

Fundamental Instrumentation

: PO1 ~ PO6

P-01

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

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P-02

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

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P-03

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

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P-04

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

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

AT Frontier

P-05

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

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

AT Frontier

P-06

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

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Life & Informatics

: PO7 ~ P25

P-07

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

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P-08

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

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P-09

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

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<p>P-10 Global changes in lipids of brain tissues from p53 KO mice: cortex, hippocampus and hypothalamus</p> <p>Sang Tak Lee¹, Jong Cheol Lee¹, Je Kyung Seong², Myeong Hee Moon^{1*}</p> <p>¹Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea ²College of Veterinary Medicine, Seoul National University, 1 Gwanak-ro, Seoul, 08826, Korea</p>	<p>P-11 Comprehensive profiling analysis of 20 urinary neurochemicals using <i>in situ</i> derivatization and liquid chromatography-tandem mass spectrometry</p> <p>Wonwoong Lee, Hye Jung An, Youna Kim, Jongki Hong*</p> <p>College of Pharmacy, Kyung Hee University, 26 Kyunghee-daero, Dongdaemun-gu, Seoul 02447, Korea</p>
<p>P-12 Korean whole salivary proteome: a preliminary report</p> <p>Ha Ra Cho, Han Sol Kim, Yong Seok Choi*</p> <p>College of Pharmacy, Dankook University, Cheonan-si, Chungnam 31116, South Korea</p>	<p>P-13 Metabolic profiling of human atherosclerotic aorta based on liquid chromatography/mass spectrometry.</p> <p>Sunhee Jung^{1,2}, Miso Nam^{1,2}, Do Hyun Ryu², Geum-Sook Hwang^{1,3*}</p> <p>¹Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Book ah hyun-ro 150, Seoul, 120-140, Republic of Korea ²Dept of Chemistry, SungKyunKwan University, SeoBoo-to 2066, Suwon, 440-746, Republic of Korea ³Department of Life Science, Ewha Womans University, Seoul 120-750, Republic of Korea</p>
<p>P-14 Targeted and global metabolic analysis of rat urine from high tryptophan availability models</p> <p>Yu Ri Cho¹, Mi Jung Ji¹, Mi Yeon Lee¹, Suk Youn Son¹, Ki Soo Lee¹, Soo Hyun Lee², and Hyun-Mee Park¹</p> <p>¹Advanced Analysis Center, Korea Institute of Science and Technology, Korea ²Department of Medical Record and Health Information Management, Kongju National University</p>	<p>P-15 Intact glycopeptide analysis of targeted serum haptoglobin</p> <p>Seunghyup Jeong^{1,2}, Unyong Kim^{1,2}, and Hyun Joo An^{1,2*}</p> <p>¹Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea ²Asia-Pacific Glycomics Reference Site, Daejeon, Korea</p>
<p>P-16 Evaluation of Single Particle ICP-MS for Screening Nanoparticles in Environmental Samples</p> <p>Sang-Jun Lee^{1,2}, Seok-Won Jang¹, Sung Ik Yang^{1*}, Yong-Hyeon Yim^{2*}</p> <p>¹Department of Applied Chemistry, Kyung Hee University, Yongin, 17104 Republic of Korea ²Center for Inorganic Analytical Chemistry, Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 305-340 Republic of Korea *E-mail: siyang@khu.ac.kr, yhyim@kriss.re.kr</p>	<p>P-17 Proteomic Analysis to Identify Interactomes of Human N-alpha-acetyltransferases 40 (hNAA40) using LC-MS/MS</p> <p>Yeirin Lee¹, Hyun Seok Kim^{2*}, and Sang-Won Lee^{1*}</p> <p>¹Department of Chemistry, Korea University, Seoul, 02841, South Korea ²Department Bioinspired Science, Ewha Womans University, Seoul, 03760, South Korea</p>
<p>P-18 Proteomic analysis to reveal the mechanism of E-cadherin loss in a gastric cancer mouse model</p> <p>Seung-Ik Ko¹, Min-Sik Kim² and Sang-Won Lee^{1*}</p> <p>¹Department of Chemistry, Korea University, Seoul, 136-701, Republic of Korea ²Department of Applied Chemistry, Kyunghee University, Gyeonggi-do, 446-701, Republic of Korea</p>	<p>P-19 Quantitative mouse retinal proteome analysis of Vascular Endothelial Growth Factor (VEGF)-induced vascular hyperpermeability by LC-MS/MS</p> <p>Jingi Bae, and Sang-Won Lee*</p> <p>Department of Chemistry, Korea University, Seoul, 136-701, South Korea</p>

<p>P-20 Increasing Sensitivity and Accuracy in Co-fragmented Peptide Identifications from Tandem Mass Spectra using Multiplexed Post-Experimental Monoisotopic Mass Refinement (mPE-MMR)</p> <p>Inamul Hasan Madar, Seung-Ik Ko, Hokeun Kim and Sang-Won Lee* <i>Laboratory of Gaseous Ion Chemistry, Department of Chemistry, Research Institute for Natural Sciences, Korea University, Seoul 136-701, South Korea</i></p>	<p>P-21 Relative metabolite ratio of di(2-ethylhexyl) phthalate in obese children.</p> <p>Wiwon On ^{1,2}, Sang Won Lee², Mi jung Park³, Jeongae Lee¹, Heesoo Pyo^{1*} ¹<i>Molecular Recognition Research Center, Korea Institute of Science and Technology</i> ²<i>Department of Chemistry, Korea University</i> ³<i>Department of Pediatrics, Sanggye Paik Hospital, Inje University College of Medicine</i></p>
<p>P-22 Label free quantitative proteomics using peptide isotope peak intensities in mass spectrometry</p> <p>Ki Na Yun^{1,2}, Gun Wook Park¹, Ju Yeon Lee¹, Eun Sun Ji¹, Mee-Jung Han³, Han Bin Oh², Jong Shin Yoo¹, Jin Young Kim¹ ¹<i>Biomedical Omics Group, Korea Basic Science Institute, Ochang, Korea</i> ²<i>Department of Chemistry, Sogang University, Seoul, Korea</i> ³ <i>Department of Biomolecular and Chemical Engineering, Dongyang University, Yeongju, Korea</i></p>	<p>P-23 A metabolomics-driven approach reveals metabolic responses and mechanisms in the rat heart following myocardial infarction</p> <p>Miso Nam^{1,2}, Sunhee Jung^{1,2}, Do Hyun Ryu², Geum-Sook Hwang^{1,3} ¹<i>Integrated Metabolomics Research Group, Western Seoul Center, Korea Basic Science Institute, Seoul, 03759, Korea</i> ²<i>Department of Chemistry, Sungkyunkwan University, Suwon, 16419, Korea</i> ³<i>Department of Chemistry and Nano Science, Ewha Womans University, Seoul, 03760, Korea</i></p>
<p>P-24 Site-specific characterization of N-glycoproteins in human and mouse plasma samples by LC-MS/MS</p> <p>Hyun Kyoung Lee^{1,2}, Ju Yeon Lee¹, Gun Wook Park^{1,2}, Jin Young Kim¹ and Jong Shin Yoo^{1,2} ¹<i>Korea Basic Science Institute, O-chang Cheongju, Korea</i> ²<i>Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea</i></p>	<p>P-25 Size-dependent analysis of urinary exosomal lipids by flow field-flow fractionation and nanoflow ultrahigh-performance liquid chromatography tandem mass spectrometry (nUPLC-ESI-MS/MS)</p> <p>Joon Seon Yang, Myeong Hee Moon* <i>Dept. of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, South Korea</i></p>
<p>Mass Spectrometry in Elemental Analysis : P26 ~ P40</p>	
<p>P-27 Isotopic analysis of uranium particles for NUSIMEP-7 using SEM-TIMS combined with simultaneous measurement</p> <p>Jong-Ho Park^{1,2*}, Kahee Jeong³ ¹<i>Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, 111 Daedeok-daero-989, Yuseong-gu, Daejeon, 34057, Korea</i> ²<i>Department of Radiochemistry & Nuclear Nonproliferation, University of Science and Technology, 217 Gajeong-ro, Yuseong-gu, Daejeon 34113, Korea</i> ³<i>Chemistry & Environment Group, Central Research Institute, Korea Hydro & Nuclear Power, 70 Yuseong-daero-1312, Yuseong-gu, Daejeon 34101, Korea</i></p>	<p>P-26 Comparative study on extraction method of fragrance allergens in water using GC-MS/MS</p> <p>IN JA LEE*, Haksun Kwon, Chi-hwa An, Jae-Chan Ahn, Bogsoon Kim <i>Seoul Water Institute, Seoul Metropolitan Government, 04981, Korea</i></p>
<p>P-29 Comparative analysis of human milk oligosaccharides by pasteurization and lyophilization</p> <p>Ye Rin Jin^{1,2}, Nari Seo^{1,2}, Tuyen Nguyen³, Nam Mi Kang⁴, Jae Han Kim³, and Hyun Joo An^{1,2*} ¹<i>Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea</i> ²<i>Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea</i> ³<i>Department of Food and Nutrition, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea</i> ⁴ <i>College of Nursing Konkuk University, 268 Chungwondae-ro, Chungju, 27478, Korea</i> <i>*E-mail: sugar@cnu.ac.kr Tel: 82-42-821-8547, Fax: 82-42-821-8541</i></p>	<p>P-28 Targeted lipidomics approach applied to characterize the lipid metabolism of autophagic liver cells</p> <p>Seung Cheol Park¹, Jae Won Lee¹, Ah Young Lee², Myung-Haing Cho², Kwang Pyo Kim^{1*} ¹<i>Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea</i> ²<i>Laboratory of Toxicology, Research Institute for Veterinary Science and College of Veterinary Medicine, Seoul National University, Seoul, Republic of Korea.</i></p> <p>P-30 Alteration of diacyl and ether phosphatidylcholines and phosphatidylethanolamines in the plasma and tissues of HBV mouse model</p> <p>Sue Ah Noh¹, Jae Won Lee¹, Hyuck Jun Mok¹, Hong Seok Kang², Kyun-Hwan Kim², Kwang Pyo Kim^{1*} ¹<i>Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea</i> ²<i>Department of Pharmacology, School of medicine, Konkuk University, Seoul 143-701, Republic of Korea</i></p>

<p>P-31 UPLC-MS/MS Based Profiling of Eicosanoids in RAW264.7 Cells</p> <p><u>Yu-Ri Choi¹</u>, <u>Jae Won Lee¹</u>, <u>Hyuck Jun Mok¹</u>, <u>Seung Cheol Park¹</u>, <u>Hyung Don Kim²</u>, <u>Kwang Pyo Kim^{1*}</u></p> <p>¹<i>Department of Applied Chemistry, College of Applied Science, Kyung Hee University, Yongin, 446-701, Republic of Korea</i> ²<i>Department of Herbal Crop Research, National Institute of Horticultural and Herbal Science, RDA, Eumseong 369-873,</i></p>	<p>P-32 Steroidal CYP enzyme activities in human amniotic fluid by GC-MS</p> <p><u>Soyun Han^{1,2}</u>, <u>Ju-Yeon Moon³</u>, <u>Jae-Hong Kim²</u>, <u>Man Ho Choi¹</u></p> <p>¹<i>Molecular Recognition Research Center, KIST</i> ²<i>College of Life Sciences and Biotechnology, Korea University</i> ³<i>Department of Pharmacy, The Catholic University of Korea</i></p>
<p>P-33 Characterization of site-specific N-glycoproteins in Dried Blood Spot by LC-MS/MS and customized database</p> <p><u>Na Young Choi^{1,2*}</u>, <u>Eun Sun Ji¹</u>, <u>Gun Wook Park¹</u>, <u>Heeyoun Hwang¹</u>, <u>Ju Yeon Lee¹</u>, <u>Hyun Kyoung Lee^{1,2}</u>, <u>Jin Young Kim¹</u> and <u>Jong Shin Yoo^{1,2}</u></p> <p>¹<i>Biomedical Omics Group, Division of Bioconvergence Analysis, KBSI, Ochang, Korea</i> ²<i>Graduated School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea</i></p>	<p>P-34 Platinum analysis in the kidney of mouse treated with the newly developed anticancer drugs</p> <p><u>Sunghwa Choi¹</u>, <u>Eunji Song¹</u>, <u>Eunmi Choi¹</u>, <u>Jiyeon Kim¹</u>, <u>Youngmi Yang¹</u>, <u>Narae Keum^{1,2}</u>, <u>Minyoung Lee^{1,3}</u>, <u>Heh-In Im⁴</u>, <u>Sang joon Lee⁴</u>, <u>Youn Soo Sohn⁵</u>, <u>Kyungsu Park^{1*}</u></p> <p>¹<i>Advanced Analysis Center, Korea Institute of Science and Technology,</i> ²<i>Department of chemistry, Yonsei University,</i> ³<i>Department of Chemistry, Graduate school, Kyung Hee University</i> ⁴<i>Center for Neuroscience, Brain Science Institute. Korea Institute of Science and Technology,</i> ⁵<i>C&Pharm, Rm 211 Science Building B, Ewha Womans University,</i></p>
<p>P-35 Analysis of inorganic element content compared to foreign fruits</p> <p><u>Sunghwa Choi¹</u>, <u>Eunmi Choi¹</u>, <u>Jiyeon Kim¹</u>, <u>Youngmi Yang¹</u>, <u>Eunji Song¹</u>, <u>Narae Keum^{1,2}</u>, <u>Minyoung Lee^{1,3}</u>, <u>Kyungsu Park^{1*}</u></p> <p>¹<i>Advanced Analysis Center, Korea Institute of Science and Technology</i> ²<i>Department of chemistry, Yonsei University</i> ³<i>Department of Chemistry, Graduate school, Kyung Hee University</i></p>	<p>P-36 Chromium Speciation in Wooden Containers and Packing Materials Using HPLC-ICP-MS</p> <p><u>Na-rae Keum^{1,2*}</u>, <u>Eun-mi Choi¹</u>, <u>Ji-yeon Kim¹</u>, <u>Young-mi Yang¹</u>, <u>Eun-ji Song¹</u>, <u>Sung-hwa Choi¹</u>, <u>Min-young Lee^{1,3}</u>, <u>Kyung-su Park^{1*}</u>, <u>Ki-Jung Paeng^{2*}</u></p> <p>¹<i>Advanced Analysis Center, Korea Institute of Science and Technology</i> ²<i>Department of Chemistry, Graduate school, Yonsei University</i> ³<i>Department of Chemistry, Graduate school, Kyung Hee University</i></p>
<p>P-37 Observations on human milk oligosaccharides affected by pasteurization or lyophilization</p> <p><u>Ye Rin Jin^{1,2}</u>, <u>Nari Seo^{1,2}</u>, <u>Tuyen Nguyen³</u>, <u>Nam Mi Kang⁴</u>, <u>Jae Han Kim³</u>, and <u>Hyun Joo An^{1,2*}</u></p> <p>¹<i>Graduate School of Analytical Science and Technology (GRASST), Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea</i> ²<i>Asia-Pacific Glycomics Reference Site, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea</i> ³<i>Department of Food and Nutrition, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Korea</i> ⁴<i>College of Nursing Konkuk University, 268 Chungwondae-ro, Chungju, 27478, Korea</i> [*]<i>E-mail: sugar@cnu.ac.kr, Tel: 82-42-821-8547, Fax: 82-42-821-8541</i></p>	<p>P-38 Development of LC-MS/MS method for quantitation of alpha-Galactosylceramide.</p> <p><u>Soo Hyun Lee¹</u>, <u>Ki Young Choi²</u> and <u>Taegwon Oh²</u></p> <p>¹<i>Department of Medical Record and Health Information Management, Kongju National University, 56 Gonju Daehak-ro Gongju-si Chungcheongnam-do, Korea</i> ²<i>Cellid, Inc., 1 Gwanak-ro, Gwanak-gu, Seoul, Korea</i></p>
<p>P-39 Development of new chemical separation method for uranium age-dating of UO₂ materials</p> <p><u>Eun Ju Choi^{1,2}</u>, <u>Sang Ho Lim^{1,2}</u>, <u>Sun-Ho Han¹</u>, <u>Ranhee Park¹</u>, <u>Jinkyu Park¹</u>, <u>Chi-Gyu Lee¹</u></p> <p>¹<i>Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, Korea</i> ²<i>Radiochemistry & Nuclear Nonproliferation, University of Science & Technology, Korea</i></p>	<p>P-40 Simultaneous determination of chlorogenic acid isomers and metabolites in rat plasma using LC-MS/MS</p> <p><u>Won-Gu Choi</u>, <u>Ju-Hyun Kim</u>, <u>Ju-Yeon Moon</u>, <u>Tae Yeon Kong</u> and <u>Hye Suk Lee[*]</u></p> <p><i>Drug Metabolism and Bioanalysis Laboratory, College of Pharmacy, The Catholic University of Korea, 43 Jibong-ro, Wonmi-gu, Bucheon-si, Gyeonggi-do, 420-743,</i></p>

Medical/Pharmaceutical Science : P41 ~ P50

P-41

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

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

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

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Ju-Hyung Park, Hophil Min, Changmin Sung, Oh-Seung Kwon,
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P-44

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

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P-45

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

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

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Integrated omics for development of Nm23 activator, NMAC1

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P-48

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

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P-49

The Plasma lipidomic profiling from patients with atrial fibrillation

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P-50

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

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**Food Environment
: P51 ~ P62**

P-51

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

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P-52

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

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P-53

Simple, Instant Determination of Fish and Seafood Freshness

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Simple, Instant Evaluation of Beef Freshness

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

AT Frontier

P-55

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

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P-56

A Comparative Study of Heavy Metal Concentration in Nut products.

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P-57

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

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<p>P-58 Analysis of isoflavone patterns by food processing conditions in Korean soybean (<i>Glycine max</i> L.) varieties using UPLC-DAD-QTOF/MS</p> <p>Heon Woong Kim, Min Ki Lee, Seon Hye Lee, Young-Jin Kim, Hwan Hee Jang, Sung Hyen Lee, Jeong-Sook Choe, Jung Bong Kim*</p> <p><i>National Institute of Agricultural Sciences, RDA, 166, Nonsaengmyeong-ro, Iseo-myeon, Wanju</i></p>	<p>P-59 Characterization of flavonoid glycosides from Korean common sage (<i>Salvia plebeia</i> R. Br.) by UPLC-DAD-QTOF/MS</p> <p>Seon-Hye Lee¹, Heon-Woong Kim¹, Min-Ki Lee¹, Young Jin Kim¹, Youn-Soo Cha², Jeong-Sook Choe¹, and Jung-Bong Kim^{1*}</p> <p>¹<i>National Academy of Agricultural Science, Rural Development Administration, 166, Nonsaengmyeong-ro, Iseo-myeon, Wanju-gun, Jeollabuk-do, Republic of Korea</i> ²<i>Department of Food Science and Human Nutrition, Chonbuk National University, 567 Baekje-daero, deokjin-gu, Jeonju-si, Jeollabuk-do, Republic of Korea</i></p>
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<p>P-72 Effect of Ca(II) on the conformation and aggregation process of alpha-synuclein</p> <p><u>Jong Yoon Han</u>, and Hugh I. Kim</p> <p><i>Deptartment of Chemistry, Korea University, Seoul 02841, Korea</i></p>	

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

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

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

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

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

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

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

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

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

AT Frontier

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

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

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

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

AT Frontier

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Korean whole salivary proteome: a preliminary report

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

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

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

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

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

Intact glycopeptide analysis of targeted serum haptoglobin

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

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

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

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

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

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

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

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

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

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

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

As a result, we identified a total 205,730 non redundant peptides, 8,685 proteins with 479 DEPs. Among them, $\beta 2$ integrin was up-regulated by VEGF treatment, but the alteration was inhibited by co-treatment of VEGF and anti-VEGF antibody which also confirmed by western blotting analysis. Finally, we experimentally demonstrated that inhibition of the $\beta 2$ integrin pathway salvaged VEGF-induced retinal vascular hyperpermeability, thus $\beta 2$ integrin can serve as an effective therapeutic target for retinal vascular hyperpermeability.

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

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

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

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

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

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

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

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

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

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Myocardial infarction (MI) is caused by myocardial necrosis resulting from prolonged ischemia. However, the biological mechanisms underlying MI remain unclear. We evaluated metabolic and lipidomic changes in rat heart tissue from sham and MI at 1hr, 1day and 10day after coronary ligation, using global profiling based on metabolomics. A time-dependent increase or decrease in polar and lipid metabolite levels was measured. The S-adenosylmethionine (SAM) concentration and the SAM/S-adenosylhomocysteine (SAH) ratio gradually decreased in a time-dependent manner and were significantly downregulated 10 days after MI. Transcriptome analysis revealed that the levels of coenzyme Q (*Coq*)-3 and *Coq*5, both of which are SAM-dependent methyltransferases, were decreased in the MI groups. These results suggested that dysregulation of SAM may be related to down regulated COQ biosynthetic pathway. In addition, short-chain (C3) and medium-chain (C4-C12) acylcarnitine levels gradually decreased, whereas long-chain acylcarnitine (C14-18) levels increased, owing to a defect in β -oxidation during ischemia. These changes are related to energy-dependent metabolic pathways, and a subsequent decrease in adenosine triphosphate concentration was observed. The comprehensive integration of various omics data provides a novel means of understanding the underlying pathophysiological mechanisms of MI.

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

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

This study provided a method to characterize the site-specific N-glycosylation of human and mouse plasma. We compared site-specific N-glycosylation in human and mouse plasma samples using LC-MS/MS with GPA (GlycoProteome Analyzer) system¹. As reported previously, we confirmed that the sialic acid of N-glycopeptides was almost entirely Neu5Gc in mouse plasma, while in human plasma was Neu5Ac. Especially, a unique trisialylated biantennary N-glycopeptide (peptide_Hex₂HexNAc₂NeuGc₃+Man₃GlcNAc₂) was specifically identified from several glycoproteins in mouse plasma. The trisialylated biantennary glycoform was recently reported in mouse serum, although it could not determine the binding position of the third Neu5Gc. We first report that it is directly linked to GlcNAc with evidence of specific oxonium ions and glycopeptide fragment ions in MS/MS spectra. This clearly proves that the new structure of trisialylated biantennary N-glycopeptide found only in mouse plasma.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Comparative analysis of human milk oligosaccharides by pasteurization and lyophilization

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

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

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

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

Acknowledgement

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Analysis of inorganic element content compared to foreign fruits

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

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

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

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

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

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

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

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

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

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

Observations on human milk oligosaccharides affected by pasteurization or lyophilization

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

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

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

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

Acknowledgement

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

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Selective, sensitive, and validated analytical methods for the quantitative evaluation of chemicals for new drug candidates are critical for the successful conduct of nonclinical and/or biopharmaceutics and clinical pharmacology studies. α -Galactosylceramide (GalCer) is a promising drug candidate as it has been identified as a ligand recognized by V α 14 natural killer T (iNKT) cells and that has been reported to show anti-tumor activity and various immunological effects in infectious diseases, autoimmune disease and graft versus host disease in mice. In the present study, a confident liquid chromatography tandem mass spectrometry (LC-MS/MS) method has been developed for identification, confirmation and quantitation of GalCer. As application of established LC-MS/MS method, the stability of GalCer was evaluated with the method. For step forward, the method will be validated in accordance with the criteria defined in Bioanalytical method validation in Guidance for industry by FDA.

Development of new chemical separation method for uranium age-dating of UO₂ materials

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

In this study, we have developed new chemical separation method using UTEVA resin and optimized separation conditions. This new chemical separation method is expected to be more versatile than previous method using TEVA resin or ion exchange chromatography because it is possible to evaluate Pu age by analyzing $^{241}\text{Am}/^{241}\text{Pu}$ as well as $^{230}\text{Th}/^{234}\text{U}$ at the same time. For testing this method, we prepared simulated uranium samples. Elution curve and recovery yield were obtained from newly developed separation schemes. The optimal volumes of Th eluent (5 M HCl) was 6 mL and the recovery yield was 99.5 %. In addition we also verified this method with UO₂ reference materials and isotopic ratio measurements of $^{230}\text{Th}/^{234}\text{U}$ were performed using MC-ICP-MS equipped with desolvation system (Aridus- II).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Integrated omics for development of Nm23 activator, NMAC1

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

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

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ROS (Redox oxidative species) are not only byproduct of respiration, but also key molecules of cell survival including signaling, proliferation, differentiation and apoptosis. However, cellular targets of ROS are still unclear. In this study, we identified the ROS target proteins in signaling pathway and their regulation mechanism employing 2D-gel electrophoresis and nanoUPLC-ESI-q-TOF tandem MS. We also found that redox sensitive proteins are readily oxidized to diverse modifications at reactive Cys residues, which regulate their stability. Oxidized redox sensitive proteins are readily ubiquitinated and then degraded via proteasome and autophagy. The molecular mechanism of protein degradation was investigated by confirming the ROS-induced structural changes employing hydrogen/deuterium exchange (HDX) mass spectrometry. The results suggest that redox sensitive proteins are regulated by oxidation induced ubiquitination and degradation as another means of quality control.

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The Plasma lipidomic profiling from patients with atrial fibrillation

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

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

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

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

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

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

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

The aim of this study is to simultaneously determine thiamine and biotin in infant formula using isotope dilution-liquid chromatography mass spectrometry. Acid hydrolysis at room temperature was performed to extract thiamine and biotin in infant formula. Thiamine-[¹³C₃] and biotin-[²H₂] standard materials were spiked as internal standard. Waters X-bridge C18 column (4.6 x 150 mm, 3.5 µm) was selected for proper separation of thiamine and biotin, and 10 mmol/L ammonium formate in H₂O, pH 3.8 and methanol were decided as mobile phases. The post-column infusion method was used to study matrix effects originating from sample matrix in electrospray ionization mode.

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

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

Simple, Instant Determination of Fish and Seafood Freshness

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

AT Frontier

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

Simple, Instant Evaluation of Beef Freshness

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

AT Frontier

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

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

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

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

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

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

A Comparative Study of Heavy Metal Concentration in Nut products.

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

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

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

We evaluate linearity, Limit of Detection, Limit of Quantification, Accuracy and Precision to verification of analysis method using a Certified Reference Material.

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

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

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

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

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

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

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

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

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

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

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

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

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

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Growing number of the abuse of diuretics in dietary supplements has become a global problem due to wide distribution and serious negative health effect. In this study, rapid screening method combined with simple sample preparation was developed for detection and confirmation of 29 sulfonamide diuretics by ultra-high performance liquid chromatography quadrupole / time of flight mass spectrometry (UHPLC-Q/TOF-MS). Simple cleanup using liquid-liquid partition was effectively eliminated significant interferences from dietary supplements. The separation of 29 sulfonamide diuretics was achieved within 10 min using 2.6 μm fused-core C18 particles in a 100 x 2.1 mm column with mobile phase (A : 10 mM ammonium formate in water; B : 100 % acetonitrile). The MS/MS spectra of sulfonamides were preferentially interpreted to find common ion and neutral loss fragment. As results, common fragment ion at m/z 77.9650 $[\text{SO}_2\text{N}]^-$ and neutral molecule loss of SO_2NH were observed. These characteristic fragmentations could be used as rapid screening of sulfonamide diuretics and diagnostic ion for elucidation of new emerging sulfonamide class drugs in dietary supplements. Screening of sulfonamides in supplements was rapidly performed by extracted common ion chromatogram (ECIC) of m/z 77.9650 and neutral loss scan of SO_2NH based on narrow mass window within mass tolerance ± 5 ppm, avoiding false positive and/or negative results. Overall calibration curves within dynamic range for all targets were shown to be linear correlation coefficient $R^2 > 0.995$ and limits of detection ranged 0.08-11.18 ng/mL for all sulfonamides. The developed method will be helpful for the protection of the abuse of sulfonamide diuretics in dietary supplements, ensuring public health and consumer safety.

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

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Perfluoroalkyl and polyfluoroalkyl substances (PFASs) including perfluorooctanoic acid (PFOA), perfluorooctanesulfonic acid (PFOS) and perfluorohexane sulfonic acid (PFHxS) are widely used in many manufacturing and various industrial applications. The PFASs was known to cause neurotoxicity, hepatotoxicity, and reproductive and developmental toxicities. The aim of this study was to develop and validate a simultaneous determination method of PFOA, PFOS, and PFHxS for rat plasma and tissues using a UPLC-MS/MS system. The analytes and internal standards (IS) were simply extracted by liquid-liquid extraction after protein precipitation with acetonitrile. UPLC analysis was carried out under the following conditions: a Kinetex[®] 2.6 μ m C₈ 100 Å column, mobile phase of methanol and 5 mM ammonium acetate buffer with gradient elution, and a flow rate of 0.3 mL/min. The three analytes were detected using electrospray ionization tandem mass spectrometry with multiple reaction monitoring (MRM) mode. The chromatograms showed good resolution, selectivity, and no interference in rat biological samples. The standard curves for PFOA, PFOS, and PFHxS in rat plasma and tissue samples were linear over the ranges concentration of 1–10,000 ng/ml with correlation coefficients greater than 0.994. Precision and accuracy with inter- and intra-batch coefficients of variation (CVs) were not exceeding $\pm 15\%$. The validated simultaneous determination method of the 3 PFASs was accepted criteria of the international guidance and successfully applied to characterize the pharmacokinetics and tissue distribution of PFOA, PFOS and PFHxS in rats after a single oral or IV administration. The 3 PFASs were highly distributed in the liver and kidney.

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

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

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

Glycan signatures of human saliva

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In recent years, saliva has received particular attention among researchers especially in the field of forensic sciences. Saliva encountered at crime scene is one of the most significant evidence for crime investigation and thus, to identify saliva from other human fluids and non-human fluids is very important. Conventional methods including enzymatic amylase and starch-iodine test to determine saliva have low sensitivity in trace samples and lack of specificity due to cross-reaction with other fluids. In order to overcome weakness in saliva identification, various studies have been attempted based on biochemical components. Glycoproteins which are highly sensitive to the biochemical environment are a major constituent in saliva and play an important and vital role in maintenance of oral health. Here, we have explored the possibility if glycan can be used as a bio-signature to identify and differentiate human saliva compared with other fluids. Briefly, N-glycans in human saliva (male: 7 and female: 11, age: on average 27) were enzymatically released and were enriched by PGC-SPE. The global characterizations of human saliva N-glycans were carried out by nano LC-PGC chip/Q-TOF MS. We could determine highly fucosylated N-glycans are saliva-specific molecule. Sensitivity was evaluated by comparisons of glycan profiles of 2.5 to 100 μ L of saliva. In future work, we will expand this approach to find glycan signatures for differentiating the human blood and semen.

(1,480 / 1,500)

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

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

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

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

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

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

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

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

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

Real-time Resolution of Analytes, without Chromatographic Separation

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

AT Frontier

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

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

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

Study of variations in human saliva N-glycans

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

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

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