxacillin and the cephalosporins) via horizontal gene transfer of mecA gene and natural selection. One of them is methicillin-resistant *Staphylococcus aureus* (MRSA). To diagnose outbreaks of MRSA, the bacterium should be cultured from body-fluid samples of "unknown fever" patients including blood, urine or sputum to perform confirmatory tests early-on. However, there has been no protein biomarker for quick and easy diagnosis of MRSA from patint specimen. And phenol-soluble modulins (PSMs), a group of toxic proteins that are produced by MRSA are an important virulence factor. Therfore, in-time detection of PSM in MRSA-infected patients is important clinical unmet needs. So far, initial treatment of the infection is often based upon suspicion and techniques by the treating physician using quantitative PCR procedures, which takes long time as confirmatory tests early-on. And only qualitative detection of PSM isoforms have been performed based on UV-HPLC analysis system and requires a lot of cell culture media, which takes time Herein, proteome of 2 kinds genotype of two kinds of S. aureus (MRSA and MSSA) was analyzed using high resolutiuon mass spectrometry coupled with nanoflow liquid chromatography (Nano LC). And SWATH (Sequential Windowed Acquisition of All Theoretical Fragment Ion Mass Spectra) - MS was developed to quantify several isoforms of PSMs in small volume of culture media (20ul) of Streptococos aureus isolated from sepsis patients. MRSA specific proteins can be applied as a valuable resource to develop rapid diagnosis of MRSA using patient's blood or urine, enabling easy and quick diagniosis. This research was suppoorted by a grant of the Korea Health technology R&D Project through the Korea Health Industry Development Institute (KHIDI), funded by the Ministry of Health & Welfare, Republic of Korea. (Grant Number: HI15C2918).

Symposium-4-C

Rapid Detection of Antimicrobial Resistance by MALDI-TOF MS

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Antimicrobial susceptibility test (AST) methods currently used in hospitals can be divided into the phenotypic and genotypic ones. Phenotype methods using culture are considered as a gold strandards, but it takes a long time to report the results. Genotype methods are faster and more sensitive than phenotype methods, but high cost and skilled engineers are needed. MALDI-TOF MS is very promising to provide the rapid and sensitive AST results within a few seconds, but it has not been commercialized yet.

MALDI-TOF MS can identify the microorganism by comparing the protein profile in the microorganism with the database of the protein profile already established for each microorganism by analyzing the protein profile with MALDI-TOF MS. However, it is very difficult to detect the changes of the protein profile which is finely changed by the antimicrobial resistance.

This presentation will cover the research trends and results on how to perform AST based on MALDI-TOF MS. These methods can be categorized into: 1) a method of measuring the function according to the resistance mechanism of the resistant strain and 2) a method of measuring the change of elements constituting the resistant bacteria. A typical example for measuring the function of resistant bacteria is to measure the modification of the beta-lactam antibiotics by beta-lactamase-producing isolates. Other methods measuring component changes of resistant bacteria were based on the presence of a specific protein peak among the protein profiles of the resistant bacteria. In other words, it depends on the detection of the biomarkers of resistant bacteria.
In this presentation, we would like to show some examples of the MRSA(Methicillin-Resistant Staphylococcus Aureus) and CRE(Carbapenem-Resistant Enterobacteriaceae) determination based on MALDI-TOF MS.

Symposium-4-D

Aberrant Glycosylation is Associated with Gastric Cancer and Precancerous Diseases

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Gastric cancer is one of the most commonly occurring malignancy and leading cause of cancer death in Korea. Classically, CEA, CA19-9, and CA 72-4 have been used for non-invasive gastric cancer screening. However, current protein markers are not only non-specific for gastric cancer, but also low specificity and sensitivity. Glycosylation is the most common post-translational modification and plays an important role in various biological processes. Glycans in blood are secreted from cells in the form of glycoprotein and these glycans are changed depending on health condition and diseases including cancers. Aberrant glycosylation is the mainly observed in various type of cancer both cancer cells and the serum of patients. Glycan profiling of whole serum is already developed and widely used in cancer biomarker study. However, targeted glycoproteomic approach is needed in clinical field for better sensitivity and specificity. In previous study, we targeted serum haptoglobin and explored the glycan alterations between gastric cancer patient and healthy control. Based on these glycan signatures, we studied aberrant glycosylation on intact glycoprotein haptoglobin without enzymatic release and enrichment process for rapid, high-throughput clinical screening. Like glycan level, intact haptoglobin represent significant differences between cancer patients (n = 44) and healthy controls (n = 44) and we found high grade marker (AUC = 0.81 to 0.93). Based on previous study, here, we have applied to large set of samples not only gastric cancer patients but also various kinds of precancerous gastric diseases (including atrophic gastritis, gastric ulcer, and gastric dysplasia) for precancerous gastric disease and cancer biomarker discovery. Samples were analyzed by UHPLC-Q-TOF MS with only denaturation process for sample preparation. Standards shows high reproducibility (n = 19, CV < 10%). The cancer and gastritis score were evaluated to distinguish each disease from control group. Furthermore, we developed algorithmic approach for diagnosis of gastric cancer and gastritis using both cancer score and gastritis score. This study can provide the information to distinguish and diagnose gastric cancer and other precancerous gastric diseases.

Symposium-4-E

Korean Whole Saliva Proteome: Identification, Characterization, and Quantitation

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While more than 3,000 proteins have been identified by proteomic studies to discover biomarkers from human saliva, there has not been any study to build Korean saliva proteome. Also, while ethnic differences in the human plasma proteome have been lately reported, such trial on human saliva proteome has not been reported. Thus, here, Korean whole saliva (WS) samples collected from 22 healthy South Korean adult volunteers (11 male and 11 female) were analyzed by a nLC-Q-IMS-TOF system to construct the Korean WS proteome for the first time. Additionally, the influence of human oral microbiome to the Korean WS proteome was evaluated. As a result, a total of 674 proteins, not affected by human oral microbiome were indexed in the catalogue and its 358 proteins were determined as distinct Korean WS proteins. The significant uniqueness of the Korean WS proteome was observed in gene ontology, too. Additionally, since 46 of the 358 distinct Korean WS proteins were found to be associated with the top 10 deadly diseases in South Korea, the potential value of ethnicity-specific human saliva proteins as biomarkers for diseases highly prevalent in that ethnic group was confirmed. From the nLC-Q-IMS-TOF analyses of the pool of all samples, quantitative information of 93 proteins, ranging from 5.89×101 ng/mL (immunoglobulin heavy chain) to 1.59×104 ng/mL (α-amylase 1), were obtained for the first time. Therefore, the present results can contribute to the development of disease biomarkers from human saliva by not only providing the expanded information for human saliva proteome but also suggesting ethnicity-controlled salivary proteomics as a new direction for disease biomarker research with probably higher success rate.

Symposium-5-A

Comparative Lipidomics of 5-Fluorouracil Sensitive and Resistant Colorectal Cancer Cells

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Fluorouracil (5-FU) is a drug that is a pyrimidine analog which is used in the treatment of colon cancer. 5-FU based chemotheraphy have shown good effects for most colorectal cancer. However, colorectal cancer develops resistance to 5-FU. The purpose of the present study is to investigate cause of resistance to 5-FU by integrating multiple layers of information, the multi 'omics' approach which can expand the limit of our understanding of 5-FU resistant mechanism in colorectal cancer. To analyse lipidome changes associated with 5-FU resistance, we performed lipidome analysis in DLD-1 (5 FU treat +/no treat -) and DLD-1/5-FU (5-FU treat +/no treat -) cell lines. We quantified amounts of sphingomyelines and ceramides in DLD-1 cell and DLD-1/5-FU cell using triple quadrupole mass spectrometer. Using integrated analysis of changes in lipidome of colorectal cancer cell lines, we show that 5-FU resistant cell line is characterized by changes in lipid metabolism.

Symposium-5-B

LC/MS/MS Assay for Immunogenicity Screening in a Therapeutic Glycoprotein: Identification and Characterization of Non-human Glycan Epitope

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Therapeutic glycoproteins represent a great accomplishment for the treatment of various cancers and autoimmune diseases. Biotherapeutics are frequently produced in mammalian expression systems (CHO, NS0, Sp2/0, etc) to obtain human-like glycosylation, which can directly affect the drug's stability, immunogenicity, PK/PD, and bioactivity. However, non-human glycan epitopes such as NeuGc and alpha-galactose strongly modulating immunogenicity in a therapeutic protein are often contained in products. Therefore, non-human glycan variants of a glycoprotein product should be adequately analyzed and controlled to ensure product quality and to regulate of potential immunogenicity for process development and manufacturing procedures of therapeutic glycoproteins. Here, we developed LC- MS/MS based immunogenicity assay for monitoring of non-human glycan epitopes in various biopharmaceutical products. Representative commercial therapeutic proteins produced by CHO cell and Sp2/O cell were selected for rapid screening and structure-specific quantitation of non-human glycan epitopes, and in parallel human IgG were used as the control to confirm human-like glycan structures. Instrument parameters including LC gradients and tandem MS employing CID were optimized for isomeric and isobaric structure separation and production of enough fragment signals. Experimental MS/MS spectra were compared with *in-silico* fragments to select diagnostic fragments that could be used to predict the presence or absence of non-human glycan epitopes such as NeuGc and terminal alpha-Gal. This assay was successfully applied to screen non-human glycan epitopes on various biotherapeutic glycoproteins produced by various cell-based expression systems. In particular, several NeuGc-sialylated glycans as well as alpha-Gal epitopes were discovered in mAbs produced by mouse Sp2/0 cells. This approach provides excellent separation and quantitation of non-human glycans and can be applied controlling immunogenicity-related risks in the development of biotherapeutics.

Symposium-5-C

Metabolic heavy water labeling for lipidomics

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In most quantitative mass spectrometry (MS), complete labeling of target analytes with heavy isotopes is designed for simple distinction of isotope-labeled compounds from unlabeled counterparts in a mass spectrum. However, achieving complete metabolic isotope labeling is challenging mainly due to high cost and long time, especially for higher organisms. An alternative method to introduce an isotope to biomolecules is indirect deuterium labeling via heavy water (^2H_2O) administration, which results in strikingly different patterns of mass spectra because of partial isotope enrichment.

We have developed novel analytical platforms for relative quantification for lipids on a global scale using metabolic partial ^2H_2O labeling. In order to assess the reproducibility and robustness of our new relative quantification strategy, unlabeled and labeled lipids from HeLa cells were mixed in various mixing ratios. Quantification of equimolar mixtures of HeLa cell lipids revealed high reproducibility and accuracy across three biological and three technical replicates. Two orders of magnitude of dynamic range for relative quantification could also be achieved with HeLa cells variously mixed from 10:1 to 1:10 between unlabeled and labeled lipids. The two critical parameters affecting the accuracy and reliability of the relative quantification were the number of detectable mass isotopomers and the degree of deuterium labeling.

Finally, an in-house software written in C++ and python was developed to streamline the data processing from calculating the peak area of extracted ion chromatogram of each mass isotopomer of lipid ions to the relative quantification of equimolr mixtures of unlabeled and labeled lipids.

Symposium-5-D

Metabolomic Analysis in Plasma of Mouse Model with Asthma by Mass Spectrometry and Pattern Recognition

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Asthma is well known as a multifaceted chronic disease caused by an alteration of various genetic and environmental factors, which is increasing in incidence worldwide. However, the biochemical mechanisms of asthma are not completely understood. Thus, we performed of metabolomic study for understanding of the biochemical events by monitoring of altered metabolism and biomarkers in asthma. In mice plasma, 27 amino acids(AAs), 24 fatty acids(FAs) and 17 organic acids(OAs) were determined by ethoxycarbonyl/methoxime/tert-butyldimethylsilyl derivatives with GC–MS. Their percentage composition normalized to the corresponding mean levels of control group. They then plotted as star symbol patterns for visual monitoring of altered metabolism, which were characteristic and readily distinguishable in control and asthma groups. The Mann-Whitney test revealed 25 metabolites, including eight AAs, nine FAs and eight OAs, which were significantly different ($p < 0.05$), and orthogonal partial least-squares-discriminant analysis revealed a clear separation of the two groups. In classification analysis, palmitic acid and methionine were the main metabolites for discrimination between asthma and the control followed by pipecolic, lactic, α-ketoglutaric, and linoleic acids for high classification accuracy as potential biomarkers. Therefore, these explain the metabolic disturbance in asthma for AAs and FAs including intermediate OAs related to the energy metabolism in the TCA cycle.

Symposium-5-E

Extending a substrate range of *Saccharomyces cerevisiae* using metabolomics-guided strain engineering

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For economically viable cellulosic bioprocesses, it is necessary to develop a strain capable of fermenting mixed sugars derived from cellulosic hydrolysates. Moreover, it is also necessary to utilize those mixed sugars simultaneously in order to broaden production capabilities. One of the most widely used industrial microorganisms, *Saccharomyces cerevisiae* is a robust and ethanologenic yeast host with versatile genetic engineering tools available. However, the yeast has a limited substrate range as well as concreate glucose repression mechanisms, which hinder efficient fermentation of mixed sugars. This presentation will focus on metabolic engineering approaches to extend a substrate range of the yeast. Specifically, we will discuss several examples demonstrating that metabolomics can greatly facilitate metabolic engineering processes.

Cellulosic sugars primarily consist of glucose and xylose, C6 and C5 sugars, respectively. While glucose is readly and efficiently fermented by *S. cerevisiae*, xylose cannot be utilized by the yeast unless the yeast is metabolically engineered to do so. Our recent metabolomic analysis of xylose-metabolizing engineered *S. cerevisiae* suggested that the degree of sedoheptulose accumulation correlates with the inefficiency of xylose metabolism. Integrating with trascriptomic analysis, we identified a novel transcriptional regulation mechanism of the pentose phosphate pathway, involved with oxidative stress response as well as sedoheptulose accumulation. This finding can be applied to not only industrial strain development but also yeast physiology research.

Symposium-6-A

<KEYNOTE SPEAKER>

미세먼지 국가전략프로젝트 사업단 연구현황

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중국이 산업화로 급격한 경제성장을 이루면서 동북아시아 지역이 극심한 대기오염에 시달리고 있다. 중국의 풍하 측에 위치한 한국은 중국으로부터 대기오염물질의 이동에 따른 영향을 빈번하게 받고 있다. 이에 따라 미세먼지에 대한 국민적 관심이 매우 높아 국가가 우선적으로 해결하여야 할 대표적 사회문제로 부각되어 2017년 8월부터 미세먼지 국가전략프로젝트 사업단이 발족되어 패키지 개념으로 과학기술 기반 미세먼지 해법을 모색하기 위해 연구를 수행하고 있다. 당면한 미세먼지 현안문제에 대응하기 위하여 미세먼지의 발생·유입, 측정·예보, 집진·저감, 보호·대응 등 4대 분야에 대해 15개 총괄/단위과제가 수행되고 있다. 발생유입 분야에서는 대기 중 미세먼지의 2차 생성과정을 현장관측과 스모그 챔버 연구를 통해 규명하는 연구를 수행하고 있다. 또한, 중국, 일본의 현지측정을 병행하여 미세먼지의 이동과정을 설명할 수 있는 지표물질을 찾아내고자 한다. 미세먼지는 미량의 다양한 화학성분으로 구성되어 있으므로, 정밀 정성·정량 분석기술이 필요한 연구 분야이다.

Symposium-6-B

Mechanistic Studies of Secondary Aerosol Formation Using Mass Spectrometry

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Atmospheric particulate matter (PM) affects human health and climate; however the formation is poorly understood because a large fraction is secondary. Main components of PM are ammoniums, sulfates, nitrates, organics and aerosol liquid water (ALW). Since organics are a myriad of individual compounds spanning a wide range of chemical and thermodynamic properities, they are the most challenging to be characterized. To simulate the formation of LA-type urban PM, smog chamber experiments of photochemistry of alkanes at high NO_x and low RH conditions) were conducted. Secondary organic aerosol (SOA) were organonitrates, which were characterized by a thermal desorption particle beam mass spectrometer. Alkyl nitrates and hydroxy nitrates were the first generation SOA, which was formed via gas-particle partitioning after becoming semivolatile. PM is also formed or aged through aqueous chemistry in ALW, a main component of hygroscopic aerosols, which are common in East Asia. Since this aqueous chemistry is connected to the gas-phase reaction, PM in East Asia is formed through multiphase chemistry. Highly water soluble volatile organic compounds (VOCs) dissolve in ALW and form SOA through radical or non-radical reactions. Reaction vessel and smog chamber experiments were conduted, and aqueous chemistry products were identified by using a high resolution mass spectrometer. Aqueous-phase photochemistry of glyoxal and methylglyoxal leads to the formation of dicarboxylic acids or multifunctional compounds. Lastly, through multiphase photochemistry at high NO_x and high RH in a smog chamber, nitric acid formed from NO_x dissolves in ALW leading to organonitrate formation and hygroscopic growth, which is considered the important mechanism for high concentration PM formation in Seoul.

Symposium-6-C

초고분해능 질량분석기를 이용한 이차유기에어로졸 특성 규명

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대기 중 미세먼지에 포함되어 있는 유기입자는 대기질과 기후변화 등 대기환경에 매우 밀접하게 연관되어 있다. 유기에어로졸은 생성 기원에 따라 입자 형태로 대기에 배출된 일차유기에어로졸(primary organic aerosol : POA)과 가스상 유기화합물의 대기 화학반응을 통해 입자상으로 변환된 이차유기에어로졸(secondary organic aerosol : SOA)로 구분된다. SOA 는 주로 다양한 형태의 산화된 유기 혼합물로 구성되어 있으며, 생성 경로에 따라 올리고머 및 질소 함유 성분도 상당한 수준으로 포함될 수 있다. SOA 의 화학조성은 유기화합물 전구체와 생성 반응 형태에 크게 영향을 받는다. 본 연구에서는 대표적 생물기원 유기화합물인 α-피넨의 SOA 생성 특성과 화학조성을 평가하였다. 특히 SOA 의 물리화학적 특성과 밀접한 관련이 있는 올리고머 성분과 질소 함유 성분에 대해 초점을 맞추었다. SOA 에 함유된 개별 성분의 분석에 초고분해능 질량분석기를 활용하였다. 경북대학교에서 개발한 스모그 챔버와 흐름반응기를 이용하여 다양한 반응조건에서 α-피넨의 SOA 를 생성하고, 테프론 코팅된 유리섬유 필터를 이용하여 SOA 시료를 채취하였다. 채취된 SOA 시료를 유기용매를 이용하여 추출한 다음 초고분해능 질량분석기인 FT-ICR MS 과 Orbitrap MS 을 이용하여 분석하였다. 검출된 각 성분에 대해 원자 수, 원소비, 질소 규칙 등 기준을 만족시키면서 측정과 이론적 질량의 오차가 가장 적은 화학식을 결정하였다. SOA 생성 조건에 따라 m/z 가 800 이하인 815 – 3501 개의 모노머와 다이머 성분이 확인되었다. NOx 가 없는 조건에서 생성된 SOA 는 대부분 전형적인 산화된 유기물(CHO)이었고, NOx 가 있는 조건에서는 질소를 함유한 성분(CHON)이 32% 정도까지 증가하였다. 다양한 반응에서 공통적으로 검출된 주요성분(예 : $C_9H_{14}O_6$, $C_{10}H_{14}O_6$, $C_{10}H_{16}O_5$, $C_{17}H_{26}O_7$, $C_{19}H_{28}O_9$, $C_{10}H_{15}NO_8$, and $C_{10}H_{15}NO_9$)은 α-피넨 SOA 의 마커성분으로 활용될 수 있을 것이다. CHON 성분의 O/C 원소비, 유기물/유기탄소 질량비(OM/OC), 탄소산화상태는 CHO 보다 높게 나타났다. 이것은 SOA 의 질소가 산화된 형태(예, $-ONO_2$)로 존재한다는 것을 나타낸다. 탄소 수에 따른 OM/OC 와 이중결합등가(double bond equivalent) 양상은 올리고머 생성반응이 매우 다양하다는 것을 보여준다.

Symposium-6-D

초미세먼지 유기지표성분 특성 및 기여량 분석

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도시 대기 중 PM2.5 농도에 기여하는 일반적인 원인으로는 (1) 도로변 발생 성분, (2) 식생 연소, (3) 식물성 유리 성분, (4) 석탄 화력발전소를 비롯한 각종 연소 성분, (5) 장거리 이동 성분, 그리고 (5) 광화학적 반응에 의한 2차 생성물 등이 있다. 이를 위해, 오래전부터 수용모델을 이용하여 기여량에 대한 많은 연구가 진행되어 왔지만, 이온성분 및 중금속성분에 국한된 입력 자료, 불확실성 산출의 제한 그리고 유기지표성분 부재 등으로 상대적으로 큰 불확실성을 내포하고 있다. 본 연구에서는 (1) 2018년 1월 한국 및 중국 동시 포집 시료, (2) 2015년 광주지역에서 계절별 포집한 시료, (3) 2016년 국내 KORUS-AQ기간 중 포집한 시료에 대해 유기지표성분(PAHs, alkanes, hopanes etc.) 등을 GCMS, LCMSMS 등을 이용, 종합적으로 분석하여, Chemical Mass Balance (CMB)와 Positive Matrix Factorization (PMF) 결과의 비교 분석 및 CMB-PMF 복합 수용모델을 이용하여, 대도시 주오염원 PM2.5 기여량을 분석하였다.

Symposium-6-E

Deciphering Chemical Information of Aerosol-derived Organic Substances Using Ultra-High Resolution FT-ICR Mass Spectrometry

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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 extremely 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 hazardous substances. The results of regional variations and size-segregated chemical variations of organic matter in ambient aerosols would be utilized to understand the particle formation mechanisms and their toxicity in human health.

Symposium-6-F

Characteristics of fine particle contamination in Ulsan, Korea: influence of local pollution and long-range transport

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Ulsan is the largest industrial city in Korea, emitting large amounts of particulate matter and precursors such as volatile organic compounds (VOCs). Recently, the highest $PM_{2.5}$ concentrations have been frequently observed in Ulsan without the influence of long-range transport from China. The recent high pollution events were probably due to local primary emissions and secondary formation, enhanced by low wind speed, high relative humidity, and strong solar radiation. In this presentation, we will overview the contamination characteristics of fine particle in Ulsan and introduce recent research activities in our group for evaluating local pollution and long-range transport. Not only instrumental analytical data, but also various statistical and modeling results will be discussed.

Symposium-7-A

Targeted and Non-targeted Metabolomics Approach to Comprehensive Understanding of the Effects of Brewing Conditions on Green Tea Infusions

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The effects of different brewing conditions on green tea infusions were comprehensively examined. To this, antioxidant assay and both non-targeted and targeted metabolomics analyses were performed using green tea infusions brewed at 60˚C and 90˚C for 5-300 min. The antioxidant capacities of the tea infusions depended more on temperature than time. Metabolic profiles were significantly changed by both temperature and time; the effects of time became evident at 95˚C starting after 30 min based on the profiles obtained by ultra-high performance liquid chromatography-quadrupole-time-of-flight mass spectrometric (UHPLC-Q-TOF-MS) analysis. Multivariate statistical analysis identified 33 differential compounds from various classes, including amino acids, organic acids, phenolic acids, flavonoids, and catechins. Hierarchical clustering analysis of the differential compounds showed that infusions brewed at 95˚C for greater than 30 min produced distinct profiles. It also revealed that prolonged brewing time led to alterations in relative levels of isomers, namely, *p*-coumaroylquinic acid, galloyl glucose, and catechin isomers. Eight major catechins that were identified and exhibited the most dramatic changes among the differential markers were further quantified by UHPLC-QqQ-MS. With brewing at 95˚C, the highest total catechin level was achieved at 10 min, after which the levels of four epi-form catechins decreased and those of four nonepi-form catechins increased. These results imply that catechins underwent epimerization during brewing. Overall, the current study suggests that green tea infusions and aqueous extracts of green tea should be evaluated not based on certain classes of compounds but based on a comprehensive understanding of non-targeted and targeted analyses and relevant activity assays.

Symposium-7-B

Surface labeling mass spectrometry for GPCR singaling analysis

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Protein-protein interactions and conformational changes of a signaling protein are major mechanisms of cellular signal transduction. To understand the precise signaling mechanism, studies have investigated the structural mechanism of signaling proteins using various biochemical and/or biophysical techniques such as X-ray crystallography, nuclear magnetic resonance (NMR), electron microscopy, and electron paramagnetic resonance. In addition to these techniques, surface labeling mass spectrometry techniques (e.g. hydrogen/deuterium exchange mass spectrometry (HDX-MS) or radiolytic footprinting mass spectrometry (FP-MS)) have been successfully used for conformational analysis of signaling proteins. These techniques have been useful tools for studying protein-protein interaction interfaces and conformational changes during a signaling protein activation. Although these techniques do not provide 3-D structural information, they analyze dynamic protein conformations that are difficult to be analyzed with other techniques. GPCR signal transduction involves extensive protein-protein interactions and conformational changes of related signaling proteins. In this seminar, I will discuss the conformational mechanisms of GPCR signaling analyzed by surface labeling mass spectrometry techniques.

Symposium-7-C

Photoisomerization in the Gas Phase Studied by Laser Spectroscopy and Tandem Ion Mobility Mass Spectrometer

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Ruthenium complexes involving sulfoxide ligands can undergo linkage isomerization upon light absorption, accompanied by dramatic changes in their optical properties. These remarkable photochromic properties are sensitive to the nature of the ligand as well as to that of the solvent. We used tandem ion mobility spectrometry coupled to mass spectrometry to gain direct experimental insight into the isomerization pathways connecting the different linkage isomers of an isolated ruthenium complex with two dimethyl-sulfoxide ligands. We find that the isomerization behavior of the solvent-free complex differs from that previously reported in the solution-phase, which is in line with recent theoretical predictions.

Symposium-7-D

Electrospray Ionization Mass Spectrometry Coupled With Gas Chromatography

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In this presentation, gas chromatography-electrospray ionization mass spectrometry (GC-ESI/MS) is introduced as novel ionization techniue and potential alternative analytical tools for screening of various substances. GC-ESI/MS configuration was developed and optimized. Several applications using GC-ESI/MS are presented: 1) on-line simultaneous H/D exchange of gas-phase molecules, 2) ionization and simultaneous analysis of anabolic steroids as trimethylsilyl derivatives and 3) ionization behavios of gas-phase polycyclic aromatic hydrocarbons.

This work was supported by Korea Institute of Science and Technology

Symposium-7-E

<KEYNOTE SPEAKER>

Expanding the Repertoire of Ion Activation Methods for Glycosaminoglycans

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Glycosaminoglycans (GAGs) are an important class of carbohydrates that play a central role in a number of biological processes, and their structural analysis is a target of substantial research effort [1]. Taken as a whole, glycosaminoglycans (GAGs) represent a challenging class of molecules to analyze due to their heterogeneity, the lability of sulfation modifications and the difficulty of distinguishing subtle structural differences, such as uronic acid stereochemistry. The last few years has seen considerable progress in GAG analysis by mass spectrometry with the introduction of supercharging methods for stabilizing sites of sulfation [2], chemical modification methods to replace sulfates with more stable functional groups [3], and novel methods of ion activation, such as electron detachment dissociation (EDD) [4]. We have investigated the applicability of EDD for fully characterizing several classes of GAGs with a single stage of tandem mass spectrometry. EDD has shown great utility for analyzing oligosaccharides from chondroitin/dermatan sulfate, heparan sulfate, and heparin. Generally speaking, EDD provides more structural detail than more widely used ion activation methods such as collision induced dissociation (CID) or infrared multiphoton photodissociation (IRMPD), and is less likely to lead to sulfate decomposition. Recently found that CID is useful for GAG analysis under selected circumstances. Specifically, CID has been useful for the analysis of full-length chondroitin sulfate saccharides from bikunin, for which the degree of sulfation is low compared to the degree of polymerization (0.3 sulfates per disaccharide repeat) [4]. Highly sulfated heparins have remained the most challenging of all GAG oligosaccharides to analyze. Surprisingly, we have recently found that CID is useful for this challenging class of GAGs if all of the ionizable protons are replaced by sodium ions [5]. Most recently, we have explored the utility of newer ion activation approaches that are compatible with FTMS instrumentation, specifically negative electron transfer dissociation (NETD) [6] and ultraviolet photodissociation (UVPD). This presentation will focus on a comparison these newest methods of ion activation with earlier approaches to sequencing GAGs.

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Symposium-8-A

<GUEST SPEAKER>

Overview of Proteomic Data Analysis

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As mass spectrometry-based proteomic datasets grow, scientists need high throughput computational resources to resolve bottlenecks in data analysis. Many research laboratories, however, do not have access to privately owned computer clusters to deal with large volumes of data. Even with a computer cluster, often it is too slow to run some types of data analyses such as a big database search or an unknown modification search. We developed a comprehensive solution, Integrated Proteomics Pipeline(IP2), to allow scientists to analyze proteomics data quickly from protein identification, quantitative analysis, to functional analysis through single user interface. The platform analyzes high-throughput proteomics data efficiently with high performance computing resources such as cloud or local parallel computational cluster. Unlike other proteomics data analysis tools, IP2 takes advantage of the High Performance Computing (HPC) massive cloud or parallel computing provided for proteomics data analysis. Also, IP2 provides user friendly web interfaces that allow our scientist to easily analyze mass spectrometry-based proteomics data. With some additional features (such as results summary, quality control parameters, enhanced multiple experiment comparison) added to IP2, scientists can significantly improve the quality and productivity of high-throughput proteomics data analysis. IP2-GPU algorithm utilize tens of thousands of GPU cores to dramatically improve search speed. Complicated post-translational modification (PTM) search, in which is extremely slow or closely impossible on regular computers can be analyzed in a timely manner using powerful IP2 computational tools.

A number of different data analysis software are integrated into the platform providing a single and consistent user interface to allow a user to process the big biomedical data in an easy way. The platform provides highly sensitive protein identification results with ProLuCID search engine. It also supports most quantitative analyses including 15N, SILAC, iTRAQ, TMT and label-free by using Census, a comprehensive quantitative analysis tool. Researchers can organize experiments with project organization tools and compare large number of samples quickly and confidently to identify proteins/peptides of interest. Largely, the IP2 provides three different functions for data analysis – protein/peptide identification, quantitative analysis, and functional analysis.

Protein Identification

We developed a protein identification software, ProLuCID that implements a three-tier scoring system to assess the quality of a match between a given peptide sequence and an acquired MS/MS spectrum. First, a binomial probability is used as a preliminary scoring scheme to select candidate peptide-spectrum matches (PSMs). Second, a modified cross-correlation score (XCorr) is calculated for each candidate PSM identified by the binomial probability. Finally, ProLuCID uses the distribution of the XCorr values for all of the selected candidate PSMs to compute a Z-score for the PSM with the highest XCorr. The ProLuCID Z-score combines the discriminative power of XCorr and DeltaCN, the standard parameters for assessing the quality of a PSM using the popular SEQUEST algorithm, and displays significant improvements in specificity over XCorr. ProLuCID also takes advantage of high-resolution MS/MS spectra leading to further improvements in PSM identification specificity when compared to low resolution MS/MS data.

Isobaric Labeling Analysis

Over the last decade, proteomic analysis by mass spectrometers has become an essential tool for addressing important biological questions. Initially, mass spectrometers were used to identify components of a proteome, but now they are commonly employed to quantitate proteomic differences induced by different biological conditions. Accurate quantitation benefits from a higher resolution mass spectrometer, which often reduces instrument scanning speed. . Census was initially developed to analyze MS data using metabolic labeling for quantitation, but it is also capable of analyzing MS data with isobaric tags.

Census version 2 can analyze isobaric labeling such as Tandem Mass Tag (TMT) or Isobaric Tags for Relative and Absolute Quantification (iTRAQ) with features including a reporter ion impurity correction, a reporter ion intensity threshold filter and an option for weighted normalization to correct mixing errors. TMT/iTRAQ analysis can be performed on experiments utilizing HCD only, CID/HCD dual scans or HCD MS3 data. To improve measurement accuracy, we implemented weighted normalization, multiple tandem spectral approach, impurity correction, and dynamic intensity threshold features.

Label-free Analysis

Compared with isotopic labeling approaches, label-free quantitative proteomics is cost-efficient and requires significantly less effort to prepare samples. With advances in high-resolution mass spectrometry, label-free analysis is gaining momentum.

However, it is hard to find analysis tools that can accurately measure peptide abundance from label-free data. To address the challenge of the label-free data analysis, we have developed chromatogram-based label-free algorithms to find statistically significant protein/peptides from different samples analyzed using the latest mass spectrometry technology. Census aligns chromatograms using identified peptides, retention time and accurate precursor masses. After alignments, Census groups peptides to calculate their ratios between different samples. The challenge in labelfree analysis is how to quantify peptides that are identified in some samples but not in all samples, because typically chromatograms are re-constructed from identified precursor mass information. This can cause problems in later stage analysis by calculating statistical p-value with incorrect standard deviation. Our new algorithm addresses this problem, extracting chromatograms for missing peptides using accurate precursor mass and retention time. We, then, applied statistical analysis to calculate p- and q-values.

Extremely large protein database search (Metaproteomic Data from Microbiomes)

As microbiome databases grow very large and mass spectrometry instruments generate very large datasets of high-resolution data, limited computational resources have made data analysis for identifying and quantifying proteins in microbiomes a challenge. Database search engines typically pre-process protein sequence database by indexing in-silico peptides by mass in order to speed up protein identification. NoSQL databases allow simple "horizontal" scaling to a computational cluster of machines. This design is optimal for distributed analysis as an MS dataset can be divided into chunks that are processed independently on cluster nodes, with individual nodes each querying the same proteomic database over a local network. We developed ProLuCID-ComPIL to process extremely large metaproteomics databases using NoSQL database techniques with fast search engine. We organized our protein data into three distributed MongoDB databases. Protein sequences were stored in a protein database and digested *in silico* using trypsin specificity. The resulting peptide sequences were grouped by identical peptide mass or sequence and stored in mass or sequence databases, respectively.
We downloaded protein files from publicly available microbiome databases and concatenated them to build a 35 GB fasta file. The fasta file was appended with decoy sequences and had a final size of 70GB. We indexed and uploaded the database file to MongoDB. The final database size in MongoDB is 1.088 TB (a 75 GB protein database, 258 GB mass database, and 755 GB sequence database). We searched E.coli data against MongoDB database using ProLuCID-ComPIL. For evaluation, we compared peptides identified from ProLuCID search engine to peptides identified from ProLuCID-ComPIL search. 96% of E.coli peptides from ProLuCID were overlapped with ProLuCID-ComPIL search results.

ProteinInferencer

ProteinInferencer is a novel algorithm that was developed to assess protein identifications based on a large number of MS experiments. It computes a global false discovery rate (FDR) and a local false discovery rate for the analyzed datasets. It also differentiates subset proteins and computes total protein sequence coverage, spectral count, and peptide count for each protein group. An option to output MS/MS spectra to the COPa spectrum library with a well-controlled FDR will also be added to ProteinInferencer. A manuscript on ProteinInferencer has been recently published in the Journal of Proteomics.

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Symposium-8-B

Secondary structural analysis of peptides and proteins using ion mobility-mass spectrometry combined with gas-phase infrared spectroscopy

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Mass spectrometry has been a routine tool for identifying and analyzing various biological molecules. Most recently, the structural studies of peptides, proteins, and their assemblies using MS-based methods firstly came to light in the developments of native mass spectrometry using very soft nano-electrospray ionization and have been significantly extended by emerging ion mobility mass spectrometry. However, the key question in this field has been whether the structures of small to medium-sized proteins can be conserved after transfer to the gas phase via ionization. A clarification of this problem is important since it would allow very sensitive native mass spectrometry to be used to address problems relevant to structural biology.

In this work, firstly, a combination of ion mobility-mass spectrometry and gas-phase infrared spectroscopy was used to investigate the secondary and tertiary structure of proteins transferred from solution to the gas phase.[1] The results show that for low charge states under gentle ionization conditions, aspects of the native secondary and tertiary structure can be conserved. Based on this result, we further applied this experimental method to investigate amyloidogenic peptide aggregates and succeeded the first direct seconday-structure analysis of every individual amyloid intermediate from dimer up to dodecamer.[2] Our data reveled that oligomers of the fibril-forming short peptide segments, which consist of 4-9 peptide strands, can contain a significant amount of β-sheet. These results clearly suggest that the ion mobility-mass spectrometry combined with gas-phase infrared spectroscopy can be used to investigate the secondary structures of proteins, peptides, and their aggregates.

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Symposium-8-C

Molecular insights of amyloid fibrillation and inter-fibrillar aggregations of α-synuclein associated with hard divalent metal cations

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Human α-synuclein (αSyn) is an intrinsically disordered protein, whose aggregation is associated with the pathogenesis of several neurodegenerative diseases, such as Parkinson's disease, and Lewy body dementia. Although the detailed αSyn aggregation process in the patients' brain is not fully understood, various hard divalent metal cations have been shown to accelerate αSyn aggregation. Especially, dyshomeostasis of Ca^{2+} was suggested to be a pathological cause of αSyn aggregation. To understand the molecular role of Ca^{2+} and hard divalent metal cations in αSyn aggregation, the structural change of αSyn in the presence of Ca^{2+} was examined using ion mobility-mass spectrometry (IM-MS) and solution small angle X-ray scattering (SAXS). Our results demonstrated that binding of multiple Ca^{2+} ions induces the structural change of monomeric αSyn to expose fibrillation-prone NAC domain to water, and furthermore provokes interfibrillar aggregation mainly *via* electrostatic interaction. Based on the results from multiple biophysical techniques, we presented the mechanism of divalent metal cation-mediated αSyn aggregation. Overall, our study provides the molecular details of structural transition and aggregation mechanism of αSyn in the presence of hard divalent metal cations. Our results would be valuable for understanding the role of dysregulated Ca^{2+} and other divalent metal cations in the pathology of αSyn-related diseases.

Symposium-8-D

Mass spectrometry for Biomedical Research

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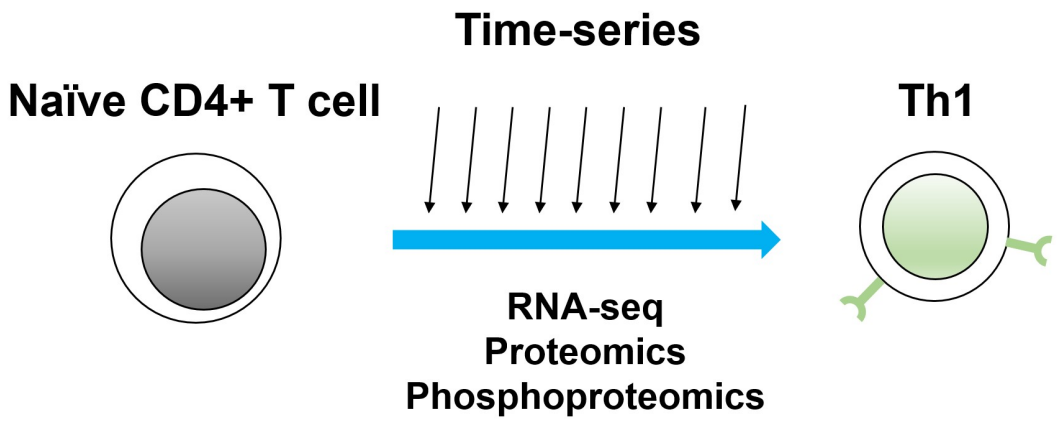
Cellular function is coordinated by complex interactions of essential biomolecules such as DNA, RNA and proteins. Technological advances in genomics, epigenomics, transcriptomics and proteomics have enabled massively parallel measurements of such cellular molecules. Recently we have carried out a unified multi-omic analysis of the genome, epigenome, transcriptome and proteome using a single human cell type to gain a coherent view of molecular status of the cell. During the analysis, we have encountered a difficulty of comparing two states of the cell type since RNA-protein abundance showed a poor correlation. Here, I describe new analysis of human primary naïve CD4+ T cells that were differentiated into Th1. RNA-seq, proteomics and phosphoproteomics were carried out in this time-course experiment of naïve CD4+ T cells differentiation. This analysis provided mechanistic insights into how several molecules involved in T cell receptor signaling are regulated at the RNA, protein and phosphorylation levels.



Symposium-8-E

Comprehensive RNA-interactome profiling in multicellular samples using formaldehyde-crosslinking

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RNA interactome profiling in light-impermeable multicellular samples has not been fully accessible with conventional ultraviolet crosslinking (UVX). Herein, we report that a kinetic-controlled formaldehyde treatment *in vivo* allows for sufficiently specific crosslinking of RNA to proteins with substantially enhanced efficiency compared to UVX. Owing to the good membrane permeability of formaldehyde, *in vivo* formaldehyde crosslinking enables comprehensive profiling of the RNA interactome (>700 proteins) even for previously unconquered light-impermeable samples such as *Xenopus laevis* oocytes/embryos.

KSMS

2018 한국질량분석학회 여름정기학술대회 및 총회

POSTER PRESENTATION

포스터 발표 및 우수포스터상 안내

■ **포스터 게시 및 철거**

- 게시: 23일(목), 08:00 ~ 10:00 까지
- 철거: 23일(목), 19:00 ~ 이후

- 포스터 발표자는 아래의 포스터 번호 및 배치도를 참고하여 포스터를 게시하고, 23일(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: 2018년 8월 24일 (금), 폐회식
- 부상: 상장 및 상금 5 만원

■ **분야별 포스터 번호**

분야	포스터번호
Fundamental & Instrumentation	001 ~ 011
Life & Informatics	012 ~ 023
Biological & Environment	024 ~ 060
Medical/Pharmaceutical Science	061 ~ 091
Food	092 ~ 103
General	104 ~ 132

1. Fundamental Instrumentation : P001 ~ P011

P-001

Ambient laser desorption of mouse hippocampal tissue slice on graphene layer substrate for high spatial resolution mass spectrometric imaging

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P-002

Hyphenation of thin layer chromatography (TLC) with mass spectrometry (MS) - a powerful tool for herbal medicinal products (HMPs)

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P-003

Development of a portable GC/ITMS for on-site VOC detection

Bongyoon Yi[1,2], Wanseop Jeong[1,2], Seung Yong Kim[1], Jae Yeong Eo[1], Byoung Seob Lee[1], Byeongwon Kang[2,*], and Hyun Sik Kim[1,*]

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P-004

An emission model for cold election ionization in portable ITMS

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P-005

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

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P-006

Development of a Gas Mixing System for the Production of Fire-Hazardous Standard Gas

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P-007

Mechanism Studies of FRIPS Mass Spectrometry

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P-008

Elucidating of hydrodesulfurization of polycyclic aromatic sulfur hydrocabon compounds in crude oil using ion mobility mass spectrometry

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P-009

Energy-resolved Collision-induced Dissociation Study of Na^+-bound G-quartets with Mixed Ligands, $[Na(Guanine)_n(9\text{-methylguanine})_m]^+$

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P-010

Anomaly in Collision-induced Dissociation of Proton-bound Hoogsteen Base Pairs of Cytosine and Guanine by Proton Transfer

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P-011

Signal reduction due to solvent composition of molecular ions generated from aromatic compounds in (+) atmospheric pressure photoionization mass spectrometry.

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2. Life & Informatics
: PO12 ~ PO23

P-012

Profiles of oxidized phospholipids in exosome from oxidatively stressed cells by flow field-flow fractionation and nUHPLC-ESI-MS/MS

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P-013

Effect of aging on lipid alteration in serum, kidney, and heart from mice by nUHPLC-ESI-MS/MS

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P-014

Optimization for quantitative analysis of glycan in yeast using metabolic isotope labeling of polysaccharides with isotopic glucose (MILPIG) by mass spectrometry

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P-015

***In-vivo* isotopic glucose labeling of glycan in fungi using metabolic isotope labeling of polysaccharides with isotopic glucose (MILPIG) for quantitative mass spectrometry**

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P-016

Proteomic Analysis of Cervicovaginal Fluid for Early Detection of Preterm Birth by 2D-nLC-ESI-MS/MS

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P-017

Optimizing extraction efficiency of serum steroids in advanced GC-MS/MS-based profiling

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P-018

Metabolic signitures of adrenal steroids in serum and saliva measured by polarity switching LC-MS

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P-019

GC-MS-based metabolic signitures of Cushing's syndrome in serum cholesterols

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P-020

Plasma lipid metabolites profiling for internet gaming disorder in korean males

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P-021

Discovery of a unique metabolic profile for activated Wnt / beta-catenin signaling

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P-022

Computational Characterization of Core and Outer Fucosylated N-Glycoproteins with LC-MS/MS and IQ-GPA

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P-023

A Web-based MS/MS Spectral Library dedicated to Structure Elucidation of Natural Products

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3. Biological & Environment : PO24 ~ PO6O

P-024

Observation on Regenerated Bony Rays of Zebrafish Caudal Fin using Time-of-Flight Secondary Ion Mass Spectrometry

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P-025

Direct MS Analysis of Drugs of Abuse in Urine Using Biocompatible Solid Phase Microextraction (BioSPME)

Frank Michel*[,1], Emily Barrey[2], Craig R. Aurand[2], Candace Price[2], Sara Smith[2]

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P-026

Improved LC/MS of peptides by innovative particle design and dedicated mobile phase additives

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P-027

Improved LC/MS/MS analysis with on-line SPE for removal of phospholipids from protein precipitation biological fluid samples

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P-028

Quantitative analysis of lead in soils by fsLA and ICP-MS

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P-029

Structural Profiles of Gangliosides in Developing Human brain via Negative Ion Mode Nano- LC/MS/MS

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P-030

Identification of Missing Proteins in Human Olfactory Epithelial Tissue by LC-MS/MS

Ji Eun Jeong[1,2], Heeyoun Hwang[1,2,3], Hyun Kyoung Lee[1,2], Ki Na Yun[1,4], Bonghee Lee[5,6], Young-Ki Paik[7], Gi Taek Yee[8], Jin Young Kim[1], and Jong Shin Yoo[1,2*]

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P-031

Validation of Analytical Methods Using LC-MS to Characterize HGH [Human Growth Hormone]

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P-032

Validation of Analytical Methods Using LC-MS to Characterize Bevacizumab

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P-033

Validation of Analytical Methods Using LC-MS to Characterize Trastuzumab

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P-034

Comparison of lipid profiling of *Drosophila* head using MALDI-MSI(Matrix assisted laser desorption ionization-mass spectrometry imaging) and ESI-MS(electrospray ionization mass spectrometry)

Hyun Jun Jang[1,2], Jeong Hyang Park[3], Jeong Hee Moon[4], Ga Seul Lee[4], Joon Sig Choi[2], Sohee Yoon[1*]

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P-035

Quantitative Proteomic Analysis of 2D and 3D Cultured Colorectal Cancer Cells: Profiling of Tankyrase Inhibitor XAV939-Induced Proteome

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P-036

Multiresidue analysis of PHTs, VOCs, phenols, parabens, PAHs, pyrethroid insecticides and tobacco smoke in human urine by LC-ESI/MS/MS

Seunghwa Lee[1,2], Kang Mi Lee[1], Minho Yang[3], Sang Moon Han[1,2], Ho Jun Kim[1], Yong Min Cho[3], Sang Beom Han[4], Hosub Im[3], Jaeick Lee[1,*]

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P-037

Solid Phase Extraction of nerve agent degradation products using poly(METAC) plate and TOF-SIMS analysis

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P-038

Quantitative proteomics of 2D-/3D-cultured adipocyte cells and its co-cultured with macrophages using a nanoLC-ESI-MS/MS

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P-039

Strong advantages of plasma mass spectrometry to analyze ultra-trace level radioactive isotopes in small amount of environmental samples

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P-040

Comparison of organic mixtures from particulate matters collected in Korea and China by using GCxGC/high resolution mass spectrometry

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P-041

Development of simultaneous analysis of 93 persistent organic pollutants (POPs) in human serum by QuEChERS method and GC-MS/MS

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P-042

Cross-validation of sulfur-based and amino acid-based quantification methods for the development of insulin reference material

Hwijin Kim[1,2], Ji-Seon Jeong[1,3], Thi Thanh Huong Tran[1,3], Youngran Lim[2], Sung Woo Heo[2], Yong-Hyeon Yim[1,2*]

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P-043

Environmental product for reference material

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P-044

A method for quantitative analysis of nucleic acids using a nanoflow liquid chromatography-tandem mass spectrometry

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P-045

The metabolites differences in a wing polyphenic small brown planthopper revealed by metabolomic analysis

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P-046

LC/MS and LC-UV analysis of photodegradation products of tetracycline and sulfathiazole

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P-047

ICP MS Analyses of deciduous teeth for exposomics research

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P-048

Analysis of Isomeric Glycopeptides by High Temperature LC-MS/MS

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P-049

LC-MS based rapid profiling and inhibits xanthine oxidase activity from *Salbia plebeia*

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P-050

Parallel reaction monitoring of fucosylated glycopeptides of alpha-fetoprotein in human serum for early hepatocellular carcinoma by LC-MS/MS with immunoprecipitation

Kwang Hoe Kim [1, 2], Soo-Youn Lee [3], Heeyoun Hwang [2], Ju Yeon Lee [1], Eun Sun Ji [1], Hyun Joo An [2], Jin Young Kim [1, *] and Jong Shin Yoo [1, 2,*]

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P-051

Proteomic analysis of exosomal proteins from rat Schwann cell

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P-052

Spatial distribution of siloxanes in coastal sediment and identification of procedural contamination sources in GC/MS analysis

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P-053

Characterization of site-specific O-glycopeptides in fibroin heavy chain from silkworm cocoon using high resolution LC-MS/MS

Hyun Kyoung Lee[1,2*], Gun Wook Park[1], Ji Won Lee[1,2], Jin Young Kim[1], Yong Koo Kang[3], Jin Hwan No[4], Kyoung Tai No[4,5] and Jong Shin Yoo[1,2]

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P-054

Automated screening of organic pollutants in airborne particulate matter using GC×GC-TOFMS

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P-055

LC-MS/MS-based DIA method approach for proteome analysis on synechocystis sp. PCC6803 and PCC7338

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P-056

Validation and application of analytical tools for stable carbon isotope analysis of crude oils in molecular level using ultra-high resolution mass spectrometry

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P-057

Performance evaluation of ICP-MS for Ra-226 determination

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P-058

Development and validations of the simultaneous analytical method of nine environmental phenol compounds in human urine samples using liquid chromatography – tandem mass spectrometry

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P-059

Selection of functional metabolites of Torreya nucifera by comparison of metabolites

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P-060

Quantitative proteomic analysis of molecular and functional alterations in the human neuronal cell culture model of Alzheimer's disease

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4. Medical/Pharmaceutical Science : PO61 ~ PO91

P-061

Simultaneous LC-MS/MS analysis of three alkanolamines found in cosmetics

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P-062

Rapid determination of β-lapachone in clinical samples using LC-MS/MS

Bo Kyung Kim[1], Hyun Ji Han[1], Mi-Ri Gwon[1,2], Boram Ohk[1], Sook Jin Seong[1], Seungil Cho[1,3], Young-Ran Yoon[1,2,3]

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P-063

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

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P-064

Diagnosis of gout and pseudogout using inorganic TiO2 matrices for LDI-ToF mass spectrometry

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P-065

Diagnosis of galactosemia by MALDI-TOF mass spectrometry using a parylene-matrix chip

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P-066

Development of sensitive β-lactamase assay for *E.coli* using a parylene-matrix chip

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P-067

Quantitative and sensitive carbapenem susceptibility test using MALDI-TOF based on a parylene-matrix chip

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P-068

Better sensitivity in LC/MS by improved sample preparation and HPLC method for determination of vitamin D metabolites in plasma

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P-069

Isolation, Characterization and Quantitative Analysis of Major Compound in Different Parts of *Hovenia dulcis* using Ultra-Performance Liquid Chromatography Coupled with Orbitrap Mass

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P-070

Urinary Metabolomic Profiling to Discover Potential Biomarkers of Acute Cellular Rejection in Kidney Transplant Recipients

Sun-Young Kim[1], Bo Kyung Kim[1], Mi-Ri Gwon[1], Sook Jin Seong[1], Boram Ohk[1], Woo Youl Kang[1], Hae Won Lee[1], Hee-Yeon Jung[2], Jang-Hee Cho[2], Chan-Duck Kim[2], Young-Ran Yoon[1] and Seungil Cho[1]

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P-071

Optimization of analysis conditions for native disulfide bond using mass spectrometry

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P-072

Simultaneous analysis of highly acidic glycans in biotherapeutics using PGC-SPE and LC-MS/MS

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P-073

Detection of Neu5Gc in Human Serum via MRM-MS

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P-074

Synergistic antibacterial activity of phenolic compound-antibiotic combination and their quantitative determination by LC-QTOF-MS

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P-075

Rapid and sensitive determination of apixaban in human plasma using LC-MS/MS

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P-076

Rapid and sensitive determination of empagliflozin and dapagliflozin in human plasma using LC-MS/MS

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P-077

Rapid and sensitive determination of dexamethasone in culture media using LC-MS/MS

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P-078

Development and validation of HPLC-MS/MS method for the determination of 9-cis and trans-β-carotene in rat plasma using solid phase extraction.

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P-079

Relative quantification of lipids in mouse serum for the discovery of preterm birth and miscarriage biomarker via metabolic heavy water labeling

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P-080

High-throughput discovery of anti-inflammatory components in Aster Yomena

Sol Bi Park[1,2], Ho Jae Lee[2], Si Hyun Seong[3], Min Sun Kim[1], Sang Wan Seo[2,*], and Hyun Sik Kim[1,*]

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P-081

Quantitative analysis method for metabolic markers of Preterm births and miscarriage

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P-082

Development of Screening Software for Illicit Drugs and Analogues

Inae Jang and Han Bin Oh*

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P-083

Visualization of the distribution of small molecule in pig-to-nonhuman primate islet xenotransplantation model by MALDI-MS imaging

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P-084

Metabolic change of serum polyamines after Mediterranean diet and contrave treatment on overweight breast cancer patients

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P-085

Estabilishment of stability conditions to analyze vitamin B12 using LC-MS/MS

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P-086

Global absolute quantitation of human whole saliva proteins using nLC-Q-IMS-TOF with MS^E

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Global identification of proteins in Korean Whole Saliva

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Non-targeted metabolite profiling of maternal plasma for accurate diagnosis of preeclampsia

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P-089

Synthesis of ^{14}C labeled peptides used for quantification of peptides using nano-tracing technique and accelerator mass spectrometry

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P-090

Lectin affinity selection for plasma glycoprotein analysis of healthy elderly groups

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P-091

Discovery of predictive serum biomarker cadidates for tyrosine kinase inhibitors response in metastatic renal cell carcinoma by using mass spectrometry-based proteomics approaches

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P-092
Novel GlcNAc-containing oligosaccharides in Aspergillus oryzae β-galactosidase-treated bovine whey permeate

Hyeyoung Lee,[1,2] Juliana Maria Leite Nobrega de Moura Bell,[2] and Daniela Barile[2]

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P-093
Comparative analysis of recovery of heavy metal concentration by sample pretreatment methods

Eunji Kim, Sunghwa Choi, Minyoung Lee, Yuri Lee, Eunmi Choi
Jeongeun Park, Kyungsu Park*

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P-094
Study on the safety of hazardous substance according to oil extraction methods

Jeong-Yun Hwang*, Hye-Eun Lee , Tae-Hun Kim, Sheen Hee Kim,
Jang Duck Choi, Gil-Jin Kang

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P-095
Determination of the geographical origins of various propolis samples via UPLC combined with high-resolution FT-ICR mass spectrometry

Cho Hyun Kim,[1,2*] Mee Young Kim,[3] Seung-Wan Lee[3] and Kyoung-Soon Jang[1,4]

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P-096
Validation of tocopherol analysis in leafy vegetables using Standard addition-isotope dilution liquid chromatography mass spectrometry method (SA-IDMS-LC/MS)

Minkyung Sung[1, 2], Joonhee Lee[1], Byungjoo Kim[1], Jeongkwon Kim[2]

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P-097
Analysis of Polycyclic Aromatic Hydrocarbons in Olive Oil using Isotope Dilution-Gas Chromatography/Mass Spectrometry

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P-098
Determination of ciguatera fish poisoning toxins (ciguatoxin) in fish by liquid chromatography-tandem mass spectrometry

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P-099
Simultaneous determination of five urushiol analogues in lacquer tree extract by using LC-MRM and QuEChERS with EDTA

Ha Ra Cho[1], Dong Yoon Kim[1], Hyo Chun Lee[1], Seung Muk Hyun[2],
Sang Beom Han[2], Yong Seok Choi[1*]

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P-100
Novel methods to analyze residual neomycin, streptomycin, and dihydrostreptomycin in acacia honey, manuka honey, and mixed flower honey by using LC-MRM with WCX SPE

Han Sol Kim[1], Ha Ra Cho[1], Hyo Chun Lee[1], Sang Beom Han[2],
Ho-Chul Shin[3], Yong Seok Choi[1*]

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P-101
Primary and secondary metabolic profiles according to regional characteristics of *Glycine max* in Korea

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Comparision of aroma components by coffee producer using GC-MS

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Development of qualitative and quantitative system for simultaneously screening 395 pesticide residues by high resolution mass spectrometry

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P-104

MALDI-MS analysis of small molecules using N-doped carbon dots as matrix

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Application of MOF-5 and UiO-66 as MALDI matrices for analysis of small molecules

Yeoseon Kim, Jinseong Oh, Dabin Lee, Sol Han, Hyemin Choi, Jungseok Hoe, and Jeongkwon Kim*

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Detection of small molecules using MALDI-ToF mass spectrometry with TiO_2 nanowire solid matrix

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Trace element analysis of optical fiber

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P-108

Analysis of iso-maltooligosaccaride by matrix-assisted laser desorption/ionization mass spectrometry using ionic liquid matrices

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Construction of Isomer-Specific and Region-Specific Mouse Brain Ganglioside Library using UHPLC-QTOF MS/MS

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P-110

Effect of matrices and drying processes sample preparation in MALDI-MS

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P-111

Biomarker discovery of coronary artery disease : serum protemic profiling

Arum Park[1], Jiyeong Lee[2], Sora Mun[1], Hyo-Jin Kim[1], Yoo-Jin Lee[1], Yoo-Rim Lee[1], Sang Hyun Park[3], Hee-Gyoo Kang[1, 2]

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Biomarker discovery of large artery atherosclerosis stroke: serum proteomic profiling

Jiyeong Lee[1], Arum Park[1], Sora Mun[2], Hyo-Jin Kim[2], Yoo-Jin Lee[2], You-Rim Lee[2], Soo Joo Lee[3], Hee-Gyoo Kang[1,2]

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Biomarker discovery of rheumatoid arthritis: serum proteomic profiling

Sora Mun[1], Jiyeong Lee[2], Arum Park[2], Hyo-Jin Kim[1], Yoo-Jin Lee[1], You-Rim Lee[1], Mi-Kyoung Lim[3], Hee-Gyoo Kang[1,2]

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Production of high purity gallium metal for compound semiconductor and trace elements quantification

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Introduction to B-10 isotope ratio analysis for the reactivity of reactor core

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Mass spectrometric study on the source of error in quantification of fatty acids

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Development of extraction method for dried blood spot

You-Rim Lee[1], Ae Eun Seok[1], Hyo-Jin Kim[1], Yoo-Jin Lee[1], Sora Mun[1], Sung Hee Hyun[1,3], Ho Joong Sung[1,2], Hee-Gyoo Kang[1,2,*]

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Understanding the DMSO effect on the drug efficiency of cisplatin using ICP-MS

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

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Validation of Analytical Method for Determination of Cyanide in Rat Blood Using Gas Chromatography-Tandem Mass Spectrometry

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Intense signal problem on TDC based LC/qTOF system

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Evaluation of quantitation performance of paper cone spray ionization (PCSI) mass spectrometry (MS)

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Analysis of trace elements in high-purity alumina powder using gravimetric standard addition method with internal standard by inductively coupled plasma optical emission spectroscopy

Eunhwa Kim[1,2], Cheongah Go[1], Hyungsik Min[1], Myungsub Han[1], Sungwoo Heo[1], Youngran Lim[1], Taekyu Kim[2], Kyoungseok Lee[1,*]

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Development of an Analytical Method for the Identification of Saliva-Specific Glycans in Trace Amounts of Human Saliva

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P-124

Study on analysis method of polyol in Polyurethane foam by Matrix-assisted laser desorption/ionization-Time of flight (MALDI-TOF)

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Understanding the DMSO effect on the drug efficiency of cisplatin using ICP-MS

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Effective determination of famphur in honey by gas chromatograph/mass spectrometer

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P-127

Characterization of polymer additives by high resolution-GC/MS

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Structure determination of Zn phthalocyanine compounds based on demetallization reaction

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Single-Injection Screening of 664 Forensic Toxicology Compounds using an Innovative Benchtop High Resolution Mass Spectrometer

Oscar G. Cabrices[1], Alexandre Wang[1], Xiang He[1], Holly McCall[1], Laura Baker[1], Adrian Taylor[2].

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Development of protein characterization analytical method for antibody drug fragments

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Simultaneous analysis of ginsenosides in fermented black ginseng, using LC/MS/MS

Ji-young Kim[1], Jung Dae Lee[2], Jin Ju Park[1], Hyang Yeon Kim[1], Jeong Eun Lim[1] and Kyu-Bong Kim[1]

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In-vitro antibacterial and antioxidant properties of flower, leaf, and stem extracts of *Agastache rugosa*

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Poster - 1

Ambient laser desorption of mouse hippocampal tissue slice on graphene layer substrate for high spatial resolution mass spectrometric imaging

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We report an ambient MS imaging system with efficient desorption procedures by using 532 nm-continuous wave (CW) laser and graphene layer substrate for ambient desorption and subsequent ionization step with an aid of plasma system. In order to facilitate the desorption process in this system, the use of a suitable material respond to the 532 nm laser is essential, so that a graphene layer was used as a light absorbing substrate at a visible wavelength. The graphene layer absorbs mainly the light energy in the UV wavelength, but also absorbs the visible wavelength quite well, so that the visible laser can be used as an ambient desorption source with the help of a graphene layer. Graphene can respond to multiple wavelengths because of broad and strong light absorption property in the visible region of light, which can widen the availability of light source for sample desorption. Instead of using gold nanoparticles that serve as light energy reservoirs inside the specimen, the fabrication of a light absorbing layer on the substrate allows for fast and simple specimen preparation with no additional pre-treatment, so that biological specimens that have difficulty in analysis due to complicated specimen preparation can be successfully analyzed with this MS method.

Poster - 2

Hyphenation of thin layer chromatography (TLC) with mass spectrometry (MS) - a powerful tool for herbal medicinal products (HMPs)

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TLC allows sample preparation and chromatographic separation in one step. This is possible because of the high sample matrix tolerance of this technique. TLC can be coupled directly to mass spectrometry (MS) via various approaches [1]. As a result, the advantages of TLC to separate many samples in parallel without time-consuming sample preparation are now combined with the powerful and versatile detection method mass spectrometry (MS). Several techniques for coupling TLC with MS will be discussed such as elution-based systems for direct solvent extraction from the plate, and the desorption-based approach MALDI (matrix-assisted laser desorption/ionization) using a laser beam for the spatial scanning of the plate. A consequence of the hyphenation of MS with TLC are increased requirements on TLC plates in terms of purity and sensitivity MS compatibility [2]. All data presented was acquired on newly developed HPTLC plates dedicated for MS detection.

Herbal Medicinal Products (HMPs) often consist of a highly complex mixture of both active and inactive ingredients resulting from the extraction of medicinal plants. The development of appropriate analytical separation methods can therefore be an arduous task. HPLC analysis is often challenged by the high matrix content of the samples. This work focuses on the advantages of TLC-MS analysis for these highly matrix-loaden phytopharmaceuticals.

[1] W. Schwack, J. Chromatogr. A. 1217 (6600-6609), 2010
[2] G. Morlock, J. Liq. Chromatogr. Rel. Techn. 37 (2892-2914), 2014

Poster - 3

Development of a portable GC/ITMS for on-site VOC detection

Bongyoon Yi[1,2], Wanseop Jeong[1,2], Seung Yong Kim[1], Jae Yeong Eo[1], Byoung Seob Lee[1], Byeongwon Kang[2,*], and Hyun Sik Kim[1,*]

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A portable gas chromatography (GC) was developed. It showed that real-time volatile organic compounds (VOCs) detection was possible with fast ramping temperature gradient provided with a low thermal heating system. The low thermal heating system was realized by coating the carbon nanotube (CNT) heating paste on an anodized aluminum bobbin and then electric currents were provided through gold and copper electrodes on the nanotube-paste. Also, we applied a new membrance interface to connect the low thermal GC and the portable ion trap mass spectrometer (ITMS) to achieve enhanced sensitivity and accurate molecular identification within a restricted size of portable GC/MS. By using a nitrogen carrier gas, VOCs were flowed through and were separated due to an interaction between the VOCs and the column coating materials of GC column, and then were splitted into /or pass through sequentially a photo-ionization detector (PID) and the ITMS. The GC eluent gas could not be injected directly due to restricted performance of a portable ion pump. At this time, the membrane interface allowed an operation of the ITMS efficiently only with a mini-ion getter pump. The membrane interface also provided a concentrating effect because it has a higher permeability to VOCs than carrier gases such as N_2. We present two different configurations of two different ion detectors, and in addition, various advantages of a simultaneous detecting system for on-site VOC detection.

Poster - 4

An emission model for cold election ionization in portable ITMS

Byoung Seob Lee[1], Wanseop Jeong[1,2], Bongyoon Yi[1,2], Seung Yong Kim[1], Jae Yeong Eo[1], and Hyun Sik Kim[1,*]

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A portable Gas Chromatography Mass Spectrometer (pGCMS) has been developed for in-situ analysis of various gas in our group. The pGCMS is composed with a low thermal GC and a miniaturized ion trap mass spectrometer. For the portability of pGCMS, the size of ion trap was reduced and electrons were generated in energy saving mode with cold electron ionization source provided by secondary electron emission from microchanle plate electron multiplier induced by 260 nm UV photons from light-emitting diode (LED). The electron behaviors in cold electron ionization source are main design factor to improve the performance of the ion trap. The various emission models of cold electrion behavior were studied and a user defined emission model for the design of ion trap were adopted to investigate the electron behaviors inside ion trap using OPERA-3D. Probably, the simulation results provided useful information to explain cold electron generation and its applications.

Poster - 5

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

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Phosphorylation is one of the most important post-translational modifications (PTMs) of proteins, which modulates a wide range of biological functions and activity of proteins. The analysis of phosphopeptides is still one of the most challenging tasks in proteomic research by mass spectrometry. In this study, phosphopeptide enrichment carried out on a digital microfluidic (DMF) chip was demonstrated by analyzing phosphopeptides in the tryptic digested *β*-casein (bovine) and ovalbumin (chicken). This approach was made using a magnetic bead (MB)-based titanium dioxide (TiO_2)-solid phase extraction (SPE) procedure. TiO_2-MB was employed to selectively enrich phosphopeptides from tryptic digests of *β*-casein and ovalbumin. The enriched phosphopeptides were detected using matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF MS). To evaluate the efficiency of the proposed enrichment method, the result is compared with the mass spectrometric data obtained from nano LC-ESI-MS analysis of the same phosphopeptides. This study shows that the phosphopeptide enrichment analysis can be automated and analyzed with a small sample volume on the DMF chip.

Poster - 6

Development of a Gas Mixing System for the Production of Fire-Hazardous Standard Gas

Hwa-yong Jang, Han Bin Oh*

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As the fire occurs, various kinds of toxic gases are generated and different material generates different toxic chemicals. During the investigation of the fire, investigators are easily exposed to toxic gases for a long time. Due to the lack of methodology or instruments enabling the real-time identification of toxic gases present in the field, respiratory-related industrial accidents of on-site police officers are constantly occurring every year. Related government departments have been developing a portable sensor capable of identifying and measuring the amount of poisonous gas in the field so that it can be used to prevent investigators from being exposed to hazardous environments. To test the accuracy and efficiency of the device, we are currently developing of a gas mixing system which is designed to provide standard fire-hazardous gases. The system is equipped with a mass flow controller (MFC) that enables the precise control of the amount of flow and a vacuum gauge that accurately measures gas pressure in the order of a few mtorr. Developed device is expected to allow a reproducible production of standard gases. Accuracy of the concentration of standard gas prepared by developed samples will be evaluated by GC analysis in the future.

Poster - 7

Mechanism Studies of FRIPS Mass Spectrometry

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A method of free radical initiated peptide sequencing (FRIPS) is a radical-based tandem mass spectrometry method in which a radical cation precursor leads to backbone dissociation of peptides upon thermal activation. Its fragmentation characteristics are similar to those of odd-electron peptide backbone dissociation methods such as electron capture dissociation (ECD)/electron transfer dissociation (ETD). Although peptide sequencing and other applications using TEMPO-mediated FRIPS have been long studied, but its fragmentation mechanism study based on the theoretical calculations has not been yet performed. In this study, free radical initiated peptide sequencing (FRIPS) fragmentation behavior of o-TEMPO-Bz conjugated GGR as a simple model was carefully studied using tandem mass spectrometry experiments and a new group-theoretical computation approach. In particular, for computations, the so-called 'ACE-reaction' algorithm, which was recently coded for automatic predictions and exhaustive search of low-energy reaction pathways, was used. The low-energy reaction pathways were thoroughly explored through DFT calculations.

Poster - 8

Elucidating of hydrodesulfurization of polycyclic aromatic sulfur hydrocabon compounds in crude oil using ion mobility mass spectrometry

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Ion-Mobility Mass Spectrometry (IM-MS) in Synapt G2 HDMS has been proved to be efficient way to characterize complex mixture such as crude oil. However, identifying gas phase structure of molecules such as polycyclic aromatic hydrocarbons (PAHs) or polycyclic aromatic sulfur-containing hydrocarbons (PASHs) isomeric species in heavy crude oil is still difficult due to the molecular complexity of petroleum and due to the difficult of getting standard compounds for accurate information. However, it has been recently reported that peak width obtained from ion mobility spectra can be used to investigate structural diversities of compounds. Based on the recent study, we combine IM-MS and theoretical calculation to investigate the structure of compounds from heavy crude oil. Hydrotreated oil samples were provided by SK innovation. Expecially, the theoretical CCS values of mass peaks were calculated by using Sigma program.

Poster - 9

Energy-resolved Collision-induced Dissociation Study of Na^+-bound G-quartets with Mixed Ligands, $[Na(Guanine)_n(9\text{-methylguanine})_m]^+$

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Collision-induced dissociation (CID) of square-planar Na^+-bound complexes of G-quartets with mixed ligands of guanine (G) and 9-methylguanine (9mG), $[Na{\cdot}G_n{\cdot}9mG_m]^+$ (n = 0 - 4, m = 0 - 4; $n + m = 4$) were investigated using tandem mass spectrometry. The mass spectrum of $[Na{\cdot}G_n{\cdot}9mG_m]^+$ produced by electrospray ionization (ESI) exhibited pronounced generation of mixed clusters of Na^+-bound monomers, dimers, and G-quartets, wherein Na^+-bound trimers were essentially missing. Similarly, CID of G-quartets hardly produced fragments of Na^+-bound trimers from the square-planar complexes. Those suggest that a great stability is gained by forming a complete hydrogen bonding network in G-quartets, which agrees well with a large predicted stepwise enthalpy of formation by complexation with the fourth ligand to be as large as 55 kcal/mol. The stability gained by hydrogen bonding between G moieties in G-quartets further suggests that Na^+-bound dimeric fragments may be formed from neighboring, hydrogen-bonded ligands; which in other words suggests preferential neutral loss of hydrogen-bonded G dimers in CID. It further allowed to address the stereochemistry of G-quartets, of which population for *cis*- and *trans*-conformers of $[Na{\cdot}G_2{\cdot}9mG_2]^+$ can be assessed to be 50:50 in the gas phase. The observed ratio of 50:50 agrees well that the G-quartets were likely to be formed in the solution and produced according to thermochemical stability rather than in the course of electrospray ionization via kinetic trapping.

Poster - 10

Anomaly in Collision-induced Dissociation of Proton-bound Hoogsteen Base Pairs of Cytosine and Guanine by Proton Transfer

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We report the anomalous collision-induced dissociation (CID) behavior of the proton-bound Hoogsteen base pairs of Cytosine (C), 1-methylcytosine (1-MeC), and 5-methylcytosine (5-MeC) with Guanine (G) as a common base partner, $(C:G:H)^+$, $(1\text{-}MeC:G:H)^+$, and $(5\text{-}MeC:G:H)^+$. In the results, in contrast to the other base pairs, CID of $C:H^+\cdots G$ exhibited more abundant production of $C:H^+$, the fragment protonated on the moiety with a smaller proton affinity, than $G:H^+$. This appeared to contradict general prediction based on the kinetic method. However, further theoretical exploration of potential energy surfaces found that there can be facile proton transfers in the proton-bound Hoogsteen base pairs during the CID process, which makes the process accessible to an additional product state of O-protonated C for $C:H^+$ fragments. The presence of an additional dissociation channel, which in other words corresponds to 2-fold degeneracy in the transition state leading to $C:H^+$ fragments, effectively doubles the apparent reaction rate for production of $C:H^+$. In this way, the process gives rise to the anomaly, the observed pronounced formation of $C:H^+$ in the CID of the proton-bound Hoogsteen base pair, $C:H^+\cdots G$.

Poster - 11

Signal reduction due to solvent composition of molecular ions generated from aromatic compounds in (+) atmospheric pressure photoionization mass spectrometry.

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The ionization process is essential for successful mass spectrometry (MS) analysis because it affects selectivity and sensitivity. In particular, certain solvents reduce the ionization of the analyte, reducing overall sensitivity at atmospheric pressure photoionization (APPI). The sensitivity varies greatly depending on the solvent. Density functional theory was used to calculate the enthalpy (ΔH) of the reactions between toluene and other solvents. The abundances of analyte ions present correlates well with the calculated ΔH value. Linear correlations between the abundance of toluene and analyte molecular ions were observed. Overall, the evidence presented in this study suggests that the reaction between solvent cluster(s) and toluene molecular ions are responsible for the observed signal reduction.

Poster - 12

Profiles of oxidized phospholipids in exosome from oxidatively stressed cells by flow field-flow fractionation and nUHPLC-ESI-MS/MS

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Oxidative stress is caused by excessive production of reactive oxygen species (ROS), which include oxygen derived radical species such as superoxide anion ($O_2^{\cdot-}$) and hydroxyl radical($^{\cdot}OH$) as well as hydrogen peroxide (H_2O_2). Although ROS participates in some physiological roles (e.g. signaling, host defence), high levels of ROS not only induces cellular impairment by altering DNA, RNA, proteins and lipids but is also involved with a number of diseases like cardiovascular disease (CVD) or cancer.

Exosomes are nano-sized extracellular vesicles secreted from cells. When oxidative stress is given to cells, it has been reported that exosome transports some protective RNA against oxidative stress or transfer stress signals to recipient cells. However, physiological roles or changes of lipids in exosome during oxidative stress conditions have not yet been studied.

In this study, oxidative stress was induced to human embryonic kidney cell 293 (HEK293) by treating with H_2O_2 for 72 hours. Exosome from control and oxidatively stressed conditions were analyzed by flow field-flow fractionation, which separates samples according to their sizes. Moreover, comparison of lipidomic alteration, including oxidized phospholipids in cell and exosome was conducted by nUHPLC-ESI-MS/MS.

Poster - 13

Effect of aging on lipid alteration in serum, kidney, and heart from mice by nUHPLC-ESI-MS/MS

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Lipids are not only the sources of energy production and basic building blocks of cell membrane, but also the important signaling molecules in intercellular communications. All living organisms are inevitable from aging which induces gradual reduction of lipid-regulated cellular metabolism. This is because lipid alteration in aging subjects can cause problems in cellular metabolism, leading to age-related diseases, such as cardiovascular disease, neurodegenerative disease, and diabetes mellitus. Although a number of studies have been conducted to elucidate the relationship between age-related diseases and lipids, only few studies have compared lipid changes with aging effect. In this study, lipid profiles in serum, kidney, and heart from C57BL/6 aging mice were examined. Uniformly raised 4 and 25-month-old mice were analyzed by nanoflow ultrahigh pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). More than 350 lipid species were identified in each sample types and 163 in serum, 210 in kidney, and 202 in heart were quantified. From quantification, most lipid species showing significant changes (> 1.5 fold and $p < 0.01$) were found to be down-regulated by aging, and lipid alteration in serum was more distinct than those in tissues (kidney and heart).

Poster - 14

Optimization for quantitative analysis of glycan in yeast using metabolic isotope labeling of polysaccharides with isotopic glucose (MILPIG) 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-glycan and O-glycan. These plays significant role in many biological functions such as cell-cell recognition, cell development, tumorigenesis and metastasis, etc. Because changes in the expression levels of glycans affect many physiological functions, it is important to analyze changes in expression levels of glycans by quantitative analysis. Therefore, mass spectrometry-based quantitative analysis of glycans has been developed. Many quantitative analysis of glycans by mass spectrometry typically have been used by labeling strategy such as reductive amination labeling, isotopic detection of aminosugars with glutamine (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 glycan of yeast. As a result, the isotope cluster distribution of the heavy labeled glycan was optimized with glucose concentration and incubation times. We report the conditions to reduce the broaden isotope cluster distribution for accurate quantitative analysis.

Key words: Glycan, Yeast, MILPIG, Mass Spectrometry

Poster - 15

In-vivo isotopic glucose labeling of glycan in fungi using metabolic isotope labeling of polysaccharides with isotopic glucose (MILPIG) for quantitative mass spectrometry

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N-glycosylation is one of the most important post-translational modifications occurring in living animals and fungi. Animal N-linked glycans and fungi N-linked glycans differ in structure, amount, and role. In the case of animals, N-linked glycans have heterogeneous structures and have specific functions involved in cell-cell recognition, cell division, cell development, cell transport, cell differentiation, immune response and other many important biological phenomena depending on their structures. On the other hand, in the case of fungi, N-linked glycan mediated biological functions remain obscure. In this work, the structure of the fungal N-linked glycan was confirmed by mass spectrometry. In addition, the identified glycans were labeled using the MILPIG (Metabolic Isotope Labeling of Polysaccharides with Isotopic Glucose) method. The MILPIG method is *in-vivo* labeling method that allows fungi to produce heavy-labeled glycans by using carbon source as heavy isotope glucose ($^{13}C_1$-glucose).

Poster - 16

Proteomic Analysis of Cervicovaginal Fluid for Early Detection of Preterm Birth by 2D-nLC-ESI-MS/MS

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Preterm birth (PTB) before 37 weeks of pregnancy is one of major causes of poor pregnancy outcome, resulting in perinatal mortality and neonatal morbidity. Despite medical advances, PTB has continuously increased over the last two years and the development of biomarker(s) for early detection of PTB has not been matured. In this study, we performed shotgun proteomic analysis of the cervicovaginal fluid (CVF) samples that delivered at preterm and term so as to unveil the protein biomarkers using isobaric tags for relative and absolute quantitation (iTRAQ) coupled with two dimension-nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (2D-nLC-ESI-MS/MS). We compared the CVF proteome of individual PTB and control using pooled control CVF as a spike-in reference standard. We identified 1294 CVF proteins, of which 605 were newly identified proteins. Of 990 proteins quantified in both PTB and control, 154 proteins were significantly up/down-regulated in PTB compared to control. Differently expressed proteins were subjected to Gene Ontology (GO) analysis. These promising results could lead to improved understanding of PTB etiology and discovery of biomarkers for PTB.

Poster - 17

Optimizing extraction efficiency of serum steroids in advanced GC-MS/MS-based profiling

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Although gas chromatography-mass spectrometry (GC-MS) has been recently increasingly replaced by liquid chromatography-mass spectrometry (LC-MS), GC-MS still provides better chromatographic resolution in profiling analysis. A GC-MS-based quantitative profiling of 84 urinary steroids was developed in 2009, but it is also needed to be improved both selectivity and sensitivity in limited volume of biological samples. Here, GC-triple quadrupole/MS (GC-MS/MS) combined with various sample purification techniques are introduced for advanced GC-MS-based steroid profiling of 17 androgens, 7 estrogens, 13 corticoids, 14 progestins, and 14 sterols in human serum. For selective extraction of serum steroids, a traditional solid-phase extraction (SPE) with Oasis HLB has been compared with supported liquid extraction (SLE) and silica nanoparticles (SNPs). In the negative charged SNP purification, the extraction efficiency of progestins, corticoids, and sterols was increased compared to those of Oasis HLB, while the positive charged SNP resulted in poor extraction recoveries in most serum steroids tested. The SLE provided comparable results, but it is not recommendable for relatively lipophilic steroids, sterols. Based on our experimental findings, we are going to develop the GC-MS-based steroid profiling assay to bring steroid signatures into practical and basic biomedical researches.

Poster - 18

Metabolic signitures of adrenal steroids in serum and saliva measured by polarity switching LC-MS

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Adrenal steroids are generated in adrenal glands and metabolized by various enzymes, such as hydroxylases and reductases. Profiling analysis of adrenal steroids in serum and saliva was therefore established to evaluate their metabolic functions in adrenal diseases. All steroids were separated through an 1.9 μm particle C18 column (50 × 2.1 mm) at a flow rate of 250 μL/min and quantitatively measured by the high-speed polarity switching LC-MS in MRM modes. In method validation, the linearity (r^2) was higher than 0.992 within 0.1 and 500 ng/mL dynamic range, while precision (%CV) and accuracy (%bias) were 1.1 ~ 9.8% and 85.9 ~ 112.1%, respectively. The levels of salivary steroids were compared with those of serum, and a comparison between saliva sampling techniques was also investigated. This validated assay was successfully applied to patients with Cushing's syndrome and the results from saliva were comparable to those from serum. Therefore, the present LC-MS method could be an useful tool for monitoring diseases, including Cushing's syndrome.

Poster - 19

GC-MS-based metabolic signitures of Cushing's syndrome in serum cholesterols

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Increased cholesterol level is one of complications associated with hypercortisolism. Although the excess cortisol is mostly found in all types of Cushing's syndrome (CS), the metabolic signatures of cholesterol have not been understood to date. A developed gas chromatography-mass spectrometry (GC-MS)-based quantitative profiling was, therefore, develpoed and applied to measure 19 circulating sterols (cholesterol, 4 cholesterol precursors, 4 cholesteryl esters and 10 hydroxycholesterols) and 3 plant sterols). The limit of quantification of cholesterol and cholesteryl esters ranged from 0.2 to 10.0 μg/mL, except for cholesteryl arachidonate (100 μg/mL), while hydroxycholesterols and cholesterol precursors ranged from 0.01 to 0.10 μg/mL. Linearity as the correlation coefficient was higher than 0.98. The precision (% CV) and accuracy (% bias) ranged from 3.2% to 14.6% and from 70.3% to 118.1%, respectively. The overall recoveries of CEs ranged from 43.1% to 88.3%, and the recoveries of other sterols ranged from 80.2% to 119.1%. The cholesterol signatures after surgery in CS patients showed the increased serum sterols, while 27-hydroxycholestrol was significantly decreased. This technique can be useful for making clinical diagnoses and for an increased understanding of the pathophysiology of Cushing's syndrome.

Poster - 20

Plasma lipid metabolites profiling for internet gaming disorder in korean males

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Internet gaming disorder (IGD) was behavioral addiction and psychiatric disease. It was insertion of diagnosric and statistical manual of mental disorder fifth edition (DSM-5). IGD is a new mental illness in which people with illness use computers to harm health and social life. But, it can't control desire. It can harm social, emotional, and physical aspects in everyday life. Psychiatry is generally categorized in terms of classification methods. However, bioflueid using Biomarker represents a result that pathological expression can help objective criteria.

Phospholipids have two main functions. it forms the basic structure in which all external and internal membranes were created. Another major function was provided on the basis of the vast majority of cell signaling systems. So, the purpose of the study was to identify the lipid characteristics of blood and investigate changes in plasma lipids.

Lipid profiles were 89 plasma samples (control = 28, IGD = 61) using liquid-chromatography Orbitrap mass-spectrometry (LC-Obitrap MS). Univatiate statistics presented significant between healthy controls and IGD group of 19 lipids. The lipids were fatty acid esters of hydroxy fatty acid, phosphocholine, lysophospholipids. Recombinant biomarker clusters based on multivariate statistics provided fairly good discrimination between the two groups. The results suggest the relevance of lipid metabolism by IGD and the applicability of biomarker signatures to complement clinical decisions.

Poster - 21

Discovery of a unique metabolic profile for activated Wnt / beta-catenin signaling

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Wnt signaling pathway is implicated in broad range of biological process including developmental process and adipogenesis. The signal cascade has been reported for the direct association with various types of diseases (e.g. oncogenesis and osteroporosis). Despite the strong linkage to metabolism, metabolome-wide investigation has not been conducted.

Thus, we explored metabolic dynamics in HEK 293 cell line stimulated by Wnt activation in a time-dependent manner by applying gas-chromatography time-of-flight mass spectrometry (GC-TOF MS). A total of 125 metabolites were profiled, which included carbohydrates, amino acids, fatty acids, and organic acids. The metabolic network analysis elucidated the coordinated alteration of a range of central carbon/nitrogen metabolism (glycolysis, TCA cycle, and amino acid metabolisms). Multivariate-coupled ANOVA (ASCA) systematically resolved factor-dependent metabolic regulation (Wnt treatment and time). Among them were fatty acid metabolism and nucleotide metabolism that showed unique metabolic regulation governed by Wnt signal transduction. Further research in combination with other molecular information (e.g. mRNA and proteins) will lead to better understanding of underlying mechanism veiled by the complexity of Wnt signaling pathways.

Poster - 22

Computational Characterization of Core and Outer Fucosylated N-Glycoproteins with LC-MS/MS and IQ-GPA

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Glycosylation is a major posttranslational modification of proteins and plays various roles in biological activities. In N-linked glycoproteins, fucosylation is important and closely relevant to diseases such as cancer. For example, core type fucosylated N-glycoproteins in hepatocellular carcinoma has been well reported[1]. Tandem mass spectrometry (MS/MS) with liquid chromatography (LC) is a powerful tool for characterization of N-glycoproteins and its fucosylation. Because manual analysis of N-glycoproteins is time consuming, we have developed GlycoProteome Analyzer (IQ-GPA)[2] software for automated analysis. Nevertheless, assignment of fucosylation in N-glycoprotein is not good enough to decide their core and/or outer positions. It is still remained challenge to classify the fucosylation types of N-glycoproteins.

In this study, we designed a computational method for automated fucosylation characterization of N-glycoprotein which consist of Core Fucosylation Score (CFS) and Outer Fucosylation Score (OFS). Essential diagnostic peaks such as MS/MS fragments with and without fucosylation provide important fucosylation information. Human immunoglobulin-G and alpha-1-acid-glycoprotein standards were used as core and outer fucosylation model to simulate fucosylation scores, respectively. Finally, this method was applied to characterize different fucosylation types of N-glycoproteins in human plasma samples.

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Poster - 23

A Web-based MS/MS Spectral Library dedicated to Structure Elucidation of Natural Products

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Natural products (NPs) are considered as an important source of biotechnology and medicine. Scientific and technical advances in mass spectrometry (MS) enabled us to characterize known NPs. For a decade, there has been an attention towards methods for identification of unknown substances of interest. The indispensable information in MS spectrum databases and NP databases has been unfortunately deficient to use. The limited information has led to an interest in computational approach for predicting reference MS spectra from chemical structures, extracting kernel-based feature of spectrum, and especially attempting to elucidate structures of unknown substances. Hence, we built a database containing calculated fingerprints and MS spectrum data compatible with computational approaches for structural elucidation.

The database currently catalogues 17 scaffolds that are provided by Dictionary of Natural Product and provided several data, including 2600 NPs. Data of each NP included structural and spectral terms. Each compound had about 30 spectra generated from instruments which are Thermo Scientific (Orbitrap), AB Sciex (TripleTOF), Waters (Q-TOF) with adducts which are H and Na at five different collision energies (10, 20, 40, 60, and 80 V). These data represented a total number of > 70,000 high-resolution MS/MS spectra. The final spectral data could be changed if what post-processing protocol and parameters are applied. To validate that every spectrum was correctly generated, MetFrag which provided the agreement between measured and in silico fragments was used. The database includes several descriptors for implementation of computational approach to elucidate structures of unknown compound.

Applying structural and spectral data into computational approach, information needed to be converted to different forms. Structural fingerprints were converted from structural information by CDK (Chemistry Development Kit). A web-based platform of MS/MS data pertaining to natural products was developed and named SnaPeaks (Search Natural Product PEAKS). As a main web application of SnaPeaks, a fragment search was established based on similarity function.

The SnaPeaks is demonstrated on the website, https://www.snapeaks.com/.

Poster - 24

Observation on Regenerated Bony Rays of Zebrafish Caudal Fin using Time-of-Flight Secondary Ion Mass Spectrometry

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We observed regenerated caudal fins of zebrafish using time-of-flight secondary ion mass spectrometry (ToF-SIMS). The zebrafish caudal fin is not only a very appropriate bio-specimen for mass spectrometry due to its thickness of less than 200 micrometers but also a very important organ for tissue regeneration studies. Thus, mass spectrometry methods could be widely applied to the wound healing studies using caudal fins of zebrafish due to providing plenty of biomolecular information.

ToF-SIMS images in this study were obtained using ToF-SIMS 5 (ION-TOF GmbH) equipped with liquid metal ion gun (LMIG) and gas cluster ion beam (GCIB) sources. The caudal fins were sputtered with Ar clusters and etched to 20-25 μm from the surface in the depth direction, then ToF-SIMS images of the bony ray and the inter-ray mesenchymal tissue were obtained using rastering of a Bi_3^+ ion.

ToF-SIMS analyzed both positive and negative ion modes and about 1000 specimen-related spectra were obtained from zebrafish caudal fins. Since the ToF-SIMS method detect mineral ions very well, it provided high spatial resolution ion images including Ca^+, Mg^+, K^+, and PO_2^- ions to intuitively identify the precise location of the truncated site and the regeneration shape of the bony rays of the zebrafish caudal fin at 4 days-post-amputation (dpa) and 7 dpa. Whereas the calcium and PO_2^- ions were be found to contain more in the regenerated area than in the existing area of the caudal fin at 4 dpa, there were little difference between the two areas of the caudal fin at 7 dpa. Consequently, ToF-SIMS imaging is a simple and easy approach to understanding the spatial distribution of small molecules in the regenerated caudal fin of a zebrafish.

Poster - 25

Direct MS Analysis of Drugs of Abuse in Urine Using Biocompatible Solid Phase Microextraction (BioSPME)

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The field of illicit drug testing has recently become a constantly changing environment with the rapid development of unregulated designer and synthetic compounds. These compounds are reported to generate stimulating affects similar to that of methamphetamine, heroin and MDMA. The difficulty for forensic testing facilities is the fact that these compounds are not detected under normal ELISA testing methods; therefore, more selective LC-MS based approaches are necessary.

This study demonstrates the benefits of Biocompatible Solid Phase Micro Extraction (BioSPME) used in conjunction with direct mass spectrometry detection. An ambient ionization source (DART-Direct Analysis Real-Time) was coupled to a single MS system (Waters QDA). This technique offers a fast, accurate, and robust method for analyzing drugs of abuse. Linear calibration curves were observed for all analytes in full scan mode from 100-5000 ng/mL. Limits of detection were between 15-20 ng/mL and quantitation limits were between 50-100 ng/mL. The urine matrix did not negatively impact the analyte responses from the fiber. Using biocompatible SPME fibers with DART-MS on the Waters QDA provides a fast and more cost effective analysis alternative compared to LC/MS/MS systems.

Poster - 26

Improved LC/MS of peptides by innovative particle design and dedicated mobile phase additives

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One option to address the demand for higher separation efficiency and increased sensitivity in HPLC was the Fused-Core particle technology [1]. This technology allows for higher efficiency in HPLC leading to narrower, higher peaks resulting in lower sensitivity. For peptides and small proteins these particles have been developed with larger pores.

Trifluoroacetic acid (TFA) is typically used for RP HPLC/UV of peptides. The idea of this additive is to form effective ion pairs with basic moieties on the peptide and to keep the pH value well below pKa of side-chain carboxyl groups to maximize retention. However, in HPLC/MS the additive TFA is not suitable for the separation of peptides, because this additive leads to high surface tension of the mobile phase precluding efficient nebulization (spray formation) in ESI source [2]. Additionally TFA ions in gas phase form ion-pairs with the basic moieties of peptides which reduces sensitivity [2]. An alternative mobile phase additive compatible with MS is formic acid. But in general formic acid leads to poorer peak shape and lower peak capacity than when TFA is used.

In this work the theory of Fused-Core technology and its application for LC/MS separation of peptides and small will be presented. The successful application of formic acid as additive in mobile phases for improved LC/MS will also be discussed.

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Poster - 27

Improved LC/MS/MS analysis with on-line SPE for removal of phospholipids from protein precipitation biological fluid samples

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Especially for HPLC-MS in bioanalysis a sound sample preparation such Solid Phase Extraction (SPE) is essential to achieve accurate and reproducible results due the high matrix burden of the samples. Usually SPE is conducted off-line and often requires significant manual effort resulting in low reproducibility. On-line SPE processes are a viable alternative for this approach.

In this work the development of on-line SPE cartridges using two RP chemistries, C8 and RP-Amide, is described. The on-line SPE cartridges were applied to the LC/MS analysis of three thyroids in human serum. The results show significantly higher (>25%) LC/MS response of all three thyroids with both chemistries in comparison to the analysis without clean-up. The RP-Amide cartridge leads to higher response than the C8 cartridges. The reproducibility (relative standard deviation, RSD) of the LC/MS signals from 120 consecutive injections of 100 ng/mL of each thyroid spiked in human serum is 5.5%-9.1% and 4.7%-8.8% with C8 and RP-Amide cartridges, respectively. The applicability of on-line SPE with LC/MS is also demonstrated with cannabis analytes in human plasma and plant extract, as well as drugs and metabolites in urine samples.

The above studies show that on-line SPE allows sample clean-up and concentration with excellent reproducibility and chromatographic performance. The technology promises to reduce the tedious manual sample preparation and improve robustness and reliability of analytical methods.

Poster - 28

Quantitative analysis of lead in soils by fsLA and ICP-MS

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It is important to determine lead in soils, which is used as an indicator for soil pollution. Inductively Coupled Plasma-Mass Spectrometer (ICP-MS) is the powerful technique for trace elements analysis. For this technique, the appropriate digestion method should be selected. Unfortunately, it is complicated and difficult to digest soils completely for ICP-MS. Laser Ablation (LA)-ICP-MS which has advantages such as simple sample preparation steps and less time-consuming has become attractive over the past decades. This study aimed to analyze lead in soils quantitatively by using ICP-MS and to test feasibility of femtosecond LA-ICP-MS.

Several methods were compared by using Certified Reference Materials (CRMs). US EPA method 3050B showed better accuracy and precision than other methods. For fsLA-ICP-MS, external calibration using diluted CRMs was obtained and quantitative analysis was performed under helium atmosphere. In order to validate these two methods, method validation was performed.

Calibration curve obtained by using diluted CRMs provided linear correlation coefficients above 0.999. Applying two analytical techniques to soil samples, the results estimated by fsLA-ICP-MS were compared with those of ICP-MS. It was confirmed that fsLA-ICP-MS is useful technique for determination of lead in soils with accuracy in the range of 91.6% to 115.1 % and precision < 25.2%. Despite of the inhomogeneity of soil samples, the results of ICP-MS and fsLA-ICP-MS displayed reasonable correlations with the determined concentration of Pb even if CRMs were diluted. Therefore, it is expected that fsLA-ICP-MS can be used for quantitative analysis of lead in soils.

Poster - 29

Structural Profiles of Gangliosides in Developing Human brain via Negative Ion Mode Nano- LC/MS/MS

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Gangliosides are attributed with diverse biological functions such as cell-cell interaction, cell recognition, neurotransmission, and signal transduction. Herein, we established an analytical platform for qualitative and quantitative analysis of gangliosides from human brain tissue by nano-LC/MS/MS for developmental mapping from neonate to adults. Briefly, each brain tissues were grinded by sonication. Homogenized brain samples were mixed with chloroform/methanol/water and centrifuged for total lipid extraction. Total lipids extracts were partitioned again with chloroform/methanol to selectively collect gangliosides. Gangliosides were further purified and enriched by C18 solid-phase extraction and they were profiled by negative ion mode nano-LC/MS using a C18 microfluidic chip. Structural information of gangliosides in both oligosaccharides composition and ceramide lipid tails was obtained by nano-LC/MS/MS. To investigate the change of ganglioside during developmental stages, sixty nine human brain tissues covering the period from 39 days to 49 years were divided into the following 7 groups: neonates to adults. Approximately 90 ganglioside compound peaks were identified in total. GD1 (d36:1 and 36:2), GT1 (d36:1), and GM1 (d36:1 and d36:2) were predominantly observed in all stages in common, accounting for over 75% of total gangliosides. Glycan portion and ceramide moieties of ganglioside were separately explored for depth profiling during brain development. GD1 was markedly decreased whereas GT1 and GM1 were slightly increased from neonates to school-ages but GD1, GT1, and GM1 kept constant level between school-ages and adults. On the other hand, we could observe explicit tendency in ceramide moieties. Long-chain ceramides such as d38:0, d38:1, d40:1, and d42:1 were significantly increased during brain development. Hierarchical clustering using normalized abundance of gangliosides revealed that adults and young adults showed high similarity while neonates and adults had little correlation.

Poster - 30

Identification of Missing Proteins in Human Olfactory Epithelial Tissue by LC-MS/MS

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The purpose of the chromosome-centric human proteome project (C-HPP) is to find and map all human proteins by using neXtProt database with LC-MS/MS. Until now, 2461 missing proteins without protein evidence that were confidently predicted but have not been detected at protein level yet and not been identified by mass spectrometry, respectively.

In this study, we first performed proteomic analyses of human olfactory epithelial tissue to identify missing proteins using liquid chromatography-tandem mass spectrometry. Since missing proteins are low abundance, the whole proteins in olfactory epithelial tissue was extracted, separated by SDS-PAGE and fractionated using bRPLC to discover the missing proteins as many as possible. Using a next-generation proteomic pipeline with a <1.0% false discovery rate at the peptide and protein levels, we identified 3,731 proteins, among which five were missing proteins (P0C7M7, P46721, P59826, Q658L1, and Q8N434). We report strong evidence of missing proteins through peptide spectrum matching by verifying MS / MS fragmentation from the LC-MS / MS analysis of the corresponding peptides. In conclusion, the use of LC-MS/MS based proteomics analysis of specific human tissue can contribute to continued research in discovering further missing proteins.

Poster - 31

Validation of Analytical Methods Using LC-MS to Characterize HGH [Human Growth Hormone]

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Synthetic human growth hormone produced by recombinant DNA technologies is used in children to treat growth retardation, for example short stature due to insufficient growth hormone secretion, Turner's syndrome or chronic renal insufficiency. In adults it is used as a treatment for growth hormone deficiency and for management of HIV-related wasting and cachexia. Several analytical methods for the characterization of growth hormone have been descried, such as liquid chromatography- mass spectrometry (LC-MS), circular dichroism spectrometry (CD), Differential scanning calorimetry (DSC), Dynamic light scattering (DLS). This protein heterogeneity results from sequence variations generated from proteolysis or transcriptional/translational errors, from post-translational modifications (PTMs), and degradation of products which are formed during processing or final product storage. For this reason, a detailed characterization and sensitive analytical techniques are necessary to assure the safety, quality and efficacy of therapeutic protein products. Mass spectrometry (MS) is widely used within structural and functional proteomics for a variety of tasks including protein quality assessment, identification, and characterization. However, the cutting-edge protein characterization method can serve as a technical barrier, the method must be validated based on regulations. This study was performed to validate standard operating procedure (SOP) method for improve analytical techniques of Human growth hormone by LC-MS based analytical method based on ICH guideline.

Poster - 32

Validation of Analytical Methods Using LC-MS to Characterize Bevacizumab

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Bevacizumab is a humanized immunoglobulin G (IgG) mAb drug against human vascular endothelial cell growth factor A (VEGF-A). It is used for treating many types of cancers. Recent studies have indicated that clinical outcomes vary among patients treated with bevacizumab and produce various side effects, such as vascular disorders. Several analytical methods for the characterization of bevacizumab have been descried, such as liquid chromatography- mass spectrometry (LC-MS), circular dichroism spectrometry (CD), Differential scanning calorimetry (DSC), Dynamic light scattering (DLS). This protein heterogeneity results from sequence variations generated from proteolysis or transcriptional/translational errors, from post-translational modifications (PTMs), and degradation of products which are formed during processing or final product storage. For this reason, a detailed characterization and sensitive analytical techniques are necessary to assure the safety, quality and efficacy of therapeutic protein products. Mass spectrometry (MS) is widely used within structural and functional proteomics for a variety of tasks including protein quality assessment, identification, and characterization. However, the cutting-edge protein characterization method can serve as a technical barrier, the method must be validated based on regulations. This study was performed to validate standard operating procedure (SOP) method for improve analytical techniques of bevacizumab by LC-MS based analytical method based on ICH guideline.

Poster - 33

Validation of Analytical Methods Using LC-MS to Characterize Trastuzumab

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Trastuzumab, a humanized monoclonal antibody, is widely used for the treatment of various cancers in humans including metastatic breast cancer and gastric cancer with over expression of cell surface human epidermal growth factor receptor 2 (HER2) receptors. This over-expression of HER2 receptors leads to abnormal cellular signaling and is responsible for the abnormal proliferation of cells resulting in malignancy. Several analytical methods for the characterization of growth hormone have been descried, such as liquid chromatography- mass spectrometry (LC-MS), circular dichroism spectrometry (CD), Differential scanning calorimetry (DSC), Dynamic light scattering (DLS). This protein heterogeneity results from sequence variations generated from proteolysis or transcriptional/translational errors, from post-translational modifications (PTMs), and degradation of products which are formed during processing or final product storage. For this reason, a detailed characterization and sensitive analytical techniques are necessary to assure the safety, quality and efficacy of therapeutic protein products. Mass spectrometry (MS) is widely used within structural and functional proteomics for a variety of tasks including protein quality assessment, identification, and characterization. However, the cutting-edge protein characterization method can serve as a technical barrier, the method must be validated based on regulations. This study was performed to validate standard operating procedure (SOP) method for improve analytical techniques of trastzumab by LC-MS based analytical method based on ICH guideline.

Poster - 34

Comparison of lipid profiling of *Drosophila* head using MALDI-MSI(Matrix assisted laser desorption ionization-mass spectrometry imaging) and ESI-MS(electrospray ionization mass spectrometry)

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MALDI-MSI is a technique for measuring the location information and intensity of bio-molecules (lipids, peptides and proteins etc.) in tissue sections of biological samples, and ESI-MS is a technique for ionizing and analyzing analytes in sample solution.

In this experiment, we measured the imaging data at the section of the Drosophila head, and compared it with the ESI spectrum of the lipid extracted from the head and brain of *Drosophila*. The *Drosophila* head is about 1 mm in size, making it difficult to measure with conventional MALDI imaging equipment. However, in a MALDI with a laser with a diameter of a few μm, a small sample can be measured. We obtained a tissue section by embedding WT flies in gelatin, spraying 1,5-Diaminonaphthalene(DAN) matrix and introducing it into MALDI imaging equipment.

In the imaging data, PE(36:3e), PE(36:2e) and PE(36:1e) were detected mainly in the brain and PE(36:4) was detected mainly in the eyes. PS(36:4), PS(36:3), and PS(36:2) were detected mainly in brain and eyes. The imaging results were compared with the normalized intensity of ESI-MS. PE(36:3e), PE(36:2e), PE(36:1e), PS(36:4), PS(36:3) and PS(36:2) detected mainly in brain showed higher intensity in brain spectrum than head spectrum of WT flies. On the other hand, PE (34: 3), PE (34: 2) and PE (34: 1) showed higher intensity in the head spectrum of WT flies.

These results indicate that lipid molecules are present at specific positions and that they have a similar tendency to ESI-MS spectrum data of lipid extracted from head and brain of WT flies.

Poster - 35

Quantitative Proteomic Analysis of 2D and 3D Cultured Colorectal Cancer Cells: Profiling of Tankyrase Inhibitor XAV939-Induced Proteome

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In this study, we present the quantitative profiling of a drug-induced proteome in 2D and 3D cultured colorectal cancer SW480 cells using two-dimensional nanoflow liquid chromatography-tandem mass spectrometry (2D-nLC-MS/MS) integrated with isobaric tags for relative and absolute quantitation (iTRAQ). We identified a total of 4854 proteins between 2D/3D cultured SW480 cells and 136/247 differentially expressed proteins (up/down-regulated in 3D compared to 2D). These differentially expressed proteins were mainly implicated in energy metabolism, cell growth and cell-cell interactions. In addition, we investigated the XAV939 (tankyrase inhibitor)-induced proteome to reveal factors involved in the 3D culture-selective growth inhibitory effect of XAV939 on SW480 cells. We identified novel XAV939-responsive proteins that were differentially expressed between 2D and 3D cultured SW480 cells. These results provide a promising informative protein dataset to determine the effect of XAV939 on the expression levels of proteins involved in SW480 cell growth.

Poster - 36

Multiresidue analysis of PHTs, VOCs, phenols, parabens, PAHs, pyrethroid insecticides and tobacco smoke in human urine by LC-ESI/MS/MS

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In this study, sample preparation and analytical method for simultaneous quantitative analysis of phthalates, volatile organic compounds, phenols, parabens, polycyclic aromatic hydrocarbons, pyrethroid insecticides and tobacco smoke in human urine was developed using ultra-high pressure liquid chromatography-electrospray ionization/tandem mass spectrometry (UHPLC-ESI/MS/MS) with polarity switching (PS) and time-dependent selected reaction monitoring (t-SRM). This study aims to reduce urine sample volume and to integrate sample preparation and analytical method of all endocrine-disrupter classes. Urine samples (500μL) were extracted via two consecutive liquid-liquid extraction (d-LLE) at different pH values following enzymatic hydrolysis. Analyses were performed by UHPLC-ESI/MS/MS with PS and t-SRM and, cycle time, dwell time, monitoring time and data points were optimized. The calibration curves of target EDs in artificial urine showed good linearity ($R^2 \geq 0.99$) and method was applied to real human urines. The present multiresidue method has the potential to be an alternative technique for the quantitation of EDs.

This study was funded in part by the Korea Ministry of Environment (MOE) as “the Environmental Health Action Program.(project number : 2017001360003)” and in part by an intramural grant from Korea Institute of Science and Technology.

Poster - 37

Solid Phase Extraction of nerve agent degradation products using poly(METAC) plate and TOF-SIMS analysis

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Nerve agents, one of the chemical warfare agents, are highly toxic and production, storage and usage of them are prohibited by Chemical Weapon Convention (CWC). Compliance of the convention have been monitored by the verification of Organization for Prohibition of Chemical Weapons (OPCW). The purpose of OPCW verification identifies the chemical warfare agents and related chemicals from the samples. Most of the nerve agents easily hydrolyzed to alkyl methylphosphonic acids (RMPA) and further degraded to methylphosphonic acid (MPA). Therefore, RMPA and MPA are good markers of nerve agents. The detection of RMPA and MPA in environmental samples requires sample preparation such as solid phase extraction and chromatographic separation. However, chromatographic methods are time consuming to analyze the sample. Therefore, in this study, we introduced functional group capable of anion exchange on the gold plate and developed a method to analyze samples quickly by using TOF-SIMS.

Poster - 38

Quantitative proteomics of 2D-/3D-cultured adipocyte cells and its co-cultured with macrophages using a nanoLC-ESI-MS/MS

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Adipocytes in human body play a role in regulating the fat storage and energy homeostasis. Excessive accumulation of adipocytes can 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 *in vitro* 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 4052 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 involving in glucose and fatty acid metabolisms, such as glucose transporter member 4, fatty acid binding protein, and acetyl-CoA carboxylase, were up-regulated, compared to that of 2D cultured-ones. Consequentially, 3D *in vitro* model offers to the alternative of 2D *in vitro* and *in vivo* models for the assessment of new medical products associated with metabolic disorder.

Poster - 39

Strong advantages of plasma mass spectrometry to analyze ultra-trace level radioactive isotopes in small amount of environmental samples

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Mass spectrometry using ICP-MS enables rapid determination of radioactivity concentration with only small amount of samples. In addition, it is a very effective method for analyzing the highly precise atom ratio among isotopes. In particular, the multiple detection system of multicollector-ICP-MS allows more precise analysis for radioactive isotopes by simultaneously measuring several isotopes. With these advantages, ICP-MS has been used as an useful atom counting technique with several advantages over decay counting techniques for the determination of long-lived radioactive isotopes, like as plutonium isotopes, neptunium-237, technetium-99, and so on. These isotopes are very important for environmental radioactivity monitoring. In this study, the analytical methods for trace levels of radioactive isotopes (^{239}Pu, ^{240}Pu, ^{237}Np, ^{99}Tc) in environmental samples were introduced, furthermore, plasma mass spectrometry and decay counting techniques were compared with each other and the strong advantages (small sample amount, short counting time, high precision, and low minimum detectable activity, and so on.) were presented.

Poster - 40

Comparison of organic mixtures from particulate matters collected in Korea and China by using GCxGC/high resolution mass spectrometry

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In Korea and neighboring China, airbone particulate matter ($PM_{2.5}$) is very serious environment problems, having primary organic pollutants directly released from emission sources and secondary organic pollutants generated from atmosphere chemical reaction. Thus, the complex organic compounds extracted from $PM_{2.5}$ collected day after day during one month in each country were analyzed to compare their identifications, relative quantities and emission sources. Samples of $PM_{2.5}$ were simultaneously collected day after day for 28 days (4-31 January 2018) in Gwangju and Beijing using a high volume air sampler. The two days of extracts were combined, filtered and concentrated under N_2 gas. Comprehensive two-dimensional gas chromatography/high resolution time-of-flight mass spectrometry (GCxGC/HRMS) was utilized to analyze the organic extracts. Approximately, 460 compounds were separated on the polar and sequencial nonpolar GC columns and identified based on the mass spectral data from NIST and Wiley libraries, and exact mass accuracy (<1 ppm) of molecular ion from high resolution data, including alkanes, carboxylic acids, hopanes, PAHs, substituted aromatics and steranes, so on. A variety of PAHs were identified in Beijing samples such as benzo[ghi]fluoranthene, benzo[a]anthracene, acepyrene, pyrene and benzo[A]yrene. Their concentrations in Beijing were more 49 to 3 times according to PAHs compounds than those in Gwangju for 16/17 days $PM_{2.5}$. Thus, it is anticipated that the issues between two countries related about the emission sources will be discussed, based on these objective results obtained for PM2.5 collected in Korea and China.

Poster - 41

Development of simultaneous analysis of 93 persistent organic pollutants (POPs) in human serum by QuEChERS method and GC-MS/MS

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Polychlorinated biphenyl (PCB), Polybrominated diphenyl ether (PBDE) and organochlorine pesticides (OCPs) are widely exist in the environment. Human exposure of POPs can cause adverse effects on endocrine andimmune system, therefore extensive profiling POPs in serum is required in health care.

In this study, we developed a simultaneous analysis of 93 POPs in human serum. We applied the QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) preparation method that widely used for food analysis to reduce preparation time and the amount of sample. Target compounds were extracted by liquid extraction with organic solvent in presence of excess amount of salt. Extracted samples were analyzed gas chromatography–electron ionization triple quadruple mass spectrometry (GC-EI-MS/MS) with multiple reaction monitoring (MRM) mode for quantitative analysis. PCBs, PBDEs and OCPs each showed 0.0025-0.025, 0.01-5, and 0.01-0.1 ng/ml of LOQ, respectively. Some compounds such as PCB-144, BDE-14 were detected at a significant level in pooled human serum, so fetal bovine serum (FBS) was applied to achieve a good linearity. Total 93 persistent organic pollutants were quantified by QuEChERS sample preparation with GC-MS/MS in human serum.

This study was funded in part by the Korea Ministry of Environment (MOE) as ‘‘the Environmental Health Action Program. (project number: 2017001360003)’’ and in part by an intramural grant from Korea Institute of Science and Technology.

Poster - 42

Cross-validation of sulfur-based and amino acid-based quantification methods for the development of insulin reference material

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Protein analysis is an essential means in clinical laboratories, pharmaceutical industries, and basic biological and medical research. In the establishement of a highter order analytical method for protein quantification, multiple stages of reduced protein such as petide, amino acid (AA), and element can be analyzed and deduce the quantity of original protein. In this study, an element (sulfur)-based reductive approach for protein quantification has been applied to determine mass fraction of insulin in a pure protein certified reference material (CRM). The absolute protein quantification using sulfur measurements was based on the isotope-dilution inductively coupled plasma mass spectrometry (ICP-MS) using enriched ^{34}S isotope as an internal standard to achieve the highest accuracy. Pressurized microwave-assisted acid digestion with concentrated nitric acid was utilized for sample digestion. Then, the mass fraction of sulfur in the candidate CRM was obtained from the isotope ratios of ^{32}S over ^{34}S which were measured by ICP-MS. In addition, the size-exclusion and reversed-phase LC methods were used with ICP-MS to characterize and quantify sulfur-containing impurities. The quantification result obtained with the present method based on sulfur analysis was in excellent agreement with the result determined via a well-established protein quantification method based on AA analysis. In the AA-based analysis, conventional acid hydrolysis combined with an ID LC-MS/MS method was used.

Poster - 43

Environmental product for reference material

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Hazardous substances detected in everyday products have a potential to cause various types of diseases to who exposed to them. This experiment was carried out in order to know how much hazardous substances are contained in everyday products we use in real life. This research selected the most commonly used products with hazardous chemicals (tetrachloroethylene) under the legal standards. Then very minute amount of specific hazardous chemicals are added to the product so that it can be used as a reference material for the detection of chemicals in the product. Reference material is prepared and evaluated for its stability and homogeneity. The stability assessment is carried out over a total of 60 days, to ensure that the concentration of the reference material remains stable. During the stability assessment, it is important to subdivide the reference material from the original stock into small volume so that possible deterioration or contamination could be avoided. After the stability of the reference material is confirmed, an assessment on material's homogeneity is carried out. Reference material is prepared in the same manner as in the stability assessment. Subsequently, the sample is subdivided into 20 or more samples with smaller volume and concentration of specific chemicals are measured for their homogeneity. Once the stability and homogeneity of the reference material is confirmed, the reference material is sent to several research agencies for the test.

Poster - 44

A method for quantitative analysis of nucleic acids using a nanoflow liquid chromatography-tandem mass spectrometry

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Nucleic acid (NA) plays an important role in a variety of biological processes in which genetic information on NA sequences of both deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) contributes to make functional macromolecules in a cell and also act as the carriers of genetic information in cells and viruses. Excepting the time-honored techniques (e.g., gel/capillary electrophoresis), quantitative profiling of nucleic acids isolated from biological matrixes is has been less frequently used in mass spectrometric (MS) method, due to their low stoichiometric abundances in cells. In this study, we introduced MS-based analytical method for qualitative/quantitative determination of NA in biological matrixes using a nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nLC-ESI-MS/MS). To this end, we developed and optimized the experimental workflow for MS-based analysis of NAs that enables to identify and quantify NAs from cell lines and viruses. Finally, we found that the method for MS-based analysis of NAs can be one of promising strategies in identifying and/or quantifying NAs, thereby being applicable to both cancer and viral diagnosis in the clinical application.

Poster - 45

The metabolites differences in a wing polyphenic small brown planthopper revealed by metabolomic analysis

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One of the leading pests of rice, small brown planthopper (*Laodelphax striatellus* : SBP) can grow up to have either short or long wings, depending on conditions. However, under the same breeding conditions, the phenotypes of the long- and short-winged SBP observed to keep the first collected phenotype. To investigate the mechanism involved in wing dimorphism, metabolomic researches have been conducted. In this study, using Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), we analyzed 80 SBP samples (n=5) from 2 solvents (methanol/chloroform), and, a different type of wing, and different sex. We previously detected ~1,500 m/z in the mass range m/z. The score plots of principal component analysis (PCA) and partial least squares-discriminate analysis (PLS-DA) showed in total, methanol fraction of ion peaks, m/z 432.24013 and chloroform fraction of ion peaks, m/z 217.04865, 333.11076, 449.17437, and 740.53309 clear discrimination between long- and short-winged SBP. Conclusion, we observed several metabolites change, and the difference of metabolites could provide clues to the relationship between physiological changes in the SBP and ecological transport.

Poster - 46

LC/MS and LC-UV analysis of photodegradation products of tetracycline and sulfathiazole

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Antibiotics released to the environment can be of an issue as they can enter the food chain posing risks to ecosystems and human health. Photodegradation has been proposed as a promising way of degrading antibiotics in environment. Antibiotics are usually present as mixtures in environment. However, previous studies usually focused on photodegradation behaviors of individual antibiotics. In this study, we investigated temporal photodegradation tendencies of antibiotics when two antibiotics are mixed together by comparing photodegradation changes when an individual antibiotic presents alone. For this purpose, we chose two most widely used antibiotics, tetracycline (TC) and sulfathiazole (STH). We performed UV-induced photodegradation of two antibiotics, individual forms and a mixed form for various time periods. Then, photodegraded products qualitatively and quantitatively analyzed by using LC-UV and liquid chromatography mass spectrometry (LC/MS) methods. Through this investigation, time-course changes of photodegraded products of TC and STH were successfully obtained and differential patterns of photodegradation were observed between individual and mixed forms.

Poster - 47

ICP MS Analyses of deciduous teeth for exposomics research

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Exposomics, a research field that tries to measure all the exposures of an individual and reveal how the measured exposures relate to health, receives increasing attention recently. There are two major challenges in exposomics analysis. First, exposomics research usually requires a longitudinal birth cohort that substantially increases cost and time. Second, it is very hard to estimate direct fetal exposures with common biomarkers such as maternal blood and urine. Recently, deciduous teeth have been proposed as novel biomarkers that partially overcome challenging issues. In this study, we tried to develop elemental analysis methods for teeth by employing various inductively coupled plasma (ICP) mass spectrometry (MS) platforms. For *in situ* inorganic chemical analysis against teeth samples, laser ablation (LA) ICP MS was used. With LA ICP MS, distribution information of various elements including Mn, Ba, Sr, and Zn were obtained directly from a deciduous tooth. As in the previous study, Zn was highly concentrated at the outer enamel edge, dentine-pulp margin and in the cervical dentine. For quantitative, multi-elemental analysis, an automated ICP DRC MS method with various reaction gases was developed and applied to acidic teeth digests. As a result, concentrations of over ten elements were successfully determined with deciduous teeth samples.

Poster - 48

Analysis of Isomeric Glycopeptides by High Temperature LC-MS/MS

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Protein glycosylation exhibits structural micro-heterogeneity according to its site specificity, which is important for protein properties and functions. The analysis of site-specific glycosylation with structural isomer remains a challenge because of structural micro-heterogeneity and abundance of glycopeptides in glycoprotein mixture. The most common approach is to analyze tryptic glycopeptides from glycoproteins by RPLC-MS/MS. In this work, the structural variation of sialic acid linkage isomer in model N- and O-glycoproteins was investigated by C18-RPLC-MS/MS at high temperature. The identified glycopeptides provided useful structural information from fragmentation spectra at retention time in high intensity by data-independent acquisition (DIA) and parallel reaction monitoring (PRM) analysis. This approach was demonstrated by characterization of acetylated sialic acids with linkage isomers in N- and O-glycopeptides. Further study of this approach will be applied to identify site-specific glycoslyation of glycoproteins in complex mixture such as serum.

Poster - 49

LC-MS based rapid profiling and inhibits xanthine oxidase activity from *Salbia plebeia*

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Salvia plebeia R. BR. is an annual or biennial grass, widely distributed in many countries, especially. It has been used as a folk medicine for the treatment of hepatitis, cough, inflammation and haemorrhoids. Phytochemical studies on *S. plebeian* revealed that it contained flavonoids, lignans, diterpenoids, aliphatic compounds and caffeic acid. Due to different cultivation areas and climatic conditions, its chemical constituents may vary significantly. In this study, we identify the active compounds in various concentrations of ethanol extract, we performed metabolite profiling using by high-resolution mass spectrometry(HR-MS) and tandem mass spectrometry (MS/MS) analysis. The analysis was followed by in-house MS/MS spectral database search to correlate both high-resolution mass spectrum and formula prediction of each component in ethanol extract with those of known compounds in natural-product databases available online. The profiling results were confirmed by comparing the MS and MS/MS spectral characteristics of the commercial standard compounds. These compounds showed inhibited the enzyme activity of xanthine oxidase, which is a key enzyme generating uric acid in the liver. These observations serve as a basis for further elaboration of the *S. plebeian* extracts for the development of new therapeutics for hyperuricemia and related disease.

Poster - 50

Parallel reaction monitoring of fucosylated glycopeptides of alpha-fetoprotein in human serum for early hepatocellular carcinoma by LC-MS/MS with immunoprecipitation

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We introduced direct analysis of fucosylated glycopeptides of α-fetoprotein (AFP) by parallel reaction monitoring (PRM) mass spectrometry (MS) combined with immunoprecipitation. α-fetoprotein (AFP) is a widely used serological marker that has been associated with hepatocellular carcinoma (HCC). In this study, we directly monitored fucosylated glycopeptides in AFP to provide a more accurate diagnosis of HCC. Because AFP is present at low concentrations in human serum, a more sensitive approach is required. In this study, two analytical methods were assessed to overcome sensitivity issues. First, LC-PRM MS combined with immunoprecipitation was performed to analyze AFP glycopeptides. Second, sialic acid was removed using a α-2,3,6,8 neuraminidase to improve the analytical sensitivity of target glycopeptides. The treatment of neuraminidase to glycopeptides for desialylation was useful to improve MS detection limit (LOD < 2 ng/mL) and to obtain reliable signal (CV < 20%) of target glycopeptides in AFP from sub μL serum. Finally, relative percentage of fucosylated AFP (AFP-fuc%) out of total glycosylated one was applied to compare sera with HCC, liver disease and healthy subjects. AFP-fuc% showed an area under the ROC curve (AUC = 0.949, p value < 0.0001) to discriminate between HCC and liver disease patients. These results suggest that our approach to target individual fucosylated glycopeptides using PRM provides an assay useful for the diagnosis of HCC.

Poster - 51

Proteomic analysis of exosomal proteins from rat Schwann cell

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Exosomes are nanometer-sized vesicle secreted by various cell types, especially in membrane proteins rich in biological fluids. Ex-vivo analysis of Exosome is becoming increasingly promising as a non-invasive tool for diagnosing and monitoring diseases and providing a new biomarker discovery platform. It is known that exosomes are present in the nervous system but it is not well known compared to other human organ or tissue studies. There is considerable support for the peripheral nervous system of the peripheral nervous system being directly influenced by Schwann cells (SCs). In order to recover the function after peripheral nerve damage, the neurons have not been identified and have no clue how the SCs contribute to the neural regeneration. Recent studies have shown that in ex-vivo, SCs-derived exosomes significantly influence axon regeneration, but there is limited evidence of the mechanism by which exosomes derived from SCs contribute to axonal regeneration. Furthermore, no studies have been performed on the comprehensive exosome analysis using proteomics techniques in the peripheral nervous system SCs. In this study, we present the first proteomic analysis of SCs exosomes. We have attempted to isolate exosome from SCs using the ultracentrifuge method. The common and specific exosomal markers CD63, CD9, Hsp70 and Hsp90 were identified from the exosome fractions in western blot. Protein profiling analysis was performed on exosome derived from primary SCs using Orbitrap Fusion mass spectrometer. The analysis identified a subset of proteins common to all exosomes such as transport (ESCRT) proteins, tetraspanins, signaling, trafficking, and endosome classifying complexes required for the cytoskeleton. The distinguishing feature found in this assay is that the neurotrophin receptor family p75NTR, TrKc, which is known as the surface antigen of dedifferentiated SCs, is present in the exosome. Also, Ncam1, Gap43 and S100, known as dedifferentiation SCs specific markers, are present in the exosome. Expression of semaphorin 3, plexin A, NRP, IgCAM, ephrin B, and ephrin B receptors, which are known as promoting axonal regeneration factors, was confirmed. The results suggest that exosome derived from SCs plays an important role in supporting axon maintenance and regeneration after nerve injury. The specific exosome protein of the primary SCs identified in this study may provide insight into potential diagnostic biomarkers involved in the disease process and regeneration of peripheral neuropathy.

Poster - 52

Spatial distribution of siloxanes in coastal sediment and identification of procedural contamination sources in GC/MS analysis

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Cyclic and linear siloxanes have been used as chemical additives in consumer and industrial products. However, several studies have reported potential toxicity of siloxanes, especially estrogen mimicry, reproductive, and liver damage in laboratory animals. Therefore, the occurrence of siloxanes in various environmental matrices can lead to negative effects on the ecosystem. The analytical determination of these compounds have been challenging because procedural contamination is highly affected during gas chromatography mass spectrometry (GC/MS) analysis. Therefore, this study was aimed to minimize the sources of background contamination of siloxanes during GC/MS analysis and analyze siloxane compounds, including 6 cyclic siloxanes (octamethylcyclotetrasiloxane–octadecamethylcyclononasiloxane) and 13 linear siloxanes (octamethyltrisiloxane–dotriacontamethyl pentadecasiloxane) in coastal sediments collected from southeastern industrial bays in Korea. The results identified that high level of cyclic siloxanes contamination was derived from the use of GC column and silicone septum of GC/MS ($\sum_6$ cVMS: 73.4±21.0 ng) or vial (38.9 ng). In particular, not only analysis, but the pretreatment process also significantly induced the contaminations. The use of silicone tube, during the concentration process, showed high levels of background contamination of $\sum_6$ cVMSs (73.4±5.8 ng). We analyzed $\sum_{19}$ Siloxanes in coastal sediments from the four industrial bays including Gwangyang, Jinhae, Busan, and Ulsan Bay. Almost all sediments had detectable levels of siloxanes and the total mean concentrations of the sites are higher than other countries. The distribution of siloxanes varied widely among the sampling sites, and compositional profiles of siloxanes were strongly affected by industrial activities in each bay. As a further study, risk assessment of siloxanes in the sediment will be carried out.

Poster - 53

Characterization of site-specific O-glycopeptides in fibroin heavy chain from silkworm cocoon using high resolution LC-MS/MS

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Silk fibroin, the structural protein of silkworm cocoon produced from bombyx mori has been reported to improve cognition function and immune system in healthy humans. Several silk proteins are known as glycoproteins but, fibroin protein is not yet known. Glycosylation is one of common post-translational modifications in a protein, which play a key role such as protein folding and protein-protein interaction. Therefore, characterization of glycosylation in fibroin protein is necessary in order to extend our understanding of its bioactivities. Fibroin protein is composed of highly repeating amino acid units of [G-A-G-A-G-S]n, and glycosylation is present at low concentration, which is difficult to analyze. So, we used HILIC enrichment and high resolution LC-MS/MS to effectively extract and identify the site-specific O-glycopeptides from nonspecific enzyme digestion of fibroin protein. A total 34 O-glycopeptides, 31 O-glycosylation sites, and 9 different O-glycans were identified from fibroin heavy chain. Most of the identified O-glycosylation sites were found at serine. Their exact O-glycosylation sites were identified by EThcD MS/MS spectra. We first report that O-glycosylation occurs in fibroin heavy chain with evidence of specific glycopeptide fragment ions in LC-MS/MS spectra. In conclusion, this new discovery of glycosylation through effective analytical method will contribute to understanding the biological systems of silkworm.

Poster - 54

Automated screening of organic pollutants in airborne particulate matter using GC×GC-TOFMS

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Comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry (GC×GC-TOFMS) has been applied to analyze complex samples such as airborne particulate matter (PM). PM samples contain thousands of compounds with unresolved carbonaceous matter (UCM), but they belong to many chemical groups such as polycyclic aromatic hydrocarbons (PAHs) and persistent organic pollutants (POPs). GC×GC is a powerful separation technology that can recognize individual chemical compounds and groups. Especially, computer-based tools with mass spectra can be applied for identification and classification of chemical compounds and groups. In this study, an automated screening method was developed based on chromatographic information on PAHs and POPs in airborne PM using GC×GC-TOFMS. First, basic search criteria of peaks and rule of classification were optimized with a special software, LECO ChromaTOF, and applied to $PM_{2.5}$ samples. Secondly, the script was written for automated classification based on fragmentation patterns, retention time, and mass spectra transformation. Finally, the efficiencies of classification methods were compared, and various $PM_{2.5}$ samples were evaluated with automated profiling. This method will be used for quick identification of persistent chemicals in PM collected during episode days.

Poster - 55

LC-MS/MS-based DIA method approach for proteome analysis on synechocystis sp. PCC6803 and PCC7338

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Synechocystis is a kind of cyanobacterium, among which pcc6803 has already undergone various studies including proteome analysis and has been utilized in various fields including biopharmaceutical field. It is expected that PCC7338, a synechocystis species, is an oceanic cultivating species and will be economically effective when used in place of PCC6803. Data independent acquisition (DIA) is introduced into the mass spectrometer by fragmenting all ions, in contrast DDA (Data-dependent Acquisition) where only ions with high intensities are selected and fragmented. There is an advantage that new objects can be found without additional method steps.

PCC6803 and PCC7338 samples were prepared and the database was constructed by DDA analysis using the HighHp RP Fractionation method. Then, based on the database, DIA analysis was carried out. At that time, skyline was used as sfotware.

As a result of DDA analysis, 6803 2421, 7338, and 2525 protein groups were identified. As a result of DIA, 7338 1878 and 6083 2379 quantitative analyzes were confirmed. We confirmed the possibility of the analysis of synechocystis by the DIA method, which is expected to be used in future studies.

Poster - 56

Validation and application of analytical tools for stable carbon isotope analysis of crude oils in molecular level using ultra-high resolution mass spectrometry

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

Poster - 57

Performance evaluation of ICP-MS for Ra-226 determination

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Ra-226, which has radio-toxic characteristics for human health, is most significant contributor to occupational radiation doses from naturally occurring radioactive material (NORM). It is well known that traditional analytical methods for the Ra-226 in environmental and NORM samples are labor intensive and have large uncertainty of measurement. Thus, the study focused on the evaluation the performance of ICP-MS and optimization of measurement condition for Ra-226 determination. The sensitivity and detection limit of ICP-MS (ICAP-RQ, Thermo Fisher, Germany) with the APEX (ESI, USA) sample introduction system were evaluated using Ra-226 standard solution from NPL (National physics laboratory, UK). The sensitivity for the Ra-226 concentration of 1 ng/L (corresponded to 37 Bq/L) with standard mode was about 1300 cps and the relative standard deviation of the measurement was 3.5 %. The effect of polyatomic interference originated from high concentration of Ba and Sr also was examined. In KED mode (using collision cell with He gas) the effect of polyatomic interference was considerably decreased. However, the signal intensity of Ra-226 was also reduced to 57% compared to standard mode. Finally, for the ICP-MS determination of Ra-226, the limit of detection was evaluated to 2 pg/L, which correspond to 74 mBq/L.

Poster - 58

Development and validations of the simultaneous analytical method of nine environmental phenol compounds in human urine samples using liquid chromatography – tandem mass spectrometry

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Environmental phenols including bisphenols, parabens, triclosan, and benzophenone are exposed to the general population through various living products such as food containers, cosmetics, medical supplies, etc. The method for simultaneous analysis developed and validated in this study includes bisphenol A/F/S (BPA/BPF/BPS), triclosan, methyl-/ethyl/butyl-/propyl-paraben, and benzophenone-3(BP-3). In this method, 0.5 mL of human urinary sample was needed. Liquid-Liquid Extraction was carried out and liquid chromatography – tandem mass spectrometry was applied, as well. Retention time for nine compounds was 8.9 minutes. Method detection limits and limit of quantitation of nine compounds 0.020 – 0.115 μg/L and 0.060 – 0.345 μg/L, respectively. Standard curves showed 0.995 – 0.999 of R-square from 0.5 – 800 μg/L. Recovery rates were calculated 80 – 113% of nine compounds. This method may be considered as a more effective way which can be applied to the nationwide biomonitoring program for the field of environmental health.

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Poster - 59

Selection of functional metabolites of Torreya nucifera by comparison of metabolites

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Torreya nucifera is a conifer species that is classified as a plant that lives in the southern part of Korea and Jeju Island. The fruit is mostly used as insect antifeedant, hair growth agent, medicinal material, and edible oil. Recent studies show that the extraction of edible oil and the unusual biological active of the fruit. In this study, mass spectrometry-based metabolic profiling was carried out to metabolically characterize the *nucifera* fruit compared to typical nuts of *juglans regia* (walnut), *pistachio vera* (pistachio), and *arachis hypogaea* (peanut). As a result, among the primary metabolites, γ-aminobutyric acid and spermidine are significantly abundant in T. nucifera compared to other nuts. In addition, unique distribution of metabolite contents was identified according to different component (e.g. nut, endodermis, and husk). The pilot study lead to detailed testing of the functional activity of gradients (e.g. radical scavenging activity) and isolate biological active compounds for higher value.

Poster - 60

Quantitative proteomic analysis of molecular and functional alterations in the human neuronal cell culture model of Alzheimer's disease

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Alzheimer's disease (AD) is characterized by amyloid plaques composed of β-amyloid (Aβ) peptides and neurofibrillary tangles composed of hyperphosphorylated tau. However, the molecular mechanism of AD pathology is yet to be fully elucidated. Recently, we developed a 3D human neuronal cell culture model recapitulating Aβ plaques and Aβ-driven tau pathology. In this study, we performed a quantitative proteomics of this cellular model to understand the early events of AD pathology. Proteins extracted from differentiated cells were fractionated into cytoplasmic and membrane fractions and then subjected to trypsin digestion. The resultant peptides were labeled with TMT isobaric mass tags, further fractionated by basic pH RPLC, and analyzed by nano LC-MS/MS. Through bioinformatics analysis, we quantify the proteome expression profile of the AD human neuronal cells overaccumulation and deposition of Aβ. Our proteomics dataset will be valuable for future investigation of the molecular mechanisms underlying Aβ-driven tau pathology in AD.

Poster - 61

Simultaneous LC-MS/MS analysis of three alkanolamines found in cosmetics

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Alkanolamines such as monoethanolamine (MEA), diethanolamine (DEA), and triethanolamine (TEA) are used as wetting agents in shampoos, lotions, creams, and other cosmetics. DEA is widely used to provide lather in shampoos and maintain a favorable consistency in lotions and creams. Although DEA is not harmful, it may react with other ingredients in the cosmetic formula after extended storage periods to form an extremely potent carcinogen called nitrosodiethanolamine (NDEA), which is readily absorbed through the skin and has been linked to the development of stomach, esophagus, liver, and bladder cancers. The purpose of this study was to develop a simultaneous quantification method for measurement of MEA, DEA, and TEA in cosmetic products. Liquid chromatography coupled tandem mass spectrometry (LC–MS/MS) was performed using a hydrophilic interaction liquid chromatography (HILIC) column with isocratic elution containing acetonitrile and 5 mM ammonium formate in water (88:12, v/v). Identification and quantification of alkanolamines were performed using MS/MS monitoring to assess the transition from precursor to product ion of MEA (m/z, 61.1 → 44.0), DEA (m/z, 106.1 → 88.0), TEA (m/z, 150.1 → 130.0), and the internal standard triethylamine (m/z, 102.2 → 58.0). Alkanolamines extractions were simplified using a single extraction with acetonitrile in the cosmetic matrix. Performance of the method was evaluated with quality parameters such as specificity, carry-over, linearity and calibration, correlation of determination (R^2), detection limit, precision, accuracy, and recovery. Calibration curves of MEA (2.9–1000 ppb), DEA (1–1000 ppb), and TEA (1–1000 ppb) were constructed by plotting concentration versus peak-area ratio (analyte/internal standard with a correlation coefficient greater than 0.99). The intra- and inter-assay accuracy ranged from 92.92 to 101.15 % for all analytes. The intra- and inter-assay precision for MEA, DEA, and TEA showed all coefficients of variance were less than 9.38 % for QC samples. Limits of detection and limits of quantification were 2.00 and 15.63 ppb for MEA, 0.49 and 1.96 ppb for DEA, and 0.49 and 1.96 ppb for TEA, respectively. This novel quantification method simplified sample preparation and allowed accurate and reproducible quantification of alkanolamines in the ng/g cosmetic weight (ppb) range for several cosmetic products.

Poster - 62

Rapid determination of β-lapachone in clinical samples using LC-MS/MS

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β-Lapachone (3,4-dihydro-2,2-dimethyl-2H-naphthol[1,2-b]pyran-5,6-dione) is a naturally occurring compound found in the bark of a South American Lapacho tree (*Tabebuia avellanedae*). Many *in vitro* studies have been performed to show its anticancer and anti-inflammatory effects for several diseases. A few researchers have developed analytical methods to determine the levels of β-lapachone and its metabolites in *in vitro* samples. Due to the complexity in human metabolism, however, clinical samples may have more complex profiles than *in vitro* samples. As a result, it is important to develop an analytical method to properly quantify the levels of β-lapachone in clinical samples. In this study, we developed an analytical method to accurately determine β-lapachone levels in human plasma, obtained from a clinical study, using liquid chromatography–tandem mass spectrometry (LC-MS/MS). We validated it with respect to its linearity, selectivity, sensitivity, accuracy, precision, recovery, and stability in accordance with the guidance for analytical method validation issued by both the US Food and Drug Administration and the Ministry of Food and Drug Safety in Republic of Korea. Then, we applied it to study the pharmacokinetics of β-lapachone in human.

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Poster - 63

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

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Newborn screening for phenylketonuria (PKU), homocystinuria (HCU), and maple syrup urine disease (MSUD) have been generally diagnosed by various detection methods including Guthrie test (substituting bacterial inhibition assay), HPLC, and LC-MS/MS. MALDI-ToF mass spectrometry could be utilized to quantify the biomarkers of the metabolic diseases by easy sample preparation and simultaneous detection.

In this work, parylene-matrix chip was developed for the qualitative and quantitative analysis of biomarkers (amino acids) using MALDI-ToF mass spectrometry by reducing the organic matrix-related noise at low mass-to-charge ratio range ($m/z<500$). [1] Parylene-N thin film was deposited on dried organic matrix (CHCA) spots with the thickness of 50~80 nm. Methanol extraction was conducted for easy and rapid sample preparation of serum sample before the mass spectrometric analysis precipitating proteins in human serum. Calibration curves were obtained by analyzing amino acids in water and serum. They showed good linearity ($R^2 > 0.98$) and the LODs were ranging from 9.0 to 22.9 μg/mL.

From these results, MALDI-ToF MS using parylene-matrix chip could be applied to the quantitative detection of amino acids for the screening of neonatal metabolic disorders with less background noise at low mass-to-charge ratio range.

Poster - 64

Diagnosis of gout and pseudogout using inorganic TiO2 matrices for LDI-ToF mass spectrometry

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Arthritis pain is often resulted from the deposition of crystals in joints or tissues. Monosodium urate (MSU) and calcium pyrophosphate dihydrate (CPPD) are frequently observed crystals in the joint space, which lead to gout and pseudogout arthropathies, respectively.

Gout and pseudogout exhibit very similar symptoms such as severe onset of pain in the affected joint followed by warmth, swelling and redness but their causes are quite different. Therefore, the accurate identification method for two kinds of arthropathic crystals is essentially required for the proper treatment as well as obvious diagnosis of these diseases. Although finding crystals in synovial fluid has been the gold standard for the diagnosis of these disorders, it contains several problems such as time-consuming analysis and high false negative results.

In this work, TiO2 nanowires developed by wet-corrosion process and TiO2 nanoparticles were used as solid matrices for the diagnosis of gout and pseudogout using LDI-ToF MS. Quantitative as well as qualitative analyses of MSU and CPPD crystals were presented and the feasibility for the diagnosis of gout and pseudogout was demonstrated.

Poster - 65

Diagnosis of galactosemia by MALDI-TOF mass spectrometry using a parylene-matrix chip

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A new quantification method of galactose was presented for the newborn screening test of galactosemia by using MALDI-TOF mass spectrometry (MS) based on parylene-matrix chip. The diagnosis of galactosemia, an inborn metabolic disease, is generally performed with various detection methods. For the quantitative analysis of galactose, the reduction potential of galactose was used to reduce o-phenylene diamine (OPD) into 2,3-diaminophenazin (DA) which could be quantitatively analyzed by MALDI-TOF MS based on parylene-matrix chip. A parylene-matrix chip was developed for the qualitative and quantitative analysis of galactose in PCB buffer and methanol using MALDI-TOF MS by diminishing noises of conventional organic matrix. Parylene-N thin film was deposited on dried organic matrix (CHCA) spots with the thickness of 50 ~ 80 nm. As the feasibility test of this method the interference of glucose and matrix proteins in serum was analyzed. Finally, the concentration of galactose spiked in human serum and the intensity of mass peak of DA were linearly correlated for the application to the newborn screening test of galactosemia.

Poster - 66

Development of sensitive β-lactamase assay for *E.coli* using a parylene-matrix chip

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β-lactamase(EC 3.5.2.6) are an important family of enzymes that confer resistance to β -lactam antibiotics by catalyzing the hydrolysis of these antibiotics. However, most current assays of β-lactamase activity are laborious and time-consuming. MALDI-TOF mass spectrometry has been used for the analysis of biomolecules with high molecular weights. MALDI-TOF mass spectrometry has many advantages, such as easy sample preparation, and low sample consumption. However, when organic matrix is evaporated and ionized during the MALDI process, the mass peaks of the resulting fragmented matrix are observed at low mass-to-charge ratio(m/z<500). The Parylene-matrix chip was developed for the quantitative analysis of small molecules and improvement of signal-to-noise ratio. The β-lactamase assay using Parylene-matrix chip measured the hydrolysis of penicillin into penicilloic acid with minimal interference of low molecular weight peaks. Finally, Penicillin-susceptible and penicillin-resistant *E.coli* were prepared and mixed with penicillin to validate the susceptibility against penicillin. The penicillin-susceptible and penicillin-resistant *E.coli* strains showed different mass signal ratios at an absolute number of 1000 *E.coli* cells.

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Quantitative and sensitive carbapenem susceptibility test using MALDI-TOF 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.

Poster - 68

Better sensitivity in LC/MS by improved sample preparation and HPLC method for determination of vitamin D metabolites in plasma

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In clinical analysis determination of vitamin D species is important, because they are markers for certain diseases and for vitamin insufficiency. The main two forms of vitamin D are vitamin D2 and D3, but for the determination usually 25-OH vitamin D3 and 25-OH vitamin D2 are used. Epimeric forms of 25-OH vitamin D3 and D2 have been discovered recently, which are biologically inactive [1]. ELISA techniques for vitamin D analysis cannot be used, because they are not able to distinguish these different forms of the vitamin D metabolites. In LC/MS the isobaric 25-OH vitamin D3 and D2 must be separated by chromatography.

This poster presents a new sample preparation method and new LC/MS method for the analysis of Vitamin D metabolites in human plasma. These new methods are especially considering the reduction of matrix impact on the ionization in MS and the chromatographic separation of all isobaric compounds. Phospholipids are often leading to ionization suppression in MS. Zirconia-coated silica has been proven successfully for the removal of phospholipids from plasma and serum samples [2,3] and was employed for this sample preparation. The ideally suited stationary phase for HPLC analysis was determined by screening of different stationary HPLC phases in the method development. The resulting Sample Prep and HPLC method allow for the direct quantitation of all vitamin D compounds including the isobaric compounds.

[1] Singh et al, J. Clin. Endocrinol. Metab. 91 (2006) 3055-61
[2] Nobutaka Hattori et al., Sci Rep. 7 (2017) 7328
[3] Junji Ohnishi et al., Human Genomics 11 (2017) 21

Poster - 69

Isolation, Characterization and Quantitative Analysis of Major Compound in Different Parts of *Hovenia dulcis* using Ultra-Performance Liquid Chromatography Coupled with Orbitrap Mass

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Hovenia dulcis (HG) is a popular traditional medicine and has been widely used in Korea and Southeast Asia for the treatment of hepatitis and diabetes. In this study, the major metabolite was isolated from HG and its chemical structure was elucidated by extensive spectroscopic data, including 1D NMR, 2D NMR, UV, IR and HR-ESI-MS analysis. Additionally, an analytical method using high performance liquid chromatography coupled with orbitrap mass spectrometer was developed for identification of the xx in HG. Our results show that calibration equation of the target compound exhibited good linear regression within the test range ($R2 \geq 0.9999$) and xx was the major constituent in different parts of HG. Interestingly, this species showed the highest amount of 20.87 mg/g of 27-*O*-protocatechuoylbetulinic acid in the roots part. It indicated that HG roots are rich in 27-*O*-protocatechuoylbetulinic acid, which could be a promising candidate for the development of nutraceutical and industrial applications.

Poster - 70

Urinary Metabolomic Profiling to Discover Potential Biomarkers of Acute Cellular Rejection in Kidney Transplant Recipients

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Acute cellular rejection (ACR) is one of the most common complications after kidney transplantation. To improve early renal allograft function, it is important to develop a noninvasive diagnostic method for ACR. However, current diagnostic methods for ACR have limitations such as invasiveness, sampling error, or nonspecificity. To complement the shortcomings of current diagnostic methods, thus, it is important to develop a noninvasive, more specific diagnostic method for ACR. This study aims to explore potential noninvasive urinary biomarkers to screen for ACR in kidney transplant recipients using untargeted metabolomic profiling.

Urinary metabolites, collected from kidney transplant recipients with non-rejection (NR) or ACR episodes, were analyzed using liquid chromatography-mass spectrometry (LC-MS). Statistical analysis revealed the differences in urinary metabolites between the two groups. ROC curve analysis showed the best performance of the training set (AUC, 0.926; sensitivity, 90.0%; specificity, 84.6%) using a panel of 5 potential biomarkers: guanidoacetic acid, methylimidazoleacetic acid, dopamine, 4-guanidinobutyric acid, and L-tryptophan. The diagnostic accuracy of this model was 62.5% for an independent test dataset.

Overall, LC-MS-based untargeted metabolomic profiling is a promising method to discriminate between ACR and NR groups. Our model, based on a panel of 5 potential biomarkers, needs to be further validated in larger scale studies.

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Poster - 71

Optimization of analysis conditions for native disulfide bond using mass spectrometry

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Disulfide bonds are one of the most common covalent posttranslational modifications of proteins. They play an important role in maintaining the three-dimensional structures of proteins, and their biological activities. Therefore, the determination of disulfide bonds becomes an important aspect of obtaining a comprehensive understanding of the chemical structure of the protein. Numerous experimental methods have been developed for the determination of disulfide bonds in proteins. However, the difficulties lie in the disulfide bonds analysis such as free thiols and disulfide bond scrambling, etc. due to the variety of the external environmental factors involved. Thus, with the experiment, I was able to solve the difficulties mentioned above and that led me to conduct more accurate research for the disulfide bonds analysis.

In the study, the optimum to analyze the native disulfide Bond needed to be searched by using mass spectrometry with standard reference materials(lgG,150kDa) which the base sequences are recognized. The search ranges for the optimum were in three major variants to perform the experiment; (1) pH 6~8(5point), (2) NEM(N-ethylmaleimide) existence (3) Urea existence. The disulfide bond analyses with various conditions were carried out using mass spectrometry among different analysis methods. Especially, it was possible to perform the analysis method with high sensitivity and resolution utilizing the Orbitrap-based system. Through this study, we expect to contribute to more accurate research of disulfide bond analysis for protein with using mass spectrometry.

Poster - 72

Simultaneous analysis of highly acidic glycans in biotherapeutics using PGC-SPE and LC-MS/MS

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Glycosylation of a therapeutic glycoprotein influences on pharmacological functions including drug's efficacy, safety, and biological activity. During product manufacturing, various media-experimental conditions can lead to alterations in glycosylation. Therefore, overall glycan profiling including both targeted and untargeted species should be performed for drug's QA/QC. In particular, acidic glycans were directly associated with *in vivo* functions. However, their analysis is still highly challengeable because of the absence of enrichment tools and ion-suppression/interference caused by different acidity in MS. We here designed an efficient strategy having high separation selectivity for parallel analysis of multiple acidic glycans using the combination of porous graphitized carbon-solid phase extraction (PGC-SPE) and high resolution LC/MS. For enhanced separation performance, diverse glycans were pre-fractionated by PGC-SPE technique according to molecular size and polarity. Subsequent LC/MS/MS analyses of differentiated species enabled informative profiling on acidic glycans providing glycan compositions, full glycan structures, and relative quantitation at once. We successfully determined both phosphorylated and sialylated glycans in a therapeutic enzyme by a single sample preparation, indicating an efficient platform to assess the glycosylation comparability between therapeutic glycoproteins involving different types of acidic glycans.

Poster - 73

Detection of Neu5Gc in Human Serum via MRM-MS

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Sialic acid expressed as an outer terminal unit on a glycan plays immunological and physiological roles such as immunological processes, hormonal response, and signal transmission. Unlike other mammalian, human cannot biosynthesize N-Glycolylneuraminic acid (Neu5Gc) due to irreversible mutation on gene CMAH. Exogenous Neu5Gc can be an immunogenic antigen in human cells and it is also reported to be found in a high level of concentration in human cancers, suggesting that immunogenic Neu5Gc is a cancer-associated glycan. Therefore, the determination of Neu5Gc from human fluids and tissue is highly important in clinical research. In this study, for the first time, we developed an analytical method using mass spectrometry to selectively identify and quantify Neu5Gc in human serum. Briefly, sialic acids were liberated from human serum by chemical hydrolysis and further enriched using solid phase extraction with a PGC cartridge. The Neu5Gc was chromatographically separated on a PGC column, then analyzed by MRM-MS. The limits of detection/ quantitation (LOD/ LOQ) for Neu5Gc and the linearity between Neu5Gc concentration and MS signal for quantitation were examined. The concentration of Neu5Gc from human serum was determined at low pico mole levels with high reproducibility (CV<6%). This result could be used for newly updated data of human serum, and moreover it is expected to be applied as a valuable reference for clinical research.

Poster - 74

Synergistic antibacterial activity of phenolic compound-antibiotic combination and their quantitative determination by LC-QTOF-MS

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Bacteria have a remarkable ability to acquire resistance against antibiotics by several mechanisms. New strategies are needed to block the development of resistance and to prolong the life of traditional antibiotics. Thus, we intended to increase the efficacy of commercially available antibiotics by combining with opportunistic phenolic compounds. Ten commercial antibiotics and 5 phenolic compounds were used against *Salmonella* Typhimurium, *Escherichia coli* and *Staphylococcus aureus* to evaluate the antibacterial combination effect. Finally, LC-QTOF-MS was used to quantify individual compounds from mixtures of antibacterial agents. Phenolic compounds demonstrated good antimicrobial activity varied with minimum inhibitory concentration depending on compounds and strains. Fractional inhibitory concentration (FIC) index of 40 sets of combination against *S.* Typhimurium, *E. coli* and *S. aureus* ranged from 0.281 to 1.016. Three combinations were selected for further investigation depending on the critically important antibiotics list of World Health Organization and the FIC index of our study. Inhibition rates of *S.* Typhimurium in presence of Gallic Acid+Ceftiofur, *E. coli* in presence of Hamamelitannin+Erythromycin, and Gallic Acid+Ampicillin demonstrated improved efficacy compared to the efficacy of those antimicrobials alone. The effect of those three combinations on the cell morphology of *S.* Typhimurium and *E. coli* were evaluated and found that those antimicrobial combinations have no effect on cell morphology. All of the three combinations showed different degrees of biofilm inhibition potential. Among them Hamamelitannin+Erythromycin combination demonstrated better inhibition potential of *E. coli* biofilm. Viability of biofilm of *S.* Typhimurium in presence of Gallic Acid+Ceftiofur, and *E. coli* in presence of Hamamelitannin+Erythromycin, and Gallic Acid+Ampicillin demonstrated improved efficacy compared to the efficacy of those antimicrobials alone. All of these five compounds were successfully quantified by LC-QTOF-MS from different compound mixtures. Based on the result of this study, it is concluded that the therapy of these combinations can be more effective than the conventional antibiotics in controlling *S.* Typhimurium and *E. coli* associated infections. Further investigations are recommended to determine the safety profile and combination antimicrobial effect in *in vivo* system.

Keywords: Combination therapy, critically important antibiotics, gallic acid, hamamelitannin, biofilm.

Poster - 75

Rapid and sensitive determination of apixaban in human plasma using LC-MS/MS

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Apixaban was determined in human plasma by LC-MS/MS using isotopic as an internal standard. To simplification of extraction steps and optimization of chromatographic condition, sample preparation method was accomplished using protein precipitation. The mobile phase was composed of water *containing* 0.1% formic acid in and acetonitrile containing 0.1% formic acid. The mobile phase condition was gradient mode and total run time was 3.0 min. The LC-MS/MS system was equipped with an electrospray source operating in the positive ion mode. The lower limit of quantification (LLOQ) was 1 ng/mL, using a sample volume of 50 μL for the analysis. The reproducibility of the method was evaluated by analyzing five replicates at four quality control (QC) levels over the nominal concentration range 1 to 1000 ng/mL. Apixaban produced a protonated precursor ion ($[M+H]^+$) at *m/z* 460, and a corresponding product ion at *m/z* 443. Internal standard produced a protonated precursor ion ($[M+H]^+$) at *m/z* 464 and a corresponding product ion at *m/z* 447. The validation, reproducibility, stability, and recovery of the method were evaluated. The method has been successfully applied to pharmacokinetic studies of apixaban in human plasma.

Poster - 76

Rapid and sensitive determination of empagliflozin and dapagliflozin in human plasma using LC-MS/MS

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Empagliflozin and dapagliflozin was determined in human plasma by LC-MS/MS using isotopic as an internal standard. To simplification of extraction steps and optimization of chromatographic condition, sample preparation method was accomplished using liquid-liquid extraction. The mobile phase was composed of methanol and 2 mM ammonium acetate and total run time was 4.0 min. The LC-MS/MS system was equipped with an electrospray source operating in the negative ion mode. The lower limit of quantification (LLOQ) was 5 ng/mL and 1 ng/mL, using a sample volume of 100 μL for the analysis. The reproducibility of the method was evaluated by analyzing five replicates at four quality control (QC) levels over the nominal concentration range empagliflozin 5 to 1000 ng/mL and dapagliflozin 1 to 1000 ng/mL. Empagliflozin produced a protonated precursor ion ($[M-H]^-$) at m/z 449, and a corresponding product ion at m/z 371. Internal standard produced a protonated precursor ion ($[M-H]^-$) at m/z 453 and a corresponding product ion at m/z 375. Dapagliflozin produced a protonated precursor ion ($[M-H]^-$) at m/z 407, and a corresponding product ion at m/z 329. Internal standard produced a protonated precursor ion ($[M-H]^-$) at m/z 412 and a corresponding product ion at m/z 334. The validation, reproducibility, stability, and recovery of the method were evaluated. The method has been successfully applied to pharmacokinetic studies of empagliflozin and dapagliflozin in human plasma.

Poster - 77

Rapid and sensitive determination of dexamethasone in culture media using LC-MS/MS

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Dexamethasone was analysis in culture media by LC-MS/MS. To simplification of extraction steps and optimization of chromatographic condition, sample preparation method was accomplished using liquid-liquid extraction. The mobile phase was composed of acetonitrile and 0.05% ammonium hydroxide solution and total run time was 3.0 min. The LC-MS/MS system was equipped with an electrospray source operating in the positive ion mode. The lower limit of quantification (LLOQ) was 0.02 ng/mL using a sample volume of 100 μL for the analysis. The reproducibility of the method was evaluated by analyzing third replicates at three quality control (QC) levels over the nominal concentration range 0.02 to 10 ng/mL. Dexamethasone produced a protonated precursor ion ($[M+H]^+$) at m/z 393, and a corresponding product ion at m/z 373. The validation, reproducibility, stability, and recovery of the method were evaluated. The method has been successfully applied to samples analysis of dexamethasone in culture media.

Poster - 78

Development and validation of HPLC-MS/MS method for the determination of 9-cis and trans-β-carotene in rat plasma using solid phase extraction.

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Carotenoids are precursors of vitamin A that contribute to health and disease prevention and β-carotene is major carotenoid existed as cis/trans stereoisomer in nature. To elucidate the ratio of each carotenoid and quantify the cis/trans β-carotene, specific and reliable analysis method is required. In present study, we developed a sensitive and rapid method to determine of 9-cis β-carotene and trans-β-carotene levels in rat plasma using high-performance liquid chromatography-mass/mass spectrometry (HPLC-MS/MS). The separation was carried out on a Acclaim™ C30 (3 μm, 2.1×100 mm, Thermo Scientific) column at 30°C. All separated compounds including the internal standard (echinenone) were eluted within 25 minute with 0.1% formic acid in water/ethanol (10/90, v/v) and 0.1% formic acid in methanol. A solid-phase extraction (SPE) method was used for the sample pretreatment to determine of 9-cis β-carotene and trans-β-carotene in rat plasma. The each step for SPE was optimized to 2-propanol/ethanol (1/1, v/v) as the extraction solvent, 50% ethanol as the washing solvent, and Hexane as the elution solvent. The analytical method was established and validated on the basis of FDA method validation guidance to apply to pharmacokinetic study of β-carotene in rats.

Poster - 79

Relative quantification of lipids in mouse serum for the discovery of preterm birth and miscarriage biomarker via metabolic heavy water labeling

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Miscarriage is a pregnancy loss before 20 gestational weeks. Preterm birth (PTB), a birth before 37 gestational weeks, causes a high rate of perinatal morbidity and mortality. Despite the threats, there is a lack of diagnostic biomarker that can identify PTB or miscarriage in the early stage of pregnancy. Herein, we presented an analytical platform for the discovery of lipidomic PTB and miscarriage markers in mouse serum by metabolic heavy water (^2H_2O) labeling. Four replicates of two mouse models (CBA/J×DBA/2 and CBA/J×BALB/c) were used for PTB/miscarriage and control groups, respectively. In the control group, the female CBA/J mice were administrated with 8% ^2H_2O enriched drinking water for four days prior to mating with BALB/c male mice. In case of PTB/miscarriage group, normal drinking water was provided for female CBA/J mice. Serum was collected from CBA/J mice in both control and PTB/miscarriage group after 16 days of mating. Serum lipid extracts from control and PTB/miscarriage groups were mixed in 1:1 ratio based on the serum volume and then analyzed by LC-MS for the relative quantification. As a result, more than 440 lipids from fatty acyl, glycerophospholipid, glycerolipid, and sphingolipid were identified in each biological replicate. Statistical analysis confirmed 11 PTB or miscarriage biomarker candidates including triacylglycerols, phosphatidylethanolamine, and phosphatidylinositol.

Poster - 80

High-throughput discovery of anti-inflammatory components in Aster Yomena

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Aster Yomena (AY), which was developed as a variety of foods, showed anti-obesity and anti-inflammatory activities in vitro and in vivo screening test in our lab. In this study, the quantitative and qualitative analyses of the fractional extracts from AY was carried out by using LC/MS. Nitric oxide (NO) production inhibition was confirmed and standardized to find new anti-inflammatory ingredients. In this study, we used a sample preparation method of the AY used for medicinal and edible purposes. Then, the 70% ethanol solvent was repeatedly used 4 times over 3 hours to extract, and then 2.5 kg of the extract was fractionated with 50%, 85% and 100% aqueous acetonitrile eluents on an open C18 coulmn, respectively. The extract fractionated with 50% aqueous acetonitrile solution showed the highest NO production inhibitory activity and then were fractionated into 15 subfractions with preparation LC. To evaluate the relative anti-inflammatory activity of those subfractions, NO production inhibitory activity were measured after LPS treatment for each subfractions. We also accumulate the ultra-high resolution Fourier transform ion cyclotron resonance mass spectrum (FT-ICR MS) of each subfraction. Using the correlation between profiles of peak intensities in the mass spectra and activities of the AY subfractions (SCAMP; Scaling of Correlations between Activity and Mass Profiles), the potential of anti-inflammatory active components were listed with increasing order of the relative anti-inflammatory efficacy.

Poster - 81

Quantitative analysis method for metabolic markers of Preterm births and miscarriage

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As of 2015, the total number of the newborns in Korea is estimated to be the second lowest in the world. As a result, births of spontaneous abortions, low birth weight infants and very low birth weight infants are rapidly increasing. Purpose of this study is to establish a qualitative and quantitative analytical method for finding biomarkers that can be used to diagnose inflammation and to monitor the treatment progress, which will eventually enlighten the main cause of miscarriage and prematurity. Formate, acetate, tyrosine, leucine and lysine have been reported as metabolic markers of preterm births and abortion. Formate and acetate were quantitatively analyzed by gas chromatography-mass spectrometry (GC- MS), The derivatized formate and acetate were analyzed using electron ionization (EI) mode of GC-MS. Calibration curves for acetate and formate were obtained using internal standards and they were detected and quantified in real urine samples. Tyrosine, leucine and lysine were quantitatively analyzed by liquid chromatography-mass spectrometry (LC-MS) by multiple reaction monitoring (MRM).

Poster - 82

Development of Screening Software for Illicit Drugs and Analogues

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Illicit drugs and analogues, like erectile dysfunction (ED) drugs, analgesics, diuretics, weight loss compounds, and psychotropic drugs, are widely spread in the online markets. To monitor these illegal drugs and analogues from the illegal market places, LC-MS/MS screening software was developed. A screening software, named as 'Spectra Match', consists of two layers. The first layer is the viewers for chromatogram and mass spectra. This first layer is coupled with the second layer in which the identification of compounds under LC-MS/MS investigation is a main function. Secondly, as an additional option, a machine learning-based classification model is included to classify unknown ED drug analogues in the software. For this the LC-MS/MS spectra for ED drug analogues were converted to binary bar-code spectra, and these bar-code spectra were trained with various machine learning techniques such as CART, random forest, KNN, SVM and ANN. Bar-code tandem mass spectra of the ED samples categorized into four groups i.e., tadalafil, sildenafil, vardenafil group, and the others, based on their structural similarities were machine-learned and a multiclass classification statistical model was constructed. This machine-learned models were included in the software as a screening tool for ED drug analogues that may be illicitly added into health supplements. This research was supported by a grant (18182MFDS425) from Ministry of Food and Drugs Safety of Korea.

Poster - 83

Visualization of the distribution of small molecule in pig-to-nonhuman primate islet xenotransplantation model by MALDI-MS imaging

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Human islet transplantation is one of the established treatments for intractable type 1 diabetes mellitus (DM1). Although short-term islet function after transplantation has been improved, the outcome of long-term islet graft function is still unsatisfactory. In this study, we investigated chemically diabetic induced rhesus monkeys (*Macaca mulatta*) were transplanted with porcine long-term islet via the jejunal veins. Liver biopsy samples from the recipient monkeys were first prepared in 12 μm thick cross-section using cryostat, applied with the DHB matrix using imageprep, and compared the distribution of lipids at a spatial resolution of 50 μm per image pixel by 9.4T Fourier-transform ion cyclotron resonance mass spectrometry imaging (9.4T FT-ICR MSI). These ion peaks of lipid (150 m/z to 1,500 m/z) were used to create mass ion visualize the differences between DM1 and healthy liver specimens. Most of these peaks corresponded to islet graft loss in the transplanted liver. Peaks at m/z 269.5307, 274.85544, 406.95419, 582.96292, 782.56915 and 797.52856 were overexpressed in DM1 liver. These data show for the first time that MSI is well-suited to visualize the spatial distribution of DM1 in a rhesus monkey model's liver. The data can be used in research and clinical practice.

Poster - 84

Metabolic change of serum polyamines after Mediterranean diet and contrave treatment on overweight breast cancer patients

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Breast cancer is the leading cause of female cancer burden, and its incidence has increased by more than 20% worldwide since 2008. Obesity is an indicator of poor prognosis for patients with primary breast cancer even after the administration of adjuvant chemotherapy. Some observational studies have suggested that the Mediterranean diet may reduce the risk of breast cancer. Contrave is an FDA-approved weight loss pill that helps reduce hunger and control cravings. Polyamines are essential for cell growth and differentiation of cells and its increased production in observed in many cancers. The liquid chromatography- tandem mass spectrometry (LC-MS/MS) based quantitative analysis of 9 polyamines in biological specimens was therefore investigated. LC-MS/MS analysis method involves chemical derivatization with dansyl chloride for improved sensitivity. LC system used gradient elution system which consists of 0.1% formic acid in water and acetonitrile at a flow rate of 0.2 mL/min. All analytes were separated through a reversed-phase C18 column (150 × 2.1 mm, 3 μm) and detected in seleted reaction monitoring mode. The linearity, which was expressed using the correlation coefficient, was greater than 0.99. The present method was applied to serum samples from four patients with breast cancer who had only mediterranean diet, five patients with breast cancer who were taking contraves together with Mediterranean diet, and six normal people who were taking contraves together with Mediterranean diet. This devised LC-MS/MS methods could be used to confirm the effect of Mediterranean diet and contrave treatment on overweight breast cancer patients.

Poster - 85

Estabilishment of stability conditions to analyze vitamin B12 using LC-MS/MS

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Vitamin B12 is a water-soluble vitamin with essential roles in red blood cell production, nerve tissue health, and brain function. Since vitamin B12 deficiency can lead to pernicious anemia and neurological abnormalities, it is administrated as analgesic to reduce deficit syndrome and menstrual cramps.

However, too much vitamin B12 has been associated with gastrointestinal problems such as bloating and diarrhea. Thus, the ability to characterize and detect quickly the level of vitamin B12 is necessary, however, accurate measurement of B12 concentrations largely depends on the environmental conditions impacting B12. Appropriate conditions need to be defined and characterized in order to accurately measure vitamin B12 concentrations in biological sample.

Measuring concentration of vitamin B12 in aqueous solutions such as plasma are inherently unstable. We investigated a variety of pre-clinical analytical conditions and measured concentration of vitamin B12 under different storage setting and times using LC-MS/MS. Our results indicated that acceptance standard required of biological method validation established by FDA and EMA. Herein, our finding illustrate and accurate quantitative analysis of vitamin B12 in biological samples thus enabling studies of vitamin B12 concentrations at both preclinical and clinical phase of development.

Poster - 86

Global absolute quantitation of human whole saliva proteins using nLC-Q-IMS-TOF with MS^E

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Saliva has potential to be widely used for the discovery of biomarkers due to its many good characteristics such as communication with blood and non-invasive nature during the sampling. However, its applications are still limited in comparison with other biological fluids such as blood. Thus, here, to expand the applications of saliva to the biomarker research, global absolute quantitation of proteins in human whole saliva (WS) by nLC-Q-IMS-TOF with MS^E was carried out. WS samples were obtained from 22 healthy Korean volunteers (11 male and 11 female) and pooled for its analyses which produced quantitative information of 93 proteins, ranging from 5.89×10^1 ng/mL (immunoglobulin heavy chain) to 1.59×10^4 ng/mL (α-amylase 1). For the validation of this study, human serum albumin in the sample was quantitated by ELISA and its result was compared with that from the nLC-Q-IMS-TOF study. As a result, there was no significant difference between two results ($1.18 \times 10^4 \pm 0.03 \times 10^4$ ng/mL from nLC-Q-IMS-TOF vs. $1.23 \times 10^4 \pm 0.07 \times 10^4$ ng/mL from ELISA, n=3, p=0.309). Since the present study is the first global absolute quantitation of proteins in human whole saliva, the resulting information can be used as the first level reference for the future human salivary protein biomarker research as well as its quantitative applications.

Poster - 87

Global identification of proteins in Korean Whole Saliva

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Proteomic studies on human saliva have been carried out for the discovery of disease biomarkers, and, as a result, more than 3,000 salivary proteins have been identified. However, there has not been any study to build Korean saliva proteome and there is a possibility of ethnic differences in human saliva proteomes. Thus, here, Korean whole saliva (WS) samples collected from 22 healthy South Korean adult volunteers (11 male and 11 female) were analyzed by a nLC-Q-IMS-TOF system to construct the Korean WS proteome for the first time. As a result, a total of 674 proteins, not affected by human oral microbiome were indexed in the catalogue and its 358 proteins were determined as distinct Korean WS proteins, not observed in the integrated human saliva protein dataset. The significant uniqueness of the Korean WS proteome was observed in its gene ontology analyses, too. Since the inter-platform reproducibility of the nLC-Q-IMS-TOF system was confirmed to be within the inner-platform repeatability range for general proteomics, these observations are obvious evidences to support ethnic differences in the human saliva proteome. In addition, 46 of the 358 distinct Korean WS proteins were found to be related with the top 10 deadly diseases in South Korea. Thus, the ethnically-specific human saliva proteins are expected to have potential to be biomarkers for diseases highly-prevalent in that ethnic group. Therefore, the present results can provide the expanded human saliva proteome and ethnicity-controlled salivary proteomics, a new approach with probably higher success rate for disease biomarker researches to the community.

Poster - 88

Non-targeted metabolite profiling of maternal plasma for accurate diagnosis of preeclampsia

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Preeclampsia is a disease that occurs after pregnancy without any known pathological cause. The complications of premature infants are a serious problem and pregnant mother as well. However, there has not been simple diagnostic criteria and authentic clinical treatment for the syndrome. Accordingly, we explored blood-based biomarkers that accurately diagnose preeclampsia, and disease-specific biochemical signature that may aid better understanding of potential pathological mechanism. Non-targeted metabolite profiling was performed on blood plasma samples (33 in preeclampsia, 68 in without preeclampsia) using gas chromatography-time of flight mass spectrometry (GC-TOF MS) in combination of automatic identification and semi-quantification based on home-built library.

The univariate statistical analysis revealed that seven blood metabolites (cholesterol, 1,3-propanediol, 6-chlorohexanol, 3-phosphoglycerate, xanthine, lyxose, glutamate) were significantly different between the two groups. The recomposition of biomarker cluster by multivariate statistical model showed excellent discrimination power that was conservatively validated by receiver operating characteristic (ROC) analysis. The area under the curve (AUC) ranged from 0.689 to 0.858 (sensitivity = 66.7, specificity = 80.9). Through metabolite profiling of maternal plasma, we have shown the possibility of diagnosing of predicting preeclampsia patient by confirming metabolites differences between the two groups.

Poster - 89

Synthesis of ^{14}C labeled peptides used for quantification of peptides using nano-tracing technique and accelerator mass spectrometry

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In the last decade, studies for the development of biodrugs such as peptides, proteins and antibodies is actively conducted rather than developing synthetic drugs. To conduct studies for ADME (absorption, distribution, metabolism, excretion) of biodrugs, it is difficult to analyze using high performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS), which is generally applied to quantify conventional synthetic drugs. However, nanotracing technique using accelerator mass spectrometry (AMS) in combination with ^{14}C-drug could be used for quantifying biodrugs without conducting any complicated process.

In this study, ^{14}C labeled peptide was prepared for the quantification by using nanotracing technique and AMS analysis. After preparing the peptide which is already known its sequence (GGKGKGG), ^{14}C-formaldehyde was used at the ratio of 1, 5, 10, 20, 50, and 100 mole to the peptide for introducing different number of ^{14}C methyl group into peptide. As a result, it was possible to synthesize ^{14}C peptide controlling the number of ^{14}C. It is expected that ^{14}C proteins and peptide which have minimum effect on its own structures and properties could be used for conducting ADME research by using ^{14}C nanotracing technique and AMS analysis. In addition, it will be applied to the research into field of various biodrugs.

Poster - 90

Lectin affinity selection for plasma glycoprotein analysis of healthy elderly groups

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This is a comparative plasma glycoproteomics between elderly healthy yoga groups to see the efficacy of yoga programs with lectin affinity selection. As the elderly population grows, yoga gets more popular as one of the exercises to improve the quality of life and health of the elderly. Glycoproteins in human plasma are known to be deeply associated with multiple diseases, cell differentiation, aging, and etc. We study the efficacy of yoga by identifying and comparing the glycoproteins in human plasma from both Advanced level group and Beginner level group before and after participation in a fall-prevention yoga program. Glycoproteins are affinity-selected from their plasma using self-packed LEL columns and then trypsin digested. After that, the proteins in both groups are identified with nLC-MS/MS and database searches. The results show that the number of plasma glycoproteins in Advanced level group is less than that in Beginner's group, demonstrating an inverse correlation between number of plasma glycoproteins and yoga experience.

Poster - 91

Discovery of predictive serum biomarker cadidates for tyrosine kinase inhibitors response in metastatic renal cell carcinoma by using mass spectrometry-based proteomics approaches

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The molecular target therapy with tyrosin kinase inhibitors (TKIs; sunitinib, sorafenib, pazopanib) is currently the first-line treatment for metastatic renal cell carcinoma (mRCC). Though a therapeutic benefit of TKIs, a majority of patients with mRCC experience variable response for TKIs. We investigated serum protein profiles collected from clear cell mRCC patients before therapy that distinguishes good response and poor response on treatment of TKIs using a mass spectrometry-based approaches. This prospective study enrolled mRCC patients scheduled for TKI therapy in Seoul National University Hospital between July 2012 and August 2013. We used 2D nanoLC & Q-TOF mass spectrometry based biomarker candidates discovery platform with pooled serum categorized into two groups by treatment response. A total of 210 unique proteins were identified in both groups and 6 proteins was upregulated in poor response group, which was associated with acute phase response, complement pathway, angiogesis. Next, we developed absolute quantification method via multiple reaction monitoring (MRM) mass specteomtery. A total of 84 MRM transitions were successfully established, and level of biomarkers in individual patients were measurd. We found 3 biomarker candidates were statistically significant. Our discovery platform sucesssfully identified predictive biomarker candidates for treatment response of TKI.

Key words: Metastatic renal cell carcinoma, Biomarker, Mass Spectrometry, Multiple reaction monitoring

Poster - 92

Novel GlcNAc-containing oligosaccharides in Aspergillus oryzae β-galactosidase-treated bovine whey permeate

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Bovine milk oligosaccharides (BMOs) in whey permeate resemble human milk oligosaccharides (HMOs), indicating that whey permeate is a potential source for milk oligosaccharides that carry HMO bioactivities. However, the recovery of oligosaccharides from whey permeate has been hindered by the low abundance of target oligosaccharides and the high concentration of undesirable lactose molecules, which overshadow the biological activity of the oligosaccharides. Lactose was hydrolyzed by Aspergillus oryzae β-galactosidase to selectively enrich the bioactive oligosaccharides through membrane separation. The generated monosaccharides were much smaller and easily separated from BMOs. High-resolution mass spectrometry analyses revealed that β-linkage-containing BMOs were degraded and that new oligosaccharides were produced during the enzymatic reaction. The synthesized oligosaccharides have N-acetylglucosamine (GlcNAc) at the reducing ends, and their degree of polymerization ranges from 5 to 11. The produced hetero-oligosaccharides could be used as the next generation of bio-therapeutic oligosaccharides and are capable of establishing a healthy intestinal microbial balance.

Poster - 93

Comparative analysis of recovery of heavy metal concentration by sample pretreatment methods

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The purpose of this study is to compare the sample pretreatment methods on contents of heavy metals in CRMs. The samples which were purchased from NIST were analyzed for comparing the recoveries of heavy metals (Pb, Cd, As, Al, Ni, Sb and Cr). In this study, the analysis was conducted about heavy metal contents of CRMs which were related to foods.

In this study, we compared three sample pretreatments which were microwave-assisted digestion, wet digestion using sulfuric acid and nitric acid and dry ashing. The analysis for heavy metals was performed using Inductively coupled plasma mass spectrometer (ICP-MS). Accuracy for the method validation was verified as participating proficiency testing.

As a result, the recoveries were 82.3 ~ 118.2%, 4.8 ~ 434.6% and -580 ~ 3109% at microwave-assisted digestion, wet digestion using sulfuric acid and dry ashing respectively. FAPAS Satisfactory results for Al, Cr and As were obtained below the Z-score 2, ensure high reliability of microwave-assisted digestion.

Poster - 94

Study on the safety of hazardous substance according to oil extraction methods

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Heavy metals (Pb, Cd, As, Al, Sn) were analysed in extracted oils (flax seed oil, sesame oil, perilla oil, soybean oil). As the extraction method, carbon dioxide extraction, solvent extraction, and compression extraction were used. These results were compared statistically with raw materials (flaxseed, sesame, perilla, soybean). Heavy metals (Pb, Cd, As, Al, Sn) were detected in all raw materials. The lead and cadmium concentrations were significantly reduced by extraction. The reduction rates of lead, cadmium, arsenic, aluminum and tin by extraction method were 40 ~ 92%, 67 ~ 100%, 64 ~ 97%, 52 ~ 99%, and 41 ~ 86% respectively. These results indicate that heavy metals in flaxseed, sesame, perilla and soybean can be reduced by the extraction method (carbon dioxide extraction, solvent extraction, squeeze extraction).

Key words: Flaxseed, Oil extraction methods, Food processing methods, Heavy metals

Poster - 95

Determination of the geographical origins of various propolis samples via UPLC combined with high-resolution FT-ICR mass spectrometry

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Propolis, the resinous substance collected by honey bees (*Apis mellifera*) from buds and resins of various plant species, is widely used in folk medicine because of its beneficial effects on various symptoms. Because the compositional diversity of propolis depends on the habitats of the plant sources, propolis samples from different origins exhibit different characteristics or biological activities. In this study, the ethanol-extracted propolis (EEP) from various propolis raw materials originating from different countries (*i.e.*, Argentina, Brazil, China and Korea) were analyzed using high-resolution 15 T Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry coupled with a reverse-phase ultra-performance liquid chromatography (RP-UPLC) system to determine the geographical origins of the propolis and the origin-specific key compounds. Based on approximately 8,000 molecular features extracted from UPLC/FT-ICR MS datasets, a partial least squares-discriminant analysis (PLS-DA) plot showed distinct separations among propolis samples from four different origins, whereas plots constructed from the UPLC analysis datasets did not. According to the variable importance in projection (VIP) scores (VIP $\geq$ 4.0) and fold change values ($\geq$2 or ≤ -2), key propolis components contributing to the discrimination of Korean propolis from Brazilian and Chinese propolis were identified. This analysis revealed the characteristic features of the different propolis samples, and these results can be used to determine the geographical origins and to assess the quality of the commercial products.

Poster - 96

Validation of tocopherol analysis in leafy vegetables using Standard addition-isotope dilution liquid chromatography mass spectrometry method (SA-IDMS-LC/MS)

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Tocopherol is an antioxidant that prevents damage to cell membranes and tissues. Primary method for analysis of tocopherol in infant formula was previously developed using standard addition-isotope dilution liquid chromatography/mass spectrometry (SA-ID LC/MS) for development of infant formula certified reference material (CRM). The aim of this study is to validate the SA-ID LS/MS method to characterize the property values of α, γ-tocopherols in spinach flour and kimchi cabbage flour CRMs.

The sample was treated with saponification and conducted liquid-liquid extraction with hexane. The separation was carried out isocratic condition with 100% methanol (10 mmol/L ammonium acetate) and Cadenza C_{18} (3 μm, 4.6 mm x 250 mm) column. Mass spectrometry analysis was conducted in the negative mode of electrospray ionization and selected reaction monitoring mode was applied.

The measurement results were agreed within their uncertainties between ID LC/MS and SA-ID LC/MS methods using deuterium labeled isotope. Also, α-tocopherol-[^{13}C] was applied on ID LC/MS in order to examine bias from using deuterium labeled isotope during SA-ID LC/MS analysis. Results of repeatability and reproducibility supported that the method is able to apply to certify the spinach flour and kimchi cabbage flour CRMs. Also, the homogeneity and stability were examined in both CRMs. SA-ID LC/MS was applied to similar type of vegetables such as kale, broccoli, leaf beet and lettuce.

Poster - 97

Analysis of Polycyclic Aromatic Hydrocarbons in Olive Oil using Isotope Dilution-Gas Chromatography/Mass Spectrometry

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Polycyclic aromatic hydrocarbons (PAHs) composed of two or more benzene ring structures have a long residence time and carcinogenic effects in humans. A major route of human exposure to PAHs is intake of fatty foods like edible oil. The edible oil can be contaminated by trace PAHs occurred during food preparation processes, such as frying, grilling, or smoking. Thus, several countries set regulations to maximum residue level in edible oil. In South Korea, the maximum residue limit of benzo(a)pyrene is below 2 μg/kg in edible oils.

The aim of this study is developing the analysis method using isotope dilution(ID)-GC/MS as a higher-order reference method for the accurate measurement of four PAHs (Benzo(a)antracene, Chrysene, Benzo(b)fluoranthene, Benzo(a)pyrene) in olive oil. Sample preparation procedure includes liquid-liquid extraction (LLE) and solid phase extraction (SPE). To optimize the sample clean-up process, we tested the clean-up performance of various cartridges for SPE such as florisil, C_{18}, silica, EZ-POP-NP dual-layer, and NH_2 cartridges. In addition, we compared the results when using deuterium and ^{13}C labeled isotopic analogues as internal standards. PAHs were quantitated by SIM mode in GC-MS (Agilent 7890 GC/Jeol JMS 800D-UF MS). The ID-GC/MS method was validated by accuracy, repeatability, reproducibility, LODs, LOQs, assessment of uncertainty, and comparison with other reference method. The developed ID-GC/MS method can also be applied to other edible oils.

Poster - 98

Determination of ciguatera fish poisoning toxins (ciguatoxin) in fish by liquid chromatography-tandem mass spectrometry

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Ciguatera fish poisoning(CFP) is the most common nonbacterial illness associated with fish consumption, affecting 50,000-200,000 people annually. Ciguatera toxin(ciguatoxin) accumulates in tissues of fish that eat the algae and bioaccumulates up the chain.

In current, there is no official analytical method for ciguatoxin in Korea. In this study, an analytical method by gradient reversed-phase liquid chromatography-tandem mass spectrometry(LC/MS/MS) has been developed for the detection and quantification of ciguatera fish poisoning (CFP) toxins (ciguatoxin) in fish. Also, we prepared the rapid and easy extraction method of ciguatoxin in fish flesh.

The test parameters included extraction solvent, clean-up method, mobile phase and mass spectrometric detection parameters. As a result, LC-MS/MS optimization and preprocessing is under review. This analytical method could have applicability in environmental monitoring studies aimed at developing a better understanding of the distribution and factors influencing ciguatera risk in Korea.

Poster - 99

Simultaneous determination of five urushiol analogues in lacquer tree extract by using LC-MRM and QuEChERS with EDTA

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Lacquer tree (*Rhus verniciflua*), known to have not only biological activities such as anti-oxidation, anti-cancer, anti-inflammation but also urushiol group allergens, is used as food material in South Korea. Thus, for its safe use as food material, the appropriate removal of urushiols prior to its use. However, its present regulatory test in Korean Food Code has limitations including miss-targeting and too high limit of quantitation. Therefore, here, an LC-MRM method to quantitate four urushiol compounds (urushiols I, II, III, and V) and laccol in lacquer tree extract, the most widely-used type of lacquer tree food material, simultaneously was developed. For extraction and purification of the targets from samples, QuEChERS with EDTA was employed, and the developed method was successfully validated in the aspects of specificity, linearity (r^2>0.990), accuracy (recovery: 84.83-102.95%), precision (relative standard deviation: 1.18-8.71%) and sensitivity (the limit of quantitation: 5 ng/g). Finally, the validated method was applied to the monitoring of the targets in 33 lacquer tree extract goods purchased from internet food markets. The present method could contribute to the establishment of the suitable regulatory system for the safe use of lacquer tree as food material in the future.

Poster - 100

Novel methods to analyze residual neomycin, streptomycin, and dihydrostreptomycin in acacia honey, manuka honey, and mixed flower honey by using LC-MRM with WCX SPE

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As global honey product use increases, the need of regulatory tests for residual veterinary drugs in various honey also emerges. Thus, in the present study, we developed novel methods to analyze residual neomycin, streptomycin, and dihydrostreptomycin in three types of honey (acacia honey, manuka honey, and mixed flowr honey). Basically, weak cation exchange solid phase extraction (WCX SPE) and multiple reaction monitoring assay (MRM) were employed for extraction/purification and instrumental analysis, respectively, in the methods. Also, the developed methods were successfully validated in the aspects of specificity, linearity ($0.989 \leq r^2 \leq 1.000$), sensitivity (LOQ≤50 ng/g), relative standard deviation, RSD (0.31%≤RSD≤10.09%), and recovery (71.37%≤recovery≤109.59%). Finally, the validated method was applied to the monitioring of the residual target compounds in 27 honey products purchased from internet food markets. The present methods could contribute to the reinforcement of food safety management system especially on honey products in South Korea.

Poster - 101

Primary and secondary metabolic profiles according to regional characteristics of *Glycine max* in Korea

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Glycine max is one of the most important crops which contain a lot of nutrients such as carbohydrates, proteins, and flavonoids. The nutritional quality and metabolic characteristics of soybean is determined by a range of environmental factors (e.g. climate and soil). Thus, the metabolic investigation may be essentially valuable.

In this study, we conducted non-targeted metabolomic analysis by using GC-TOF MS and LC-Orbitrap MS. A total of 210 metabolites were structurally identified, further employed for statistical analysis, which fairly covered a range of chemical entity, thus allowed comprehensive metabolic phenotyping.

The resultant profiles integrative of primary and secondary metabolites were differentiated by multivariate statistical model according to 7 representative cultivation regions in Korea. The metabolic cluster relocated with five metabolites (malonylgenistin, malonyldaidzin, N-acetylornithine, allysine, tryptophan) showed outstanding discrimination power for the profiles of all seven regions, which was determined by ROC analysis.

The subsequent interrogation on covarianced structures of the metabolome revealed region-specific metabolic features that systematically isolated list of metabolites and linked it to different region of the soybean cultivation. Our result suggested metabolite analysis can be applied to authentic methodology that identifies origin of agricultural products, and also provide nutritional information according to cultivation region.

Poster - 102

Comparision of aroma components by coffee producer using GC-MS

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We report on the analysis of volatile compounds by GC-MS for individual roasted coffee beans. The aim was to understand the relative abundance and variability of volatile compounds between individual roasted coffee beans of origin.

Coffee aroma is one of the most distinctive characteristics of this commodity, which is mostly consumed for its flavor. Coffee has different tastes and flavors depending on where it came from. In this experiment, we will compare the difference in the ingredients depending on where the coffee comes from We analyzed the commonly encountered raw beans in Ethiopia, Columbia, Brazil, and Kenya with GC-MS and studied which ingredients each made the difference between the smell and the taste. Volatile compounds in roasted coffee are mainly represented by aldehydes, ketones, alcohols, esters, pyrazines, furans, acids, nitrogen-containing compounds and volatile phenolic compounds.

Poster - 103

Development of qualitative and quantitative system for simultaneously screening 395 pesticide residues by high resolution mass spectrometry

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A simultaneous screening system to qualify and quantify 395 pesticide residues was developed by using a high resolution mass spectrometer. A gas chromatography-orbitrap high resolution mass spectrometer (GC-HRMS) was used to analyze 280 pesticide residues, which qualify the pesticides based on the ratios of qualifying ions to quantifying ions. 115 pesticide residues were determined by a liquid chromatography-quadrupole/orbitrap high resolution mass spectrometer (LC-MS/HRMS), which confirms target compounds using the data of specific fragment ions. Additionally, high resolution mass spectrometry enables to prove compounds based on an exact isotope mass with the resolution of 60,000 (GC-HRMS) and 70,000 (LC-MS/HRMS). The recovery of 395 pesticide residues spiked in a lettuce was acceptable in a range of expected recovery presented by Association of Official Analytical Chemists (AOAC). Therefore, the simultaneous screening system developed in this study enables to determine 395 pesticide residues in food whose complex matrix is prone to cause an interference and a contamination.

Poster - 104

MALDI-MS analysis of small molecules using N-doped carbon dots as matrix

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Matrix-assisted laser desorption/ionization (MALDI) is simple and useful soft ionization method. The matrix helps ionize analytes, where organic matrices such as 2,5-dihydroxybenzoic acid and sinapic acid are commonly used. Organic matrices are effective for large molecule analysis such as proteins and peptides. Due to strong background interferences from intrinsic matrix-related ion in the low mass region, organic matrices are not suitable for small molecule analysis in MALDI-mass spectrometry (MS). To overcome the limitation, various alternative matrices such as nanomaterials and porous silicon, carbon-based materials and metal oxides are being studied.

In this study, N-doped carbon dot (N-CD) was selected as an alternative matrix for analysis of small molecules. To synthesize N-CDs, a solution containing 1 g citric acid, 1 g urea, and 10 mL distilled water was heated in 800 W microwave for 4 min. Characterization of N-CDs was performed by Fourier-transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), UV-Vis absorption (UV-Vis), photoluminescence spectroscopy (PL), and X-ray diffraction (XRD). Glucose, sucrose, amino acids, and nilotinib were successfully analyzed using the synthesized N-CDs as matrix in MALDI analysis

Poster - 105

Application of MOF-5 and UiO-66 as MALDI matrices for analysis of small molecules

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Matrix matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI TOF-MS) is a convenient, sensitive and accurate method for determination of macromolecules. However, because the commonly used organic matrices such as 2,5-dihydroxybenzoic acid and α-cyano-4- hydroxycinnamic acid have a high matrix interference in the low molecular-weight range (≤ 500 Da), the measurement of small molecules in MALDI is greatly limited. To overcome this limitation, currently alternative matrices such as charcoals, graphenes, graphene oxides, and carbon nanotube have been used for the analysis of small molecules.

In this experiment, MOF-5 and UiO-66 were investigated as MALDI matrices. Since they have a π-π structure of the organic linker and the oxygenated function groups (-COOH and -OH), they can absorb the energy from UV laser radiation and transfer energy to small molecules. Glucose, sucrose, amino acids, PEG 400, and PEG 1450 were analyzed using the synthesized MOF-5 and UiO-66 as matrix in MALDI analysis.

Poster - 106

Detection of small molecules using MALDI-ToF mass spectrometry with TiO_2 nanowire solid matrix

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MALDI-TOF MS has been widely applied for the analysis of biomolecules with high molecular weights, such as proteins and peptides, because of its advantages on soft ionization, easy sample preparation, sensitive detection, and clinical field such as bacterial identification, newborn screening and drug monitoring. However, the conventional organic matrices are ionized themselves to produce their own peaks are called matrix noise at low mass-to-charge (m/z) ratio range (<500) while the sample analytes are ionized by pulsed laser. Moreover, the organic matrices formed non-uniform co-crystals with samples while drying on the surface of target. So, MALDI-TOF MS in the low mass range molecules is so hard. This reasons small molecular weight molecules detection so the other kinds of matrices are required. In this work, TiO_2 nanowire arrays such as solid matrix was synthesized in other to use matrix and applied to MALDI-TOF MS. TiO_2 nanowire arrays was synthesized to detect several amino acid and some small peptides by MALDI-TOF MS. TiO_2 nanowire arrays were synthesized by top-down hydrothermal process. characterizing their morphology and structures by X-ray diffraction (XRD), atomic force microscopy (AFM), scanning electron microscopy (SEM), Raman spectrometry and photo luminescence spectrometry. As a result, interference was significantly reduced and quantitative detections of several amino acid and small peptides were feasible using TiO_2 nanowire arrays.

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Keywords: TiO_2, Nanowires, Solid matrix, Mass spectrometry

Poster - 107

Trace element analysis of optical fiber

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The optical fiber is made of a transparent dielectric material such as quartz glass or plastic, which is made by elongating a long and thin, and has a refractive index distribution at a central portion. Using the refractive index of the core portion, it is used in various fields such as space, military, medical, and communication etc.. The most commonly used is silicon oxide (SiO_2) optical fiber. The refractive index of the silicon oxide optical fiber varies depending on the content of the trace inorganic elements, thereby changing the optical properties. In order to analyze these trace elements, it has been analyzed by ICP-OES (Inductively Coupled Plasma-Optical Emission Spectroscopy) mainly through acid pretreatment. However, acid-destructive analysis using ICP-OES is suitable for high-content quantitative analysis and it is only possible to analyze high-purity SiO2 impurities. And it is impossible to analyze trace quantities and distributions according to sample characteristics.

In this study, study using fsLA-ICP-MS (femtosecond Laser Ablation-Inductively Coupled Plasma-Mass Spectrometer) which has high detection sensitivity and resolution by coupling ICP-MS (Inductively Coupled Plasma-Mass Spectrometer) with a femtosecond laser that produces particles uniformly with resolution in μm. And, We also developed analytical methods for the characteristics of the samples and analyzed the content of trace inorganic elements by fiber cross section.

As a result, significant results were obtained.

Poster - 108

Analysis of iso-maltooligosaccaride by matrix-assisted laser desorption/ionization mass spectrometry using ionic liquid matrices

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Matrix-assisted laser desorption/ionization (MALDI) is an ionization source that transfers laser energy to analytes via matrix. It has been applied to the analysis of biomolecules such as proteins, peptides, lipids and carbohydrates. The successful analysis of samples using MALDI-mass spectrometry (MS) depends on the selection of proper MALDI matrix. Recently, ionic liquid matrices (ILMs) have been introduced as a potential alternative to the conventional matrices such as 2,5-dihydroxybenzoic acid (DHB), α-cyano-4-hydroxycinnamic acid (CHCA) and sinapic acid in MALDI-MS. In general, ILMs are made by mixing conventional organic matrices and base molecules. Improved shot-to-shot peak reproducibility was reported using ILMs.

In this study, we are trying to find out the dependence of the loading amount on the intensity using ILMs in MALDI-MS analysis of iso-maltooligosaccharide. ILMs were prepared by mixing DHB and bases (N-Methylaniline (NMANI) or N-Ethylaniline (NEANI) in a 1:1 molar ratio to analyze iso-maltooligosaccaride. In addition, 100 mM NaCl is functioned as a cationization agent. The peaks of iso-maltooligosaccharide were observed at *m/z* 365, *m/z* 527, *m/z* 689, *m/z* 851, *m/z* 1013, *m/z* 1175, *m/z* 1337, and *m/z* 1499. Detailed experimental results will be presented during the session.

Poster - 109

Construction of Isomer-Specific and Region-Specific Mouse Brain Ganglioside Library using UHPLC-QTOF MS/MS

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Gangliosides are anionic glycosphingolipids containing one to several sialic acid residues. Although they play an important role in neuro-biological functions including synaptic plasticity and memory formation, there have been only few studies in ganglioside due to their structural complexity and the lack of effective analytical methods. In particular, isomeric investigation of gangliosides is necessarily required in order to understand the ganglioside biology with the consideration of its biosynthesis however, isomer separation based on reversed-phase (RP) chromatography is highly challengeable. In this study, for the purpose of construction of localized mouse brain ganglioside library, we examined ganglioside from anatomically dissected nine mouse brain regions by isomer-specific LC/MS and LC/MS/MS. Briefly, gangliosides were extracted by modified Folch method with chloroform and methanol, followed by purification and enrichment by C18-SPE. Then they were identified and quantified by UHPLC (C18 column) QTOF MS. Ganglioside isomers were completely separated depending on their glycan traits on a C18 column by addition of formic acid in the mobile phase. Furthermore, tandem MS analysis was performed to confirm the identification based on diagnostic fragment ions. Through LC-MS/MS based isomeric investigation of gangliosides, region-specific mouse brain ganglioside biosynthetic pathway including 0-, a-, b- and c- series could be suggested. Interestingly, major ganglioside were distributed with distinguished qualitative and quantitative pattern for each nine brain regions. Constructed mouse brain ganglioside library is going to be used for monitoring alteration in KO mouse models including glycosylation transferase KO mice.

Keyword: Ganglioside, LC/MS/MS, Isomer-specific, Mouse brain

Poster - 110

Effect of matrices and drying processes sample preparation in MALDI-MS

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Conventional sample drying processes such as air drying (AD) or vacuum drying (VD) are generally carried out for the sample preparation in matirx-assisted laser desorption/ionization-mass spectrometry (MALDI-MS). However, these conventional sample drying processes are less reproducible because these processes produced heterogeneous distribution of sample. Recently, freeze vacuum drying (FVD) was reported to result in the homogeneous distribution of analytes because the analyte-matrix mixtures are quickly frozen and then dried under vacuum. In this experiment, spot images and mass spectra of several common standard proteins such as cytochrome *c*, myoglobin and bovine serum albumin are compared within other matrices (2,5-dihydroxybenzoic acid, α-cyano-hydroxycinnamic acid, sinapic acid, and 2-nitrophloroglucinol) prepared using either AD, VD or FVD. By applying the FVD drying process, the samples generate more homogeneous spot images, while the peak intensities were lower than those from the mass spectra using conventional sample drying processes.

Poster - 111

Biomarker discovery of coronary artery disease : serum protemic profiling

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Coronary artery disease is one of the most popular occurred disease and cause of death worldwide. Recently, several studies were tried to find novel biomarker in coronary artery disease patients using genomics, transcriptome and proteomics due to lack of specificity of current diagnostic method. Blood which was used to diagnostic or prognosis marker is the properly sample to identify potential biomarker in various disease. However, the most of studies were conducted using pooled serum sample. The pooled serum sample is difficult to represent individual status as low abundant proteins high expressed from only one sample could be selected as new biomarker. Therefore, we conducted proteomics using individual plasma sample to remove above mentioned bias. We examined 33 patients with coronary disease and 43 healthy control independently for finding novel biomarker. The LC-MS/MS was used to analyze proteins qualitatively and quantitatively. The quantitative analysis was performed by SWATH-MS acquisition. As a result, we identified 128 more than 2-fold differentially expressed proteins compared to each controls and patients. Among them, we showed several proteins were associated with immune response-lectin induced complement pathway and immune response-classical complement pathway using GeneGo Metacore. The individual analysis is going to enable accuracy analysis without bias. Therefore, we thought that several proteins obtained through the individual analysis can be used in clinical to distinguish the disease and healthy subjects more precise.

Poster - 112

Biomarker discovery of large artery atherosclerosis stroke: serum proteomic profiling

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

Poster - 113

Biomarker discovery of rheumatoid arthritis: serum proteomic profiling

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Rheumatoid arthritis is an autoimmune disease involving inflammation of the synovial membrane. Anti-citrullinated protein autoantibody and rheumatoid factor are currently used to diagnose rheumatoid arthritis. However, they have rather low specificity. Therefore, efforts have been made to develop methods for efficient diagnosis of rheumatoid arthritis. Nano-liquid chromatography-tandem mass spectrometry (LC-MS/MS) is an efficient proteomics approach to quantify serum proteins and to identify disease-specific protein expression patterns. In this study, 50 patients and 43 healthy subjects were used for biomarker of rheumatoid arthritis. Comparative analysis between patients with rheumatoid arthritis and healthy subjects was performed by SWATH-MS acquisition. Among differentially expressed proteins by more than 2-fold (p-value<0.05), the number of selected potential biomarkers for rheumatoid arthritis were 51. The result of functional analysis showed that differentially expressed proteins including complement C3, complement factor H, clusterin and vitronectin were associated with alternative complement pathway. These alternative complement pathway-related proteins will help to understand pathophysiology of rheumatoid arthritis. Further, we expect that multi-biomarkers that were confirmed from 51 differentially expressed proteins have stronger potential for diagnosis.

Poster - 114

Production of high purity gallium metal for compound semiconductor and trace elements quantification

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Gallium is used as an essential raw material for the production of high-purity III-V compound semiconductors or semi-insulators such as gallium arsenide (GaAs). Particularly, semi-insulator(GaAs) requires high purity of 8N or higher, and gallium metal used as a raw material must have a high purity of 8N or more, and a method of analysis of high purity gallium is necessary.

In this study, we quantitatively analyzed gallium crystallized at high purity using Czochralski(CZ) method. Three types of CRM selected to calculate relative sensitivity factors (RSF) for quantifying impurity elements in high purity gallium. CRM has an aluminum matrix containing gallium contents of 175, 100 and 330 ppmw, respectively. The calculated RSF for the aluminum matrix CRM was 2.65, 2.36 and 2.34, respectively. The average RSF was 2.45 and the relative standard deviation (RSD) was about 7%. Using this standard sample, for the 17 elements of Al, Ga, Mg, Si, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Ag, Cd, Sn, Pb and Bi, Quantitative analysis is possible. Finally, in the analysis of gallium crystallized by the CZ method, four kinds of impurity elements were detected as Al, Si, Cr, and Fe, and all of the other elements were below the detection limit. The quantitative analysis in GD-MS was calculated by multiplying the ion beam ratio (IBR) by RSF. The IBR of Al, Si, Cr and Fe were 5.12, 2.84, 3.09, 1.57 ppbw respectively. The RSF of Al, Si, Cr, and Fe calculated using CRM were 0.41, 0.43, 0.58, and 0.30. Therefore, the quantitative analysis for the final four elements can be expressed as (2.10, 1.22, 1.79, 0.47) ppbw, and the total amount of impurity elements is 5.58 ppbw and the final purity of gallium is about 99.9999994% (8N).

Poster - 115

Introduction to B-10 isotope ratio analysis for the reactivity of reactor core

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Boron has two stable isotopes, B-11(80.1%) and B-10(19.9%). The B-10 is used to control the reactivity of reactor core. Therefore, core management considering B-10 burnup is needed, and the inaccuracy of boron concentration leads to reduction of reliability and safety of core design such as shutdown margin. The PWR (Pressurized Water Reactor) operating in domestic controls the core reactivity by measuring the B-10 isotope ratio of the reactor coolant and correcting the boron concentration. Before startup, samples are taken from RCS (Reactor Coolant System), RWST (Reactor makeup Water Storage Tank) and BAT (Boron Acid Tank). Results of the analysis are used for core physics test, shutdown margin calculation, and expected criticality. During normal operation, samples are taken every 3 EFPM (Effective Full Power Months) from RCS to check the critical boron concentration. Before restarting, samples taken from RCS and RWST are used to calculate the expected criticality.

This paper deals with introduction to B-10 isotope ratio analysis using ICP-MS.

Poster - 116

Mass spectrometric study on the source of error in quantification of fatty acids

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Identification and quantification of fatty acids are important in fields of lipidomics and metabolomics. Although exogenous fatty acid contaminants, which leads to inaccurate quantification, have been neglected in lipidome analyses, unexpected contamination can be occurred from plasticware and glassware during the sample preparation. Therefore, quantitative measurement of the contaminants is necessary for reducing an error associated with accurate determination of the amount of endogenous fatty acids in biological samples.

Fatty acid contaminants were investigated with respect to different types of sample containing tubes, extraction solvents, and sample preparation. The contaminants were analyzed by high-performance liquid chromatography electrospray ionization quadrupole time-of-flight mass spectrometry in technical triplicate. The target molecules were palmitic acid and stearic acid that account for the largest portion of the contaminants. As a result, among sample containing tubes, glassware washed using methanol revealed the minimum contamination of fatty acids. By evaluation of different types of extraction solvents, chloroform showed the least contamination. Also, the amount of contaminants generated in the sonication step was about 57 times higher than that in the pipetting step, which is expected to be the most abundant source of the contamination.

Poster - 117

Development of extraction method for dried blood spot

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Dried blood spots(DBS) have been used for small molecule analysis for a variety of purposes due to their many advantages. DBS is an alternative to blood, but its extraction efficiency is not the same as the amount of small molecules in the blood. Therefore, in this study, we compared the extraction efficiency of small molecules of DBS compared to blood according to the type of organic solvent and the addition of step to soak out small molecules in water. The blood was obtained from four subjects, and made blood samples and DBS samples. The first step for small molecule extraction was performed by 30 minutes of incubation of plain extraction solution(P) or incubation of water then add extraction solution(W). Samples extracted by solvent precipitation method using five extraction solutions. Liquid chromatography-mass spectrometry(LC-MS)/MS analysis was performed for samples. Comparing the number of MS and MS/MS molecular features(MFs), W showed MFs greater than P in all solvents. The solvent with the highest MS/MS MFs was 80% methanol/0.1% formic acid in water(MWF)-W. MWF-P and 80% methanol in water(MW)-W had the second highest MFs. Among all identified MFs, 100 percent of the 46 MFs identified over 10 conditions were sorted and relative percent recovery was calculated. M-W was the most abundant in recovery 50~100%, followed by MW-W and MWF-W. Therefore, these three conditions seem to be the most suitable extraction method, and additional analysis is under way.

Poster - 118

Understanding the DMSO effect on the drug efficiency of cisplatin using ICP-MS

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Cisplatin (cis-[Pt(NH3)2Cl2]) is a platinum-based anticancer drug used for diverse cancers. Cisplatin is commonly administered as a single drug or in combination with other drugs to raise its efficacy. Nevertheless, cancer cells could have acquired or intrinsic resistance to cisplatin. In this reason, a large number of in vitro studies have been conducted to clarify the mechanism of the phenomena. In most of these studies, dimethyl sulfoxide (DMSO) has been utilized as solvent for the stock solution of cisplatin and other drugs at high concentration. According to a study concerning effects of solvents on the activity of cisplatin, DMSO depresses cytotoxic efficiency via ligand exchange with Cl-. However, very few studies have been published on which steps DMSO affects on. Herein, we employed an inductively coupled plasma mass spectrometry (ICP-MS) for the quantitative analysis of cisplatin to understand how DMSO directly impedes Pt-mediated toxicity. First, the cellular uptake depending on solvents was compared by quantifying the amount of cisplatin in the media and cells. Furthermore, determination of the amount of DNA-Pt adducts, which is known to be a direct cause of cell apoptosis, was performed. In quantitation of DNA-Pt adduct, cisplatin in DMSO and media showed significant difference, whereas the uptake study did not. Therefore, further studies will investigate on the structural influence of DMSO in correlation to the coordination of DNA-Pt adduct.

Poster - 119

Validation of Analytical Method for Determination of Cyanide in Rat Blood Using Gas Chromatography-Tandem Mass Spectrometry

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This study was conducted to develop the analytical method for determination of cyanide in rat blood using gas chromatography (GC) coupled with triple quadrupole tandem mass spectrometry (MS/MS). The analytical method was validated with respect to selectivity, linearity, accuracy, precision and system suitability. The cyanide was detected using a derivatization solution of 20 mM Pentafluorobenzyl bromide (PFB-Br) dissloved in ethyl acetate. The calibration curve for cyanide of a range of 10 to 200 μM using a 2,5-Dibromotoluene (2,5-DBT) as the internal standard (IS) showed a good linearity correlation (>0.996, n=3). The precision and accuracy of analytical method were acceptable within 20% (Coefficient of Variation, CV) and –20% to 20% (Relative error, RE) at quality control levels. Also, the cyanide and IS was confirmed that system suitability values were within 6.8% and 3.3%, respectively. In the analytical condition, there was no interference peak to affect the concentraton of cyanide. Consequently, as these results were acceptable ranges specified in bioanalytical method validation guideline, this method could be applied to the analytical method for determination of cyanide in rat blood.

Poster - 120

Intense signal problem on TDC based LC/qTOF system

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The dead time effect of TDC is well-known. When a ion is arrived at detector within dead time of previous detected ion, the ion is not recorded. As a result, the right side of the peak is reduced and its peak mass is shift to lower value as ion signal is increase. Moreover, the dead time effect generate ghost peak when the ion signal is much more increased. This ghost peaks affect de-isotoping method and sometimes unwanted ion can be selected for precursor.

Increasing signal intensity by introducing more sample amount is usually helpful. However, in TDC-based qTOF system, increasing sample amount beyond certain point will result in poor mass accuracy in MS spectra. On the contrary, in the viewpoint of MS/MS acquisition, more sample amount is always recommended for better spectral quality or reduced acquisition time. So, it is desirable to introduce more sample amount and find the way to reduce dead time effect in survey scan. Since most data dependent analysis changes collision energy value for survey scan and MS/MS scan, adjusting collision energy for survey scan to reduce ion signal is quite natural. The signal transmission is recorded at several collision energy settings. Then, DDA experiments were performed at these reduced survey MS signal intensities, while maintaining MS/MS sensitivitiy. The precursor selection was adjusted by signal transmission. The resultant peptide ID or search results at various collision energies are compared for E.coli digested peptides as a model system.

Poster - 121

Evaluation of quantitation performance of paper cone spray ionization (PCSI) mass spectrometry (MS)

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We developed an extractive ambient ionization method, paper cone spray ionization (PCSI), for direct mass spectrometric analysis of raw solid samples. Pyramidal-shaped, 3D paper cone serves as a sample container, an *in situ* liquid-solid extraction chamber, an analyte transport channel, as well as an electrospray tip. Here, we report fundamental aspects and quantitation performance of PCSI MS. By using simple alkyl alcohols as spraying solvents, PCSI MS rapidly generated major chemical fingerprints from various solid materials without any sample pretreatment. After confirming versatility of PCSI MS, we focused on evaluating quantitation performance of PCSI MS. In order to achieve this, we prepared model pharmaceutical powders that contain various contents of acetaminophen. We performed wicking-mode PCSI MS analysis against model powders and successfully obtained solid-liquid extraction patterns and intensity information of acetaminophen ions. From the results, we found that PCSI MS showed a good linearity.

Poster - 122

Analysis of trace elements in high-purity alumina powder using gravimetric standard addition method with internal standard by inductively coupled plasma optical emission spectroscopy

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Alumina is one of the most commonly found aluminum oxide (Al_2O_3) and has been widely utilized as advanced industrial materials. For high-tech industry, especially, high-purity alumina (HPA) is required because impurities in alumina prohibit growth of crystalline or deteriorate the crystal properties. Thus, accurate analysis of trace elements in alumina is essential to development of related technology but a little number of analytical methods for HPA were reported because HPA is hard to dissolve without contamination because of its intrinsic stability. In this study, we analyzed trace level of magnesium (Mg) and silicon (Si) in HPA as a candidate for certified reference material (CRM) through gravimetric standard addition and inductively coupled plasma optical emission spectroscopy (ICP-OES). An optimized procedure was developed for complete dissolution of alumina based on pressurized microwave digestion under 80 bar with hydrochloric acid. The whole sample preparation was completed in a day. ICP-OES was used for the analysis of Mg and Si in aluminum excess solutions and has shown more reliable intensity compared to ICP-MS which is prone to severe intensity reduction over time because of aluminum deposition and clogging on the orifice of cones in ICP-MS. Between-bottle and in-bottle homogeneities of Mg and Si in a batch of HPA reference material were confirmed respectively. For method validation, Mg and Si in NMIJ CRM 8007-a Fine Alumina Powder-high purity were also determined and the measurement results were in good agreement with the certified results. This analytical method was thoroughly validated so that can be applied to the assignment of certified values of KRISS alumina CRM.

Poster - 123

Development of an Analytical Method for the Identification of Saliva-Specific Glycans in Trace Amounts of Human Saliva

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Saliva often encountered at crime scenes provides valuable insights for criminal identification and post-mortem interval estimation. In previous study, we introduced a new approach using glycomics to overcome the lack of specificity of traditional methods for human saliva identification. We found that significant amounts of fucosylated glycans and the presence of highly fucosylated N-glycans could differentiate human saliva from other body fluids. The following studies, detection of saliva-specific glycans in trace amounts of samples and their stability, were conducted for practical applications. Herein, we have developed a platform for separating and analyzing N-glycans in dry saliva samples using protein protector cards. Briefly, dried saliva were prepared by spotting of human saliva on a protein saver card. N-glycans of dried saliva were directly released from the piece of saver card using PNGase F and enriched by SPE with a PGC. Saliva N-glycans were characterized by nano LC/Q-TOF MS. Highly fucosylated N-glycans and significant level of fucosylation previously found from liquid saliva were identically observed in dried saliva samples. Indeed, N-glycan profiles between liquid and dried saliva samples showed the significant correlation (R = 0.96) in terms of the number of glycans and their amount. The experimental reproducibility was evaluated to ensure suitability of an analytical platform and to determine detection limit (up to 2 μL) of saliva-specific glycans. (1,508/1,500)

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Study on analysis method of polyol in Polyurethane foam by Matrix-assisted laser desorption/ionization-Time of flight (MALDI-TOF)

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Polyurethane foam is used to various industrial field with other material due to outstanding insulation. It has much different form such as soft form, hard form, coating, special adhesives, sealant and elastomer. Polyurethane could be obtained by reaction between polyol and diisocyanate or polymeric isocyanate in existence of additives and catalyst. The various types of polyurethane could be made according to many kinds of polyol and diisocyanates. Thus, it is important to research physical and chemical property of polyol in polyurethane foam.

Recently, modern analytical methods (ex. GPC, NMR, GC) were used to analyze polyol. In this research, MALDI-TOF (Matrix-assisted laser desorption/ionization-Time of flight) method was applied for MS and MS/MS analysis to obtain m/z (mass to charge ratio) value and structure information of various polyor.

From MS results, we got MS spectrum and m/z values of various polyols according to acid and alcohol types. Also, we could confirm structure information of polyols from fragment pattern results.

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Understanding the DMSO effect on the drug efficiency of cisplatin using ICP-MS

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Cisplatin (cis-[Pt(NH3)2Cl2]) is a platinum-based anticancer drug used for diverse cancers. Cisplatin is commonly administered as a single drug or in combination with other drugs to raise its efficacy. Nevertheless, cancer cells could have acquired or intrinsic resistance to cisplatin. In this reason, a large number of in vitro studies have been conducted to clarify the mechanism of the phenomena. In most of these studies, dimethyl sulfoxide (DMSO) has been utilized as solvent for the stock solution of cisplatin and other drugs at high concentration. According to a study concerning effects of solvents on the activity of cisplatin, DMSO depresses cytotoxic efficiency via ligand exchange with Cl-. However, very few studies have been published on which steps DMSO affects on. Herein, we employed an inductively coupled plasma mass spectrometry (ICP-MS) for the quantitative analysis of cisplatin to understand how DMSO directly impedes Pt-mediated toxicity. First, the cellular uptake depending on solvents was compared by quantifying the amount of cisplatin in the media and cells. Furthermore, determination of the amount of DNA-Pt adducts, which is known to be a direct cause of cell apoptosis, was performed. In quantitation of DNA-Pt adduct, cisplatin in DMSO and media showed significant difference, whereas the uptake study did not. Therefore, further studies will investigate on the structural influence of DMSO in correlation to the coordination of DNA-Pt adduct.

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Effective determination of famphur in honey by gas chromatograph/mass spectrometer

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Famphur is one of the pesticides used in bee-farming. This is a highly hazardous pesticide classified by WHO and some countries are regulating this pesticides. In this study, a method for the selective determination of famphur in four kinds of honey using solid-phase extraction (SPE) and gas chromatography-mass spectrometry (GC-MS) was established. 5 g of honey was dissolved in 10 mL of water and transferred to a C18 cartridge preconditioned with ethyl acetate and water. After washing with 2 mL of purified water, and then famphur was eluted with 6 mL of ethyl acetate and determined by gas chromatograph with mass spectrometer (GC/MS). Optimization of solid-phase extraction (SPE) parameters was evaluated by the pH of the sample, the type and volume of the elution solvent. Chromatographic separation was achieved on DB-35MS column (30 m × 0.20 mm × 0.33 μm), and oven temperature was ramped up from 120 ℃ to 310 ℃ at a rate of 25 ℃/min, and then maintained for 2 minutes. The injection mode was the split (10:1), and m/z 218 was used as the quantitative ions in SIM mode. From the established extraction and GC-MS conditions, the limit of detection (LOD) and limit of quantitation (LOQ) in the spiked sample were 2 ng/g and 5 ng/g, respectively. Recovery studies were performed at 5 ng/g, 10 ng/g, 20 ng/g of fortification levels, and accuracy and precision in working range were 63.7-118.4 % and 1.0-27.7 RSD %, respectively. The calibration curves for the quantitative analysis were obtained the concentration range of 5~50 ng/g with correlation coefficients (R^2) from 0.9883 to 0.9958. The proposed method was applied to the analysis of famphur in domestic honey samples.

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Characterization of polymer additives by high resolution-GC/MS

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The plastic industry continuously develops highly sophisticated materials. Additives contribute decisively to maintain the initial properties of plastics. Polymer additives containing benzodioxaphosphocine provide excellent color stability, constant melt viscosity, and good hydrolytic stability during polymer processing. Some of these polymer additives are often observed as oxidized form with liquid chromatography/mass spectrometer (LC/MS). In order to avoid this situation, high resolution-gas chromatography/mass spectrometer (HR-GC/MS) with mass accuracy below 1 ppm is used to characterize species susceptible to oxidation. Here we discuss the applicability of HR-GC/MS technique for analysis of additives in polymer products.

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Structure determination of Zn phthalocyanine compounds based on demetallization reaction

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Dyes and pigments are widely used materials in the display industry. In general, various analytical methods such as mass spectrometry (MS), nuclear magnetic resonance (NMR), energy dispersive X-ray spectroscopy (EDS), and X-ray fluorescence (XRF) are applied to analyze the structure of dyes and pigments. However, in the case of a compound containing a metal, the low solubility in organic solvents and the peak broadening in NMR due to paramagnetic property of the metal make it difficult to elucidate the structure using LC/MS and NMR techniques. Therefore, in order to accurately determine the structure of pigments and metal-containing dyes, it is required to develop a sample pretreatment method capable of LC/MS or NMR analysis. The possibility of analyzing the structure of pigments and metla-containing dyes through the degradation of Zn phthalocyanine compounds based on the demetallization reaction was evaluated.

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Single-Injection Screening of 664 Forensic Toxicology Compounds using an Innovative Benchtop High Resolution Mass Spectrometer

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Introduction

Quadrupole Time-of-flight mass spectrometry (QTOF-MS) provides high-resolution, accurate-mass data for full-scan information of both precursor ion and all product ions. This is an ideal approach for forensic toxicology screening where unknown compounds in complex biological samples must be identified from information-rich data sets.

Herein, we present a single-injection method for screening 664 most up-to-date forensic compounds using an innovative benchtop QTOF mass spectrometer. The obtained data provided both structural information and retention times to enhance identification accuracy, especially for structurally similar isomers. Sample preparation procedures for urine and whole blood samples and library-search settings are described for confident unknown substance identification within an efficient, all-in-one workflow.

Methods

Urine and whole blood samples were spiked with stock standard mixtures and used to determine the retention time of the 664 compounds. Urine samples were diluted with mobile phase and analyzed; whole blood samples, were extracted by using protein precipitation and centrifugation; supernatant was evaporated and reconstituted in mobile phase for analysis.

Analytes were chromatographically separated using a Phenomenex Kinetex phenyl-hexyl (50 x 4.6 mm, 2.6 µm) column. Mobile Phase was ammonium formate in water and formic acid in methanol, 600 µL/min flow rate. The QTOF-MS was operated in positive electrospray mode with information dependent acquisition MS/MS methods. Samples were evaluated against a list of parameters containing the names, molecular formulas and retention times for all compounds.

Preliminary data

The performance of separation was evaluated with different mobile phases (acidic and neutral), gradient conditions, and column types. Results indicate that most of isomeric compounds were fully resolved with neutral Buffer A and a 10-min linear gradient using the phenyl-hexyl column.

Analyte retention time (RT) was a critical element for accurate identification of each forensic analyte using this screening method, the following RT reproducibility tests were conducted for each compound to evaluate the robustness of the LC condition in this method: (1) reproducibility on 3 separate columns; (2) the inter-day (n=3) reproducibility; (3) the reproducibility in neat versus matrix samples. The reproducibility tests indicated that the RTs generated from the optimized LC conditions are consistent and reproducible. RTs measured on three separated analytical columns all have %CVs of less than 5% for each of the 664 compounds. RT inter-day reproducibility (tested on 80 compounds) resulted in %CVs less than 5% over 3 days. Lastly, RT variability in human whole blood and urine samples (tested on 80 compounds) indicated that the %CV for 3 individual lots is less than 5%.

The retention time determined by the optimized LC condition combined with high-resolution mass spectrometry and MS/MS spectra, enabled accurate compound identification across the workflow. Retrospective analysis was also performed on the acquired data sets to screen for new compounds without having to re-inject samples, allowing data sets to be re-processed as new forensic targets were discovered.

Novel Aspect

High resolution Mass Spectrometry Analysis of 664 forensic compounds in a single injection using a benchtop QTOF mass spectrometer.

Poster Session: Toxicology

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Development of protein characterization analytical method for antibody drug fragments

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Antibodies and related proteins now make up the largest and fastest growing category of protein pharmaceuticals. Monoclonal antibodies (mAbs) are an important class of such proteins; specially, many new entities are antibody fragments.

In addition to the whole antibody form including both the variable region and the constant region of the antibody molecule, monoclonal antibody drugs are being developed in the form of Fab fragments, single chain Fv fragment utilizing only the variable region, and fusion proteins using constant region (Fc) conjugated in protein.

A recently discovered endopeptidase, IdeS, cleaves heavy chains below the hinge region, producing F(ab')2 and Fc fragments. Following reduction of disulfide bonds, three antibody domains (LC, Fd, and scFc) can be released for further characterization. The use of IdeS is becoming increasingly popular for the fast characterization of antibody by mass spectrometry, including correct sequence assessment, antibody Fab and Fc glyco-profiling, biosimilar comparability studies and Fc-fusion protein studies.

In this study, monoclonal antibody drug, Trastuzumab and Infliximab were separated LC, Fd, scFc fragment by RP-LC. After the separated fractions were digested using trypsin, product was analyzed peptide mapping by LC-MS/MS. And the methodologies we describe here form a solid framework for routine biosimilar verification.

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Simultaneous analysis of ginsenosides in fermented black ginseng, using LC/MS/MS

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Cosmetics market and industry are steadily growing in Korea. Fermented black ginseng has been shown to be effective in anti-wrinkles and whitening and cosmetic products containing fermented black ginseng was developed. In this study, ginsenosides were simultaneously analyzed in cosmetics. Analysis was performed simultaneously on each of raw materials (Rb, Rd, Rg3 and compound K) and formulation (Rd and Rg3) using LC/MS/MS. C8 column for raw materials and C18 for formulation were chosen for separation of ginsenosides. With the help of the high specificity and the high sensitivity of multiple reaction monitoring in negative ion mode, the present method showed specificity, linearity (r^2 of Rb, Rd, Rg3 and compound K ≥ 0.994 within 20-2000 ng/mL, 8-800 ng/mL, 3-300 ng/mL and 15-1500 ng/mL respectively for raw material and r^2 of Rd and Rg3 ≥ 0.99 within 15-1500 ng/mL and 8-800 ng/mL respectively for formulation), sensitivity (the lower limit of quantitation at 20 (Rb), 8 (Rd), 3 (Rg3) and 15 (compound K) ng/mL for raw material and 15 (Rd) and 8 (Rg3) ng/mL for formulation), intra- and inter-day accuracy (Rb, Rd, Rg3 and compound K within 85.36 - 111.74% for raw materials and Rd and Rg3 within 95.4 – 108.3% for formulation) and precision (LLOQ ≤ 17.19% and LOQ, MOQ and HOQ ≤ 13.00%). The contents of Rb, Rd, Rg3 and compound K were 5.1, 3.5, 1129.2 and 1.9 μg/mL, respectively at raw material. The contents of Rd and Rg3 were 0.3 and 4.8 μg/mL, respectively at formulation. The ginsenosides were stable for 8 months in formulation.

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In-vitro antibacterial and antioxidant properties of flower, leaf, and stem extracts of *Agastache rugosa*

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The phenolic compounds in different plant parts of *Agastache rugosa* (*A. rugosa*) were determined using Liquid chromatography–mass spectrometry (LC-MS), high performance liquid chromatography (HPLC), total phenolic, anthocyanin, and flavonoid assays. Also, antibacterial and antioxidant activities of the methanol extracts from the flower, leaf, and stem of *A. rugosa* were determined. In this study, LC-MS anaylsis showed that a total of eight phenolic compounds; namely, catechin, chlorogenic acid, caffeic acid, *trans-p*-hydroxy cinnamic methyl ester, ferulic acid, tilianin, rutin, and kaempferol, were identified in *A. rugosa* leaves. HPLC anaylsis showed that leaves contained the higher amount of phenolic compounds than the other parts. However, the total phenolic, anthocyanin, and flavonoid contents were higher in flowers. Furthermore, methanol extracts of flowers revealed that higher antioxidant and antibacterial properties.

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