



2018 한국질량분석학회 여름정기학술대회 및 총회

POSTER PRESENTATION

포스터 발표 및 우수포스터상 안내

■ 포스터 게시 및 철거

- 게시: 23일(목), 08:00 ~ 10:00 까지
- 철거: 23일(목), 19:00 ~ 이후
- 포스터 발표자는 아래의 포스터 번호 및 배치도를 참고하여 포스터를 게시하고, 23일(목) 10:50~ 11:50까지 포스터 앞에 대기하여 질문에 응해야 합니다.
- 포스터 발표자 순서: 홀수번호 10:50~11:20 / 짝수번호 11:20~11:50

■ 우수포스터 상

- 포스터 발표 회원중 심사를 거쳐 15명을 선정하여 우수포스터상을 수여합니다.
※ Brief Oral Presentation 발표자는 우수포스터 상의 우선권이 주어짐.
- 시상: 2018년 8월 24일 (금), 폐회식
- 부상: 상장 및 상금 5만원

■ 분야별 포스터 번호

분야	포스터번호
Fundamental & Instrumentation	001 ~ 011
Life & Informatics	012 ~ 023
Biological & Environment	024 ~ 060
Medical/Pharmaceutical Science	061 ~ 091
Food	092 ~ 103
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1. Fundamental Instrumentation : PO01 ~ POT1	P-006 Development of a Gas Mixing System for the Production of Fire-Hazardous Standard Gas Hwa-yong Jang, Han Bin Oh* Department of chemistry, Sogang University, Seoul 04107, Korea
P-001 Ambient laser desorption of mouse hippocampal tissue slice on graphene layer substrate for high spatial resolution mass spectrometric imaging Jae Young Kim^{1,*}, Hee Jin Lim¹, Sun Young Lee¹, Hyunmin Kim², Ji-Won Park³, Dong Kwon Lim⁴, and Dae Won Moon¹ ¹Department of New Biology, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu, Republic of Korea. ²Companion Diagnostics & Medical Technology Research Group, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu, Republic of Korea. ³Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, Daejeon, Republic of Korea. ⁴KU-KIST Graduate School of Science and Technology, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul, Republic of Korea.	P-007 Mechanism Studies of FRIPS Mass Spectrometry Jaeung Lee¹, Yeonjoon Kim², Woo Youn Kim², Han Bin Oh^{1,*} ¹Department of chemistry, Sogang University Email: tnlatnlagho@naver.com; hanbinoh@gmail.com. ²Department of chemistry, Kaist. Email: yj11@kaist.ac.kr; wooyoun@kaist.ac.kr.
P-002 Hyphenation of thin layer chromatography (TLC) with mass spectrometry (MS) - a powerful tool for herbal medicinal products (HMPs) Frank Michel^{1*}, Michaela Oberle², Michael Schulz² ¹Sigma-Aldrich Chemie GmbH, part of Merck KGaA, Eschenstr. 2, 82024 Taufkirchen, Germany; ²Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany	P-008 Elucidating of hydrodesulfurization of polycyclic aromatic sulfur hydrocarbon compounds in crude oil using ion mobility mass spectrometry Dongwan Lim¹, and Sunghwan Kim^{1,2*} ¹Kyungpook National University, Department of Chemistry, Daegu, 702-701, Republic of Korea ²Green-Nano Materials Research Center, Daegu, 702-701 Republic of Korea
P-003 Development of a portable GC/ITMS for on-site VOC detection Bongyoon Yi^{1,2}, Wanseop Jeong^{1,2}, Seung Yong Kim¹, Jae Yeong Eo¹, Byoung Seob Lee¹, Byeongwon Kang^{2,*}, and Hyun Sik Kim^{1,*} ¹Mass Spectrometry & Advanced Instrumentation Group, Korea Basic Science Institute, Cheongju 28119, Republic of Korea ²Department of Physics, Chungbuk National University, Cheongju 28644, Republic of Korea	P-009 Energy-resolved Collision-induced Dissociation Study of Na⁺-bound G-quartets with Mixed Ligands, [Na(Guanine)₄(9-methylguanine)₄]⁺ Yoon Kyung Choi,[†] Sang Yun Han[*] Department of Nanochemistry, Gachon University, 1342 Seongnam-daero, Sujeong-gu, Seongnam-si, Gyeonggi-do, 13120, Republic of Korea [*]E-mail: sanghan@gachon.ac.kr
P-004 An emission model for cold electron ionization in portable ITMS Byoung Seob Lee¹, Wanseop Jeong^{1,2}, Bongyoon Yi^{1,2}, Seung Yong Kim¹, Jae Yeong Eo¹, and Hyun Sik Kim^{1,*} ¹Mass Spectrometry & Advanced Instrumentation Group, Korea Basic Science Institute, Cheongju 28119, Republic of Korea ²Department of Physics, Chungbuk National University, Cheongju 28644, Republic of Korea	P-010 Anomaly in Collision-induced Dissociation of Proton-bound Hoogsteen Base Pairs of Cytosine and Guanine by Proton Transfer Jeong Ju Park,^{†,1} Choong Sik Lee,² Sang Yun Han^{*,1} ¹Department of Nanochemistry, Gachon University, 1342 Seongnam-daero, Sujeong-gu, Seongnam-si, Gyeonggi-do, 13120, Republic of Korea ²Scientific Investigation Laboratory, Ministry of National Defense, 22 Itaewon-ro, Yongsan-gu, Seoul, 04383, Republic of Korea [*]E-mail: sanghan@gachon.ac.kr
P-005 Efficient Enrichment of Phosphopeptides on Digital Microfluidics (DMF) Chip Using TiO₂-Magnetic Bead by MALDI-TOF MS. Jinwoo Kim, Sang Tak Lee, Hyunji Lee, Inae Jang and Han Bin Oh* Dept of Chemistry, Sogang University, Mapogu Baegbeomlo 35, Seoul, 04107, Korea	P-011 Signal reduction due to solvent composition of molecular ions generated from aromatic compounds in (+) atmospheric pressure photoionization mass spectrometry. Seulgidaun Lee¹, Donghwi Kim¹, Arif Ahmed¹, and Sunghwan Kim^{1*} ¹Department of chemistry, Kyungpook National University, 80 Daehak-ro, Buk-gu, Daegu 702-701, Republic of Korea.

2. Life & Informatics : PO12 ~ PO23	P-017 Optimizing extraction efficiency of serum steroids in advanced GC-MS/MS-based profiling <u>Soyun Han</u> ^{1,2} , Hyi Jin Jung ¹ , Jae-Hong Kim ² , Joonseok Lee ¹ , Man Ho Choi ¹ ¹ Molecular Recognition Research Center, KIST, Seoul 02792 ² College of Life Sciences, Korea University, Seoul 02841, Korea
P-012 Profiles of oxidized phospholipids in exosome from oxidatively stressed cells by flow field-flow fractionation and nUHPLC-ESI-MS/MS <u>Joon Seon Yang</u> and Myeong Hee Moon* <i>Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea</i>	P-018 Metabolic signatures of adrenal steroids in serum and saliva measured by polarity switching LC-MS <u>Chaelin Lee</u> ^{1,2} , Hugh I. Kim ² , Man Ho Choi ¹ ¹ Molecular Recognition Research Center, KIST, Seoul 02792 ² Department of Chemistry, Korea University, Seoul 02841, Korea
P-013 Effect of aging on lipid alteration in serum, kidney, and heart from mice by nUHPLC-ESI-MS/MS <u>Jung Yong Eum</u> , Jong Cheol Lee, and Myeong Hee Moon* <i>Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seoul, 03722, Korea</i>	P-019 GC-MS-based metabolic signatures of Cushing's syndrome in serum cholesterol Ayoun Lee ¹ , <u>Go Eun Kwon</u> ¹ , Chaelin Lee ¹ , Jung Hee Kim ² , Man Ho Choi ¹ ¹ Molecular Recognition Research Center, KIST, Seoul 02792 ² Department of Internal Medicine, Seoul National University Hospital, Seoul 03080, Korea
P-014 Optimization for quantitative analysis of glycan in yeast using metabolic isotope labeling of polysaccharides with isotopic glucose (MILPIG) by mass spectrometry <u>Ji-Yeon Kim</u> ¹ , Soo-Hyun Choi ¹ , Jae-Min Lim ¹ , * ¹ Department of Chemistry, Changwon National University, Changwon 51140, South Korea	P-020 Plasma lipid metabolites profiling for internet gaming disorder in Korean males <u>Chang-Wan Lee</u> ¹ , Deokjong Lee ^{3,4} , Eun-Mi Lee ¹ , Soo Jin Park ¹ , Young-Chul Jung ^{2,3} , Do Yup Lee ¹ ¹ Department of Bio and Fermentation Convergence Technology, BK21 PLUS program, Kookmin University, Seoul 02707, Republic of Korea ² The Department of Psychiatry ³ Institute of Behavioral Science in Medicine, Yonsei University College of Medicine, Seoul 03722, Republic of Korea ⁴ National Health Insurance service Ilsan Hospital, Goyang, Gyeonggi 10444, Korea
P-015 In-vivo isotopic glucose labeling of glycan in fungi using metabolic isotope labeling of polysaccharides with isotopic glucose (MILPIG) for quantitative mass spectrometry <u>Soo-Hyun Choi</u> , Ji-Yeon Kim, and Jae-Min Lim* Changwon National University, Changwon 51140, South Korea *E-mail: jmlim@changwon.ac.kr, Tel: 82-55-213-3431, Fax: 82-55-213-3439	P-021 Discovery of a unique metabolic profile for activated Wnt / beta-catenin signaling <u>Yu-Jin Kang</u> , Soo-Jin Park, Joo-Hyun Kim, Sangteak Oh, Do Yup Lee Department of Bio and Fermentation Convergence Technology, BK21 PLUS program, Kookmin University, Seoul, Korea
P-016 Proteomic Analysis of Cervicovaginal Fluid for Early Detection of Preterm Birth by 2D-nLC-ESI-MS/MS <u>Kwonseong Kim</u> , ^{1,2} Young Eun Kim, ² Han Bin Oh, ¹ Dukjin Kang ² ¹ Department of Chemistry, Sogang University, Seoul 04107, Korea ² Center for Bioanalysis, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science, Daejeon, 34113, Korea	P-022 Computational Characterization of Core and Outer Fucosylated N-Glycoproteins with LC-MS/MS and IQ-GPA <u>Hoi Keun Jeong</u> ^{1,2*} , Gun Wook Park ¹ , Heeyoun Hwang ^{1,2} , Hyun Kyoung Lee ^{1,2} , Ju Yeon Lee ¹ , Jin Young Kim ¹ , and Jong Shin Yoo ^{1,2} ¹ Biomedical Omics Research, Korea Basic Science Institute, 162 Yeongudanji-ro, Cheongwon-gu, Cheongju, 28119, Republic of Korea ² Graduate School of Analytical Science and Technology, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Republic of Korea

P-023 A Web-based MS/MS Spectral Library dedicated to Structure Elucidation of Natural Products <u>Young-Mook Kang</u>¹, Hong Kyeong Jung¹, Kwang Hoe Kim^{1,2}, Eun Sun Ji¹, Gun Wook Park¹, Sang Won Lee^{3,4}, Ki Beom Shin^{3,4}, Kyoung Tai No^{3,4}, Jong Shin Yoo^{1,2}, and Jin Young Kim^{1,*} ¹Department of Mass Spectrometry, Korea Basic Science Institute, Cheongju, 28119, Korea ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, 34134, Korea ³Biotechnology, Yonsei University, Seoul, 03722, South Korea. ⁴Bioinformatics & Molecular Design Research Center, Seoul, 03722, South Korea. *Corresponding author: jinyoung@kbsi.re.kr	P-028 Quantitative analysis of lead in soils by fsLA and ICP-MS <u>Minyoung Lee</u>[*], Eunji Kim, Sunghwa Choi, Yuri Lee, Jeongeun Park, Eunmi Choi, Kyungsu Park <i>Advanced Analysis Center, Korea Institute of Science and Technology, 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul, 02792, Republic of Korea</i>
3. Biological & Environment : PO24 ~ PO60	P-029 Structural Profiles of Gangliosides in Developing Human brain via Negative Ion Mode Nano- LC/MS/MS <u>Jua Lee</u>^{1,2}, Jaekyung Yun^{1,2}, Heeyoun Hwang³ and Hyun Joo An^{1,2,*} ¹Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea ³Korea Basic Science Institute, Daejeon, Korea
P-024 Observation on Regenerated Bony Rays of Zebrafish Caudal Fin using Time-of-Flight Secondary Ion Mass Spectrometry <u>Sun Young Lee</u>^{1,*}, Jae Young Kim¹, and Dae Won Moon¹ ¹Department of New Biology, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu, Republic of Korea.	P-030 Identification of Missing Proteins in Human Olfactory Epithelial Tissue by LC-MS/MS <u>Ji Eun Jeong</u>^{1,2}, Heeyoun Hwang^{1,2,3}, Hyun Kyoung Lee^{1,2}, Ki Na Yun^{1,4}, Bonghee Lee^{5,6}, Young-Ki Paik⁷, Gi Taek Yee⁸, Jin Young Kim¹, and Jong Shin Yoo^{1,2,*} ¹Biomedical Omics Research, Korea Basic Science Institute, Cheongju, Korea. ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea. ³Asia-Pacific Glycomics Reference Site, Chungnam National University, Daejeon, Korea. ⁴Department of Chemistry, Sogang University, Seoul, Korea. ⁵Department of Anatomy & Cell Biology, Graduate School of Medicine, Gachon University, Incheon, Korea. ⁶Center for Genomics and Proteomics & Stem Cell Core Facility, Lee Gil Ya Cancer and Diabetes Institute, Gachon University, Incheon, Korea. ⁷Yonsei Proteome Research Center and Department of Integrated OMICS for Biomedical Science, and Department of Biochemistry, College of Life Science and Biotechnology, Yonsei University, Seoul, Korea. ⁸Department of Neurosurgery, Gil Medical Center, Gachon University, Incheon, Korea.
P-025 Direct MS Analysis of Drugs of Abuse in Urine Using Biocompatible Solid Phase Microextraction (BioSPME) <u>Frank Michel</u>^{*1}, Emily Barrey², Craig R. Aurand², Candace Price², Sara Smith² ¹Sigma-Aldrich Chemie GmbH, part of Merck KGaA, Eschenstr. 2, 82024 Taufkirchen, Germany ²MilliporeSigma, part of Merck KGaA, 595 North Harrison Road, Bellefonte, PA, 16823, USA	P-031 Validation of Analytical Methods Using LC-MS to Characterize HGH [Human Growth Hormone] <u>Dong-Ho Yeom</u>[*], Chengmin Jin, Yeoun Hur <i>Research & Development Center, Digital Technology & Contract Research Organization (Dt&CRO), 28 Baengnyeong-ro 20 beon-gil, Cheoin-gu Yongin city, Gyeonggi-do, 17042, Korea</i>
P-026 Improved LC/MS of peptides by innovative particle design and dedicated mobile phase additives <u>Frank Michel</u>^{*1}, Hillel K. Brandes² ¹Sigma-Aldrich Chemie GmbH, part of Merck KGaA, Eschenstr. 2, 82024 Taufkirchen, Germany ²MilliporeSigma, part of Merck KGaA, 595 North Harrison Road, Bellefonte, PA, 16823, USA	P-032 Validation of Analytical Methods Using LC-MS to Characterize Bevacizumab <u>Dong-Ho Yeom</u>[*], Chengmin Jin, Yeoun Hur <i>Research & Development Center, Digital Technology & Contract Research Organization (Dt&CRO), 28 Baengnyeong-ro 20 beon-gil, Cheoin-gu Yongin city, Gyeonggi-do, 17042, Korea</i>
P-027 Improved LC/MS/MS analysis with on-line SPE for removal of phospholipids from protein precipitation biological fluid samples <u>Frank Michel</u>^{*1}, Candace Price² ¹Sigma-Aldrich Chemie GmbH, part of Merck KGaA, Eschenstr. 2, 82024 Taufkirchen, Germany ²MilliporeSigma, part of Merck KGaA, 595 North Harrison Road, Bellefonte, PA, 16823, USA	P-033 Validation of Analytical Methods Using LC-MS to Characterize Trastuzumab <u>Dong-Ho Yeom</u>[*], Chengmin Jin, Yeoun Hur <i>Research & Development Center, Digital Technology & Contract Research Organization (Dt&CRO), 28 Baengnyeong-ro 20 beon-gil, Cheoin-gu Yongin city, Gyeonggi-do, 17042, Korea</i>

P-034 Comparison of lipid profiling of <i>Drosophila</i> head using MALDI-MSI(Matrix assisted laser desorption ionization-mass spectrometry imaging) and ESI-MS(electrospray ionization mass spectrometry) <u>Hyun Jun Jang</u>^{1,2}, Jeong Hyang Park³, Jeong Hee Moon⁴, Ga Seul Lee⁴, Joon Sig Choi², Sohee Yoon^{1*} ¹Center for Nano-Bio Measurement, Korea Research Institute of Standards and Science (KRISS), Daejeon 34113, Republic of Korea ²Department of Biochemistry, Chungnam National University, Daejeon 34134, Republic of Korea ³Department of Brain & Cognitive Sciences, Daegu Gyeongbuk Institute of Science & Technology (DGIST), Daegu 42988, Republic of Korea. ⁴Disease Target Structure Research Center, Korea Research Institute of Bioscience and Biotechnology (KRIBB), Daejeon 34141, Republic of Korea	P-040 Comparison of organic mixtures from particulate matters collected in Korea and China by using GCxGC/high resolution mass spectrometry <u>Moonhee Park</u>¹, and Young Hwan Kim^{1,*} ¹Biomedical Omics Group, Korea Basic Science Institute, Yeongudanji-ro, Cheongju, 28119, Republic of Korea
P-035 Quantitative Proteomic Analysis of 2D and 3D Cultured Colorectal Cancer Cells: Profiling of Tankyrase Inhibitor XAV939-Induced Proteome <u>Young Eun Kim</u>^{1*}, Hyo Jin Jeon², Dahee Kim², Kwang-Rok Kim², Dukjin Kang¹ ¹Center for Bioanalysis, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science, Daejeon, 34113, Korea ²Therapeutic & Biotechnology Division, Korea Research Institute of Chemical Technology, Daejeon, 34114, Korea	P-041 Development of simultaneous analysis of 93 persistent organic pollutants (POPs) in human serum by QuEChERS method and GC-MS/MS <u>Joeeun Lee</u>^{1,2}, Minho Yang³, Yong Min Cho³, Hosub Im³, Sang Beom Han⁴, Ki Hun Kim¹, ¹Doping Control Center, Korea Institute of Science and Technology, Hwarang-ro 14-gil 5, Seongbuk-gu, Seoul, 02792, Korea ²Department of Chemistry, Sogang University, Seoul, 04107, Korea ³Institute for Life & Environmental Technology, Smartive Corporation, Dobong-ro 110na-gil, Dobong-gu, Seoul, 01454, Korea ⁴College of Pharmacy, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul, 06974, Korea
P-036 Multiresidue analysis of PHTs, VOCs, phenols, parabens, PAHs, pyrethroid insecticides and tobacco smoke in human urine by LC-ESI/MS/MS <u>Seunghwa Lee</u>^{1,2}, Kang Mi Lee¹, Minho Yang³, Sang Moon Han^{1,2}, Ho Jun Kim¹, Yong Min Cho³, Sang Beom Han⁴, Hosub Im³, Jaeick Lee^{1,*} ¹Doping Control Center, Korea Institute of Science and Technology, Hwarang-ro 14-gil 5, Seongbuk-gu, Seoul, 02792, Korea ²Department of Chemistry, Research Institute for Natural Sciences, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul, 02841, Korea ³Institute for Life & Environmental Technology, Smartive Corporation, Dobong-ro 110na-gil, Dobong-gu, Seoul, 01454, Korea ⁴College of Pharmacy, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul, 06974, Korea	P-042 Cross-validation of sulfur-based and amino acid-based quantification methods for the development of insulin reference material <u>Hwijin Kim</u>^{1,2}, Ji-Seon Jeong^{1,3}, Thi Thanh Huong Tran^{1,3}, Youngran Lim², Sung Woo Heo², Yong-Hyeon Yim^{1,2*} ¹Department of Bio-Analytical Science, Uiniversity of Science and Technology (UST), Daejeon, 34113, Korea ²Center for Analytical chemistry, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea ³Center for Bioanalysis, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea
P-037 Solid Phase Extraction of nerve agent degradation products using poly(METAC) plate and TOF-SIMS analysis <u>Hyun-Suk Kim</u>, Agency for Defense Development, Yuseong P.O.Box 35, DaeJeon, 34186, Korea	P-043 Environmental product for reference material <u>Jee-seon Moon</u>, Han Bin Oh* Dept of Chemistry, Sogang University, Seoul 04107, Korea
P-038 Quantitative proteomics of 2D-/3D-cultured adipocyte cells and its co-cultured with macrophages using a nanoLC-ESI-MS/MS <u>Sun Young Lee</u>,^{1,2} Sung Bum Park,³ Ki Young Kim,³ Jongki Hong,¹ Dukjin Kang² ¹Department of Life and Nanopharmaceutical Sciences, Kyung Hee University, Seoul 02447, Korea ²Center for Bioanalysis, Division of Metrology for Quality of Life, Korea Research Institute of Standards and Science, Daejeon, 34113, Korea ³Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, P.O. Box 107, Yuseong-gu, Daejeon 305-600, Republic of Korea	P-044 A method for quantitative analysis of nucleic acids using a nanoflow liquid chromatography-tandem mass spectrometry <u>Ji Hyun Kim</u>^{1,2}, Sun Young Lee^{1,3}, Kwonseong Kim^{1,4}, Young Eun Kim¹, Hee Min Yoo^{1,*}, Dukjin Kang^{1,*} ¹Center for Bioanalysis, Korea Research Institute of Standards and Science, Daejeon, Republic of Korea ²Department of Bio-Analytical science, University of Science and Technology (UST), Daejeon, Republic of Korea ³College of Pharmacy, Kyung Hee University, Seoul, Republic of Korea ⁴Department of Chemistry, Sogang University, Seoul, Republic of Korea
P-039 Strong advantages of plasma mass spectrometry to analyze ultra-trace level radioactive isotopes in small amount of environmental samples <u>Seong A Yim</u>^{1*} ^{1,2}Dept of Radiation Safety Research, Korea Institute of Nuclear Safety, 62 Gwahak-ro, Yuseong-gu, Daejeon, 34142, Republic of Korea	P-045 The metabolites differences in a wing polyphenic small brown planthopper revealed by metabolomic analysis <u>Eui-Gil Jung</u>¹, Gwan Seok Lee², Bo Yoon Seo², and Jong Bok Seo¹ ¹Korea Basic Research Institute, Seoul Center, Seoul. ²Department of Plant Protection, National Academy of Agricultural Science, RDA

P-046 LC/MS and LC-UV analysis of photodegradation products of tetracycline and sulfathiazole <u>Youngjoo Kal</u>¹, Seong Ho Yun², Eun Hea Jho², and Sangwon Cha^{1,*} ¹Dept of Chemistry, Hankuk University of Foreign Studies, Yongin, Kyunggi-Do 17035, Korea ²Dept of Environmental Science, Hankuk University of Foreign Studies, Yongin, Kyunggi-Do 17035, Korea	P-052 Spatial distribution of siloxanes in coastal sediment and identification of procedural contamination sources in GC/MS analysis <u>Danbi Lee</u>[*], Sung-Deuk Choi <i>School of Urban and Environmental Engineering, Ulsan National Institute of Science and Technology (UNIST), 50 UNIST-gil, Ulsan, 44919, Korea</i>
P-047 ICP MS Analyses of deciduous teeth for exposomics research <u>Eunji Seo</u>¹, Yujin Lee¹, and Sangwon Cha^{1,*} ¹Dept of Chemistry, Hankuk University of Foreign Studies, Yongin, Kyunggi-Do 17035, Korea	P-053 Characterization of site-specific O-glycopeptides in fibroin heavy chain from silkworm cocoon using high resolution LC-MS/MS <u>Hyun Kyoung Lee</u>^{1,2*}, Gun Wook Park¹, Ji Won Lee^{1,2}, Jin Young Kim¹, Yong Koo Kang³, Jin Hwan No⁴, Kyoung Tai No^{4,5} and Jong Shin Yoo^{1,2} ¹Korea Basic Science Institute, Ochang Cheongju, Korea ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea ³BrainOn Inc, Seoul, Korea ⁴Bioinformatics & Molecular Design Research Center, Seoul, Korea ⁵Department of Biotechnology, Yonsei University, Seoul, Korea
P-048 Analysis of Isomeric Glycopeptides by High Temperature LC-MS/MS <u>Eun Sun Ji</u>¹, Hyun Kyoung Lee^{1,2}, Kwang Hoe Kim^{1,2}, Gun Wook Park¹, Jin Young Kim¹, and Jong Shin Yoo^{1,2} ¹Biomedical Omics Group, Korea Basic Science Institute, Ochang, Republic of Korea ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Republic of Korea	P-054 Automated screening of organic pollutants in airborne particulate matter using GC×GC-TOFMS <u>Ho-Young Lee</u>[*], Seong-Joon Kim, Sung-Deuk Choi <i>School of Urban and Environmental Engineering, Ulsan National Institute of Science and Technology (UNIST), 50 UNIST-gil, Ulsan, 44919, Korea</i>
P-049 LC-MS based rapid profiling and inhibits xanthine oxidase activity from <i>Salbia plebeia</i> <u>Woo Jung Kim</u>, Jun Ho Shin, Yong Mun Choi, Jin Kyu Kim and Jong-Suk Lee[*] ¹Biocenter, Gyeonggido Business & Science Accelerator, Gyeonggi 16229, Korea [*]Corresponding author : leej@s@gsa.or.kr	P-055 LC-MS/MS-based DIA method approach for proteome analysis on <i>synechocystis</i> sp. PCC6803 and PCC7338 <u>Da Mi Kwon</u>[*] <i>Department of pharmacy, Gachon University, 56 Hambangmoe-ro, Yeonsu-gu, Incheon, Korea</i>
P-050 Parallel reaction monitoring of fucosylated glycopeptides of alpha-fetoprotein in human serum for early hepatocellular carcinoma by LC-MS/MS with immunoprecipitation <u>Kwang Hoe Kim</u>^{1,2}, Soo-Youn Lee³, Heeyoun Hwang², Ju Yeon Lee¹, Eun Sun Ji¹, Hyun Joo An², Jin Young Kim^{1,*} and Jong Shin Yoo^{1,2,*} ¹Biomedical Omics Group, Korea Basic Science Institute, 162 YeonGudangji-Ro, Ochang-eup, Cheongju, 28119, Republic of Korea. ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon 34134, Republic of Korea. ³Department of Laboratory Medicine and Genetics, Sungkyunkwan University School of Medicine, Seoul 06351, Republic of Korea	P-056 Validation and application of analytical tools for stable carbon isotope analysis of crude oils in molecular level using ultra-high resolution mass spectrometry <u>Seungwoo Son</u>¹, Donghwi Kim¹, Sunghwan Kim^{1*} ¹Department of Chemistry, Kyungpook National University, Daegu, Republic of Korea
P-051 Proteomic analysis of exosomal proteins from rat Schwann cell <u>Da Kyeong Park</u>¹, Young Hee Kim^{2,4}, Dowonkyoung Park¹, Jong Kuk Kim^{3,4}, Hwan Tae Park^{2,4*} and Young Hye Kim^{1*} ¹Division of Biomedical Omics Research, Korea Basic Science Institute, 162, Yeongudangji-ro, Cheongwon-gu, Cheongju-si, Chungbuk, 28119, Republic of Korea ²Department of Physiology College of Medicine, Dong-A University, 37, Nakdong-daero 550beon-gil, Saha-gu, Busan, 49315, Republic of Korea ³Department of Neurology College of Medicine, Dong-A University, 37, Nakdong-daero 550beon-gil, Saha-gu, Busan, 49315, Republic of Korea ⁴Department of Peripheral Neuropathy Research Center, College of Medicine, Dong-A University, 37, Nakdong-daero 550beon-gil, Saha-gu, Busan, 49315, Republic of Korea	P-057 Performance evaluation of ICP-MS for Ra-226 determination <u>Ji-young Park</u>, Jong Myoung Lim[*], Wanno Lee <i>Dept of Environmental Radioactivity Assessment Team, Korea Atomic Energy Research Institute, Daejeon, 34057, Korea</i>

P-058 Development and validations of the simultaneous analytical method of nine environmental phenol compounds in human urine samples using liquid chromatography – tandem mass spectrometry YounAh Kim, Daye Seo, Seoyoon Song, Minho Yang, Yong Min Cho, <u>Hosub Lim</u>* <i>Institute for Life & Environment Technology, SMARTIVE Corporation, 58, Dobong-ro 110 na-gil, Dobong-gu, Seoul 01454, Korea</i>	P-063 Newborn screening by MALDI-ToF mass spectrometry using parylene-matrix chip <u>Joo-Yoon Noh</u>, Jong-Min Park, Moon-Ju Kim, Tae Gyeong Yun, and Jae-Chul Pyun* <i>Department of Materials Science and Engineering, Yonsei University, Seoul, Korea</i> *E-mail: jcpyun@yonsei.ac.kr
P-059 Selection of functional metabolites of <i>Torreya nucifera</i> by comparison of metabolites <u>Hyung do Kwon</u>¹ and Do Yup Lee¹ ¹The Department of Bio and Fermentation Convergence Technology, BK21 PLUS Program, Kookmin University, Seoul 02707, Republic of Korea	P-064 Diagnosis of gout and pseudogout using inorganic TiO₂ matrices for LDI-ToF mass spectrometry Moon-Ju Kim, Jong-Min Park, <u>Joo-Yoon Noh</u>, Tae Gyeong Yun, and Jae-Chul Pyun* <i>Department of Materials Science and Engineering, Yonsei University, Seoul, Korea</i> *E-mail: jcpyun@yonsei.ac.kr
P-060 Quantitative proteomic analysis of molecular and functional alterations in the human neuronal cell culture model of Alzheimer's disease <u>Min-Young Song</u>, Da Kyeong Park, Soo Youn Lee, Dowonkyoung Park, Jin Young Kim, and Young Hye Kim* <i>Biomedical Omics Research, Korea Basic Science Institute, Cheongju-si, 28119, Republic of Korea</i>	P-065 Diagnosis of galactosemia by MALDI-TOF mass spectrometry using a parylene-matrix chip <u>Tae Gyeong Yun</u>, Jong-Min Park, Joo-Yoon Noh, Moon-Ju Kim and Jae-Chul Pyun* <i>Department of Materials Science and Engineering, Yonsei University, 50 Yeonsei-ro, Seodaemun-gu, Seoul, 03722, Korea</i>
4. Medical/Pharmaceutical Science : PO61 ~ PO91	P-066 Development of sensitive β-lactamase assay for <i>E. coli</i> using a parylene-matrix chip Jong-Min Park, Joo-Yoon Noh, Moon-Ju Kim, <u>Tae Gyeong Yun</u>, Jae-Chul Pyun* <i>Department of Materials Science and Engineering, Yonsei University, 50 Yeonsei-ro, Seodaemun-gu, Seoul, 03722, Korea</i>
P-061 Simultaneous LC-MS/MS analysis of three alkanolamines found in cosmetics <u>Kyung-Ran Min</u>, Kyong-Oh Shin, Maftuna Shamshiddinova, Yong-Moon Lee* <i>College of Pharmacy, Chungbuk National University, Korea</i> *Corresponding author: ymlleefn@cbnu.ac.kr	P-067 Quantitative and sensitive carbapenem susceptibility test using MALDI-TOF based on a parylene-matrix chip Jong-Min Park, Joo-Yoon Noh, Moon-Ju Kim, <u>Tae Gyeong Yun</u>, Jae-Chul Pyun* <i>Department of Materials Science and Engineering, Yonsei University, 50 Yeonsei-ro, Seodaemun-gu, Seoul, 03722, Korea</i>
P-062 Rapid determination of β-lapachone in clinical samples using LC-MS/MS Bo Kyung Kim¹, <u>Hyun Ji Han</u>¹, Mi-Ri Gwon^{1,2}, Boram Ohk¹, Sook Jin Seong¹, Seungil Cho^{1,3}, Young-Ran Yoon^{1,2,3} ¹School of Medicine, Kyungpook National University and Department of Clinical Pharmacology, Kyungpook National University Hospital, Daegu 41944, Korea ²Cell and Matrix Research Institute, School of Medicine, Kyungpook National University, Daegu 41944, Korea ³Molecular Diagnostics and Imaging Center, School of Medicine, Kyungpook National University, Daegu 41944, Korea	P-068 Better sensitivity in LC/MS by improved sample preparation and HPLC method for determination of vitamin D metabolites in plasma <u>Frank Michel</u>^{*1}, Craig R. Aurand², Hugh Cramer² ¹Sigma-Aldrich Chemie GmbH, part of Merck KGaA, Eschenstr. 2, 82024 Taufkirchen, Germany; ²MilliporeSigma, part of Merck KGaA, 595 North Harrison Road, Bellefonte, PA, 16823, USA

P-069 Isolation, Characterization and Quantitative Analysis of Major Compound in Different Parts of <i>Hovenia dulcis</i> using Ultra-Performance Liquid Chromatography Coupled with Orbitrap Mass Min-Sung Lee, Ji Ae Park, Mi Na Choi, Hun Min Song, Hea Seok Kim, Chang Nam Im, Yeong-Su Kim, Dae Wook Kim*, <i>Forest Plant Industry Department, Baekdudaegan National Arboretum, Arboretum, Bonghwa-gun 26209, Korea</i>	P-075 Rapid and sensitive determination of apixaban in human plasma using LC-MS/MS Han-Na Kim^{1*}, Soo-Ji Kim², Yeoun Hur² <i>Research & Development Center, Digital Technology & Contract Research Organization (Dt&CRO), 28 Baengnyeong-ro 20 beon-gil, Cheoin-gu Yongin city, Gyeonggi-do, 17042, Korea</i>
P-070 Urinary Metabolomic Profiling to Discover Potential Biomarkers of Acute Cellular Rejection in Kidney Transplant Recipients Sun-Young Kim¹, Bo Kyung Kim¹, Mi-Ri Gwon¹, Sook Jin Seong¹, Boram Ohk¹, Woo Youl Kang¹, Hae Won Lee¹, Hee-Yeon Jung², Jang-Hee Cho², Chan-Duck Kim², Young-Ran Yoon¹ and Seungil Cho¹ ¹<i>School of Medicine, Kyungpook National University and Department of Clinical Pharmacology, Kyungpook National University Hospital, Daegu 41944, Korea</i> ²<i>Department of Internal Medicine, Kyungpook National University Hospital, Daegu 41944, Korea</i>	P-076 Rapid and sensitive determination of empagliflozin and dapagliflozin in human plasma using LC-MS/MS Han-Na Kim^{1*}, Soo-Ji Kim², Yeoun Hur² <i>Research & Development Center, Digital Technology & Contract Research Organization (Dt&CRO), 28 Baengnyeong-ro 20 beon-gil, Cheoin-gu Yongin city, Gyeonggi-do, 17042, Korea</i>
P-071 Optimization of analysis conditions for native disulfide bond using mass spectrometry Chung Su Lim*, Byung Jun Ko, Joo-rang Woo <i>DepartmenBiodrug Analysis Team, New Drug Development Center, Osong Medical Innovation Foundation, 123 Osongsaengmyeong-ro, Heungdeok-gu, Cheongju-si, Chungbuk, Korea</i>	P-077 Rapid and sensitive determination of dexamethasone in culture media using LC-MS/MS Eun-A Kim^{1*}, Soo-Ji Kim², Yeoun Hur² <i>Research & Development Center, Digital Technology & Contract Research Organization (Dt&CRO), 28 Baengnyeong-ro 20 beon-gil, Cheoin-gu Yongin city, Gyeonggi-do, 17042, Korea</i>
P-072 Simultaneous analysis of highly acidic glycans in biotherapeutics using PGC-SPE and LC-MS/MS Yongsuk Seo, Myung Jin Oh, and Hyun Joo An* ¹<i>Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, 34134, Korea</i> ²<i>Asia-Pacific Glycomics Reference Site, Daejeon, 34134, Korea</i>	P-078 Development and validation of HPLC-MS/MS method for the determination of 9-cis and trans-β-carotene in rat plasma using solid phase extraction. Mi Yang KIM, Han Young EOM, Jong-Hwa Lee* <i>Korea Institute of Toxicology, Daejeon 305-343, Republic of Korea</i>
P-073 Detection of Neu5Gc in Human Serum via MRM-MS Jaekyoung Ko^{1,2}, Hyun Jung Jeong^{1,2}, Nari Seo^{1,2}, MyungJin Oh^{1,2}, and Hyun Joo An^{1,2*} ¹<i>Graduate School of Analytical Science and Technology, Chungnam National University, Korea</i> ²<i>Asia-Pacific Glycomics Reference Site, Korea</i>	P-079 Relative quantification of lipids in mouse serum for the discovery of preterm birth and miscarriage biomarker via metabolic heavy water labeling Byoungsook Goh¹, Ji-Yeon Park³, Joo-Hee Choi³, Jong-Hwan Park³, Tae-Young Kim^{1,2*} ¹<i>Department of Chemistry</i> ²<i>School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju, 61005, South Korea</i> ³<i>Laboratory Animal Medicine, College of Veterinary Medicine and BK 21 PLUS Project Team, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju, 61186, South Korea</i>
P-074 Synergistic antibacterial activity of phenolic compound-antibiotic combination and their quantitative determination by LC-QTOF-MS Md. Akil Hossain, Hae-Chul Park, Kwang-Jick Lee, Sung-Won Park & JeongWoo Kang* <i>Veterinary Drugs & Biologics Division, Animal and Plant Quarantine Agency, Gimcheon-si 39660, Republic of Korea</i>	P-080 High-throughput discovery of anti-inflammatory components in Aster Yomena Sol Bi Park^{1,2}, Ho Jae Lee², Si Hyun Seong³, Min Sun Kim¹, Sang Wan Seo^{2*,} and Hyun Sik Kim^{1,*} ¹<i>Mass Spectrometry & Advanced Instrumentation Group, Korea Basic Science Institute, Cheongju 28119, Republic of Korea</i> ²<i>Department of Oriental Medicine & Biotechnology, Honam University, Gwangju 62399, Korea</i> ³<i>College of Pharmacy, Chungnam National University, Daejeon 305-764, Korea</i>

P-081 Quantitative analysis method for metabolic markers of Preterm births and miscarriage <u>Yunha Ju</u> and Han Bin Oh* ^{1,2}Dept of Chemistry, Sogang University, Seoul 04107, Korea	P-087 Global identification of proteins in Korean Whole Saliva Ha Ra Cho¹, Han Sol Kim¹, Jun Seo Park¹, <u>Dong Yoon Kim</u>¹, Hyo Chun Lee¹, Seung Cheol Park², Kwang Pyo Kim², Troy D. Wood³, Yong Seok Choi* ¹College of Pharmacy, Dankook University, Cheonan, Chungnam 31116, South Korea ²Department of Applied Chemistry, The Institute of National Science, College of Applied Science, Kyung Hee University, Yongin, Kyungki 17104, South Korea ³Department of Chemistry, State University of New York at Buffalo, Buffalo, NY 14260, USA
P-082 Development of Screening Software for Illicit Drugs and Analogues <u>Inae Jang</u> and Han Bin Oh* Dept of Chemistry, Sogang University, Seoul 04107, Korea	P-088 Non-targeted metabolite profiling of maternal plasma for accurate diagnosis of preeclampsia <u>Bo Mi Lee</u>¹, Eun Mi Lee¹, Seung Mi Lee², Joong Shin Park² and Do Yup Lee¹ ¹Department of Bio and Fermentation Convergence Technology, BK21 plus program, Kookmin University, Seoul, 02702, Korea ²Seoul National University College of Medicine, Seoul, Korea Email: gook68@naver.com
P-083 Visualization of the distribution of small molecule in pig-to-nonhuman primate islet xenotransplantation model by MALDI-MS imaging <u>Eui-Gil Jung</u>¹, Jun-Seop Shin² and Jong Bok Seo¹ ¹Seoul Center, Korea Basic Science Institute, Seoul, ²Xenotransplantation Research Center, Seoul National University College of Medicine, Seoul	P-089 Synthesis of ¹⁴C labeled peptides used for quantification of peptides using nano-tracing technique and accelerator mass spectrometry <u>Gwan-Ho Lee</u>¹, Min-Seok Oh², Jong Han Song¹, Ki Soo Kee¹, Byung-Yong Yu^{1*} ¹Advanced Analysis Center, Korea Institute of Science and Technology, 5, Hwarang-ro 14-gil, Seongbuk-gu, Seoul, 02792, Republic of Korea ²Department of Stem Cell Biology, School of Medicine, Konkuk University, 120, Neungdong-ro, Gwangjin-gu, Seoul, 05029, Republic of Korea
P-084 Metabolic change of serum polyamines after Mediterranean diet and contrave treatment on overweight breast cancer patients <u>Yu Ra Lee</u>^{1,2}, Ji-Won Lee⁴, Jeongae Lee¹, Jongki Hong^{2,3}, Bong Chul Chung^{1,2,*} ¹Molecular Recognition Research Center, Korea Institute of Science and Technology, Hwarang-ro 14-gil, Seoul ²KHU-KIST Department of Converging Science and Technology, Kyungheeda-ro, Seoul ³College of pharmacy, Kyung Hee University, Kyungheeda-ro, Seoul ⁴Department of Family Medicine, College of Medicine, Yonsei University, Yongsong Severance Hospital, Eonju-ro, Seoul	P-090 Lectin affinity selection for plasma glycoprotein analysis of healthy elderly groups <u>Miseon Jeong</u>, Jihoon Shin, and Wonryeon Cho* Department of Chemistry, Wonkwang University, 460 Iksanda-ro, Iksan, 54538, Korea
P-085 Establishment of stability conditions to analyze vitamin B12 using LC-MS/MS <u>Eun-Jung Bae</u>, Youjin Seo Korea Institute of Toxicology, KRICT 141, Gajeong-ro, Yuseong-gu, Daejeon 34114, Republic of Korea	P-091 Discovery of predictive serum biomarker candidates for tyrosine kinase inhibitors response in metastatic renal cell carcinoma by using mass spectrometry-based proteomics approaches <u>Kisoon Dan</u>¹, Jeong Woo Lee², Dohyun Han¹, Sang Hoon Song³, Cheol Kwak⁴ ¹Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, Korea ²Department of Urology, Dongguk University Ilsan Hospital, Dongguk University College of Medicine, Goyang, Korea ³Department of Laboratory Medicine, Seoul National University Hospital, Seoul, Korea ⁴Department of Urology, Seoul National University College of Medicine, Seoul, Korea
P-086 Global absolute quantitation of human whole saliva proteins using nLC-Q-IMS-TOF with MS^E Ha Ra Cho, Han Sol Kim, Jun Seo Park, <u>Dong Yoon Kim</u>, Yong Seok Choi* College of Pharmacy, Dankook University, Cheonan, Chungnam 31116, South Korea	

5. Food : PO92 ~ P103	P-097 Analysis of Polycyclic Aromatic Hydrocarbons in Olive Oil using Isotope Dilution-Gas Chromatography/Mass Spectrometry <u>Hyunjeong Ju</u>^{1,2}, Song-Yee Baek¹, Byungjoo Kim¹, Jeongkwon Kim² ¹Center for Analytical Chemistry, Division of Chemical and Medical Metrology, South Korea Research Institute of Standard and Science (KRISS), Daejeon, 34113 South Korea ²Department of Chemistry, Chungnam National University, Daejeon, 34134 South Korea
P-092 Novel GlcNAc-containing oligosaccharides in <i>Aspergillus oryzae</i> β-galactosidase-treated bovine whey permeate <u>Hyeyoung Lee</u>^{1,2}, Juliana Maria Leite Nobrega de Moura Bell,² and Daniela Barile² ¹Food Science and Technology Major, Dong-Eui University, 176 Eomgwangno, Busanjin-gu, Busan 47340, Korea ²Department of Food Science and Technology, University of California-Davis, Davis, California 95616, United States	P-098 Determination of ciguatera fish poisoning toxins (ciguatoxin) in fish by liquid chromatography-tandem mass spectrometry <u>Jin Hong Yoon</u>[*], Seung A Jeong, Yu Jihn Kwon, Shin Hee Kim, Gil Jin Kang ^{1,2}Food Contaminants Division, National Institute of Food and Drug Safety Evaluation, Ministry of Food and Drug Safety Korea, Osongsaengmyeong 2-ro, Osong-eup, Heungdeok-gu, Cheongju-si, Chungcheongbuk-do, 28159, Korea.
P-093 Comparative analysis of recovery of heavy metal concentration by sample pretreatment methods <u>Eunji Kim</u>, Sunghwa Choi, Minyoung Lee, Yuri Lee, Eunmi Choi Jeongeun Park, Kyungsu Park[*] Advanced Analysis Center, Korea Institute of Science and Technology, 5 Hwarang-ro 14-gil, Seongbuk-gu, Seoul 02792, Republic of Korea	P-099 Simultaneous determination of five urushiol analogues in lacquer tree extract by using LC-MRM and QuEChERS with EDTA Ha Ra Cho¹, Dong Yoon Kim¹, <u>Hyo Chun Lee</u>¹, Seung Muk Hyun², Sang Beom Han², Yong Seok Choi^{1*} ¹College of Pharmacy, Dankook University, Cheonan, Chungnam 31116, South Korea ²College of Pharmacy, Chung-Ang University, Seoul 06974, South Korea
P-094 Study on the safety of hazardous substance according to oil extraction methods <u>Jeong-Yun Hwang</u>[*], Hye-Eun Lee, Tae-Hun Kim, Sheen Hee Kim, Jang Duck Choi, Gil-Jin Kang Food Contaminants Division, National Institute of Food and Drug Safety Evaluation, Ministry of Food and Drug Safety Korea, Osongsaengmyeong 2-ro, Osong-eup, Heungdeok-gu, Cheongju-si, Chungcheongbuk-do, 28159, Korea.	P-100 Novel methods to analyze residual neomycin, streptomycin, and dihydrostreptomycin in acacia honey, manuka honey, and mixed flower honey by using LC-MRM with WCX SPE Han Sol Kim¹, Ha Ra Cho¹, <u>Hyo Chun Lee</u>¹, Sang Beom Han², Ho-Chul Shin³, Yong Seok Choi^{1*} ¹College of Pharmacy, Dankook University, Cheonan, Chungnam 31116, South Korea ²College of Pharmacy, Chung-Ang University, Seoul 06974, South Korea ³College of Veterinary Medicine, Konkuk University, Seoul 05029, South Korea
P-095 Determination of the geographical origins of various propolis samples via UPLC combined with high-resolution FT-ICR mass spectrometry <u>Cho Hyun Kim</u>^{1,2*}, Mee Young Kim,³ Seung-Wan Lee³ and Kyoung-Soon Jang^{1,4} ¹Biomedical Omics Center, Korea Basic Science Institute, Cheongju 28119, Republic of Korea ²Department of Chemistry, Korea University, Seoul 02841, Republic of Korea ³Propolis Research Institute, Seoul Propolis Co., Daejeon 34025, Republic of Korea ⁴Division of Bio-Analytical Science, University of Science and Technology, Daejeon 34113, Republic of Korea	P-101 Primary and secondary metabolic profiles according to regional characteristics of <i>Glycine max</i> in Korea <u>Eun Mi Lee</u>¹, Byeong Gon Sin² and Do Yup Lee¹ ¹Department of Bio and Fermentation Convergence Technology, BK21 plus program, Kookmin University, Seoul, 02702, Korea ²Experiment Research Institute of National Agricultural Products Quality Management Service, Gimcheon 39660, Korea
P-096 Validation of tocopherol analysis in leafy vegetables using Standard addition-isotope dilution liquid chromatography mass spectrometry method (SA-IDMS-LC/MS) <u>Minkyung Sung</u>^{1,2}, Joonhee Lee¹, Byungjoo Kim¹, Jeongkwon Kim² ¹Center for Analytical chemistry, Division of Chemical and Medical Metrology, Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, South Korea ²Department of Chemistry, Chungnam National University, Daejeon, 34134, South Korea	P-102 Comparison of aroma components by coffee producer using GC-MS <u>Hye Min Lee</u> and Jong-Suk Lee[*] ¹Biocenter, Gyeonggido Business & Science Accelerator, Gyeonggi 16229, Korea [*]Corresponding author : hmlee@gbsa.or.kr

P-103 Development of qualitative and quantitative system for simultaneously screening 395 pesticide residues by high resolution mass spectrometry <u>Jung eun Seo</u>^{1,*}, Dong sik Jeong¹, Cheong Tae Kim¹, SeongJin Park¹ ¹Food Safety Research Team, NONGSHIM CO., LTD., Yeouidaebang-Ro, Seoul, 07057, Korea	P-108 Analysis of iso-maltooligosaccharide by matrix-assisted laser desorption/ionization mass spectrometry using ionic liquid matrices <u>Sol Han</u>, Yeoseon Kim, Dabin Lee, Hyemin Choi, and Jeongkwon Kim* Department of Chemistry, Chungnam National University, Daejeon, 34134, Korea
General : P104 ~P132	P-109 Construction of Isomer-Specific and Region-Specific Mouse Brain Ganglioside Library using UHPLC-QTOF MS/MS <u>Jaekyung Yun</u>^{1,2}, Jua Lee^{1,2}, Heeyoun Hwang^{1,2} and Hyun Joo An^{1,2,*} ¹Asia Glycomics Reference Site, Chungnam National University, Daejeon, Korea ²Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Korea
P-104 MALDI-MS analysis of small molecules using N-doped carbon dots as matrix <u>Dabin Lee</u>, Yeoseon Kim, Sol Han, Hyemin Choi and Jeongkwon Kim* Department of Chemistry, Chungnam National University, Daejeon, 34134, Korea	P-110 Effect of matrices and drying processes sample preparation in MALDI-MS <u>Hyemin Choi</u>, Yeoseon Kim, Dabin Lee, Sol Han, and Jeongkwon Kim* Department of Chemistry, Chungnam National University, Daejeon, 34134, Korea
P-105 Application of MOF-5 and UiO-66 as MALDI matrices for analysis of small molecules <u>Yeoseon Kim</u>, Jinseong Oh, Dabin Lee, Sol Han, Hyemin Choi, Jungseok Hoe, and Jeongkwon Kim* Department of Chemistry, Chungnam National University, Daejeon, 34134, Korea	P-111 Biomarker discovery of coronary artery disease : serum proteomic profiling <u>Arum Park</u>¹, Jiyeong Lee², Sora Mun¹, Hyo-Jin Kim¹, Yoo-Jin Lee¹, Yoo-Rim Lee¹, Sang Hyun Park³, Hee-Gyoo Kang^{1,2} ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, Republic of Korea. ²Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Republic of Korea. ³Department of Cardiology, Eulji University Hospital, Eulji University School of Medicine, Daejeon, Republic of Korea.
P-106 Detection of small molecules using MALDI-ToF mass spectrometry with TiO₂ nanowire solid matrix <u>Joo-Yoon Noh</u>, Jong-Min Park, Moon-Ju Kim, Tae Gyeong Yun, and Jae-Chul Pyun* Department of Materials Science and Engineering, Yonsei University, Seoul, Korea *E-mail: jcpyun@yonsei.ac.kr	P-112 Biomarker discovery of large artery atherosclerosis stroke: serum proteomic profiling Jiyeong Lee¹, Arum Park¹, Sora Mun², Hyo-Jin Kim², Yoo-Jin Lee², You-Rim Lee², Soo Joo Lee³, Hee-Gyoo Kang^{1,2} ¹Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Republic of Korea. ²Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, Republic of Korea. ³Department of Neurology, Eulji University Hospital, Eulji University School of Medicine, Daejeon, Republic of Korea.
P-107 Trace element analysis of optical fiber <u>SungHwa Choi</u>¹, MinYoung Lee¹, YuRi Lee¹, EunJi Kim¹, Eun Mi Choi¹, SangBae Lee², JaeKyun Lee³, Kyungsu Park^{1,*} ¹Advanced Analysis Center, Korea Institute of Science and Technology, ²Nanophotonics Research Center, Korea Institute of Science and Technology, Seoul 136-791, Korea ³Center for Neuro-Medicine, Korea Institute of Science and Technology, Seoul 136-791, Korea	P-113 Biomarker discovery of rheumatoid arthritis: serum proteomic profiling Sora Mun¹, Jiyeong Lee², <u>Arum Park</u>², Hyo-Jin Kim¹, Yoo-Jin Lee¹, You-Rim Lee¹, Mi-Kyoung Lim³, Hee-Gyoo Kang^{1,2} ¹Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Seongnam-si, Korea. ²Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, Korea. ³Department of Rheumatology, Eulji University Hospital, Eulji University School of Medicine, Daejeon, Republic of Korea.

P-114 Production of high purity gallium metal for compound semiconductor and trace elements quantification <u>Yang, Jaeyeol</u>^{1,2}, O, Byungsung², Jang, Minkyung^{1,3}, Yoon, Jaesik^{1,*} ^{1,*}Korea basic science institute Department of Earth and environmental research, ²Chungnam national university Department of Physics ³Chungnam national university Department of Materials science and engineering	P-120 Intense signal problem on TDC based LC/qTOF system <u>Ga Seul Lee</u>^{1,*}, Jeong Hee Moon¹ ¹Disease Target Structure Research Center, KRIBB, Daejeon 34141, Republic of Korea
P-115 Introduction to B-10 isotope ratio analysis for the reactivity of reactor core <u>Kahee Jeong</u>[*] Chemistry&Environment group, KHNP-CRI, 70-1312gil, Yuseong-daero, 34101, Korea	P-121 Evaluation of quantitation performance of paper cone spray ionization (PCSI) mass spectrometry (MS) <u>Tae-min Park</u>¹ Jun-young Park¹, and Sangwon Cha^{1,*} ¹Dept of Chemistry, Hankuk University of Foreign Studies, Yongin, Kyunggi-Do 17035, Korea
P-116 Mass spectrometric study on the source of error in quantification of fatty acids <u>Hyejin Park</u>¹ and Tae-Young Kim^{1,*} ¹School of Earth Science and Environmental Engineering, Gwangju Institute of Science and Technology, 123 Cheomdangwagi-ro, Buk-gu, Gwangju, 61005, Korea	P-122 Analysis of trace elements in high-purity alumina powder using gravimetric standard addition method with internal standard by inductively coupled plasma optical emission spectroscopy <u>Eunhwa Kim</u>^{1,2}, Cheongah Go¹, Hyungsik Min¹, Myungsub Han¹, Sungwoo Heo¹, Youngran Lim¹, Taekyu Kim², Kyoungseok Lee^{1,*} ¹Korea Research Institute of Standards and Science (KRISS), Daejeon, 34113, Korea ²Dept of Chemistry, Busan National University, Busan, 46241, Korea
P-117 Development of extraction method for dried blood spot <u>You-Rim Lee</u>¹, Ae Eun Seok¹, Hyo-Jin Kim¹, Yoo-Jin Lee¹, Sora Mun¹, Sung Hee Hyun^{1,3}, Ho Joong Sung^{1,2}, Hee-Gyoo Kang^{1,2,*} ¹Laboratory of Signal Transduction and Disease Biomarker Discovery, Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon 34824, Korea ²Department of Biomedical Laboratory Science, College of Health Science, Eulji University, Seongnam 13135, Korea ³Department of Biomedical Laboratory Science, Eulji University, Daejeon, 34824, Republic of Korea	P-123 Development of an Analytical Method for the Identification of Saliva-Specific Glycans in Trace Amounts of Human Saliva <u>Jinyoung Park</u>^{1,2}, Bum Jin Kim^{1,2}, and Hyun Joo An^{1,2,*} ¹Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon ²Asia-Pacific Glycomics Reference Site, Chungnam National University, Daejeon
P-118 Understanding the DMSO effect on the drug efficiency of cisplatin using ICP-MS <u>Gyeong Seo Min</u>, Areum Hong, Hugh. I. Kim[*] Dept of Chemistry, Korea University, Anam-ro 145, Seoul, 02841, Republic of Korea	P-124 Study on analysis method of polyol in Polyurethane foam by Matrix-assisted laser desorption/ionization-Time of flight (MALDI-TOF) <u>Yeongsuk Yoo</u>^{1,*}, Jaeyong Lee², Seung-hwa Lee², Kun Cho¹ ¹Dept of Biomedical Omis, Korean basic science institute, Yeonggudanji-ro, Cheongju, ASI/KR/KS001/CHEONGJU, Korea ²Dept of Research & business, Kumho Petrochemical, Yeonggudanji-ro, Daejeon, ASI/KR/KS015/DAEJEON, Korea
P-119 Validation of Analytical Method for Determination of Cyanide in Rat Blood Using Gas Chromatography-Tandem Mass Spectrometry <u>Min-Chul Shin</u>, Young-Sang Kwon, Jong-Hwan Kim and Jong-Su Seo[*] Korea Institute of Toxicology, Environmental Chemistry Research Group, Jinju City, Republic of Korea	P-125 Understanding the DMSO effect on the drug efficiency of cisplatin using ICP-MS <u>Gyeong Seo Min</u>, Areum Hong, Hugh. I. Kim[*] Dept of Chemistry, Korea University, Anam-ro 145, Seoul, 02841, Republic of Korea

P-126 Effective determination of famphur in honey by gas chromatograph/mass spectrometer <u>Seung-Ho Lee</u>, Jong-Sung Rho, Hyun-Woo Cho, Seung-Woon Myung* <i>Dept of Chemistry, Kyonggi University, Gwanggyosan-ro, Yeongtong-gu, Suwon, 154-42, Korea</i>	P-132 In-vitro antibacterial and antioxidant properties of flower, leaf, and stem extracts of <i>Agastache rugosa</i> <u>Chang Ha Park</u>, Sang Un Park* <i>Dept of Crop Science, Chungnam National University, 99, Daehak-Ro, Yuseong-gu, Daejeon 34134, Republic of Korea</i>
P-127 Characterization of polymer additives by high resolution-GC/MS <u>Hyun Sik You</u>¹, Yeu Young Youn², Young Hee Lim¹ ¹LG Chem/LG Science Park, 30, Magokjungang 10-ro, Gangseo-gu, Seoul, 07796, Korea ²LG Chem R&D Campus, 188, Munji-ro, Yuseong-gu, Daejeon, 34122, Korea	
P-128 Structure determination of Zn phthalocyanine compounds based on demetallization reaction <u>Yeon Hwa Lee</u>¹, Hyun Sik You², Yeu Young Youn¹, Young Hee Lim² ¹LG Chem R&D Campus, 188, Munji-ro, Yuseong-gu, Daejeon, 34122, Korea ²LG Chem/LG Science Park, 30, Magokjungang 10-ro, Gangseo-gu, Seoul, 07796, Korea	
P-129 Single-Injection Screening of 664 Forensic Toxicology Compounds using an Innovative Benchtop High Resolution Mass Spectrometer <u>Oscar G. Cabrices</u>¹, Alexandre Wang¹, Xiang He¹, Holly McCall¹, Laura Baker¹, Adrian Taylor². ¹SCIEX, 1201 Radio Rd, Redwood City, CA USA 94065. ²SCIEX, 71 Four Valley Drive, Concord, Ontario, Canada L4K 4V8.	
P-130 Development of protein characterization analytical method for antibody drug fragments <u>Jinyoung Kim</u>*, Jong Suk Lee <i>Biocenter, Gyeonggi-do Business & Science Accelerator, Suwon, Korea</i>	
P-131 Simultaneous analysis of ginsenosides in fermented black ginseng, using LC/MS/MS <u>Ji-young Kim</u>¹, Jung Dae Lee², Jin Ju Park¹, Hyang Yeon Kim¹, Jeong Eun Lim¹ and Kyu-Bong Kim¹ ¹College of Pharmacy, Dankook University, 119 Dandae-ro, Chungnam, 31116, Republic of Korea ²College of Pharmacy, Sungkyunkwan University, Sebu-ro 2066, Changan-Ku, Gyeonggi-Do, Suwon, 16419, Republic of Korea	

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

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

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

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

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

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

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A portable gas chromatography (GC) was developed. It showed that real-time volatile organic compounds (VOCs) detection was possible with fast ramping temperature gradient provided with a low thermal heating system. The low thermal heating system was realized by coating the carbon nanotube (CNT) heating paste on an anodized aluminum bobbin and then electric currents were provided through gold and copper electrodes on the nanotube-paste. Also, we applied a new membrane interface to connect the low thermal GC and the portable ion trap mass spectrometer (ITMS) to achieve enhanced sensitivity and accurate molecular identification within a restricted size of portable GC/MS. By using a nitrogen carrier gas, VOCs were flowed through and were separated due to an interaction between the VOCs and the column coating materials of GC column, and then were splitted into /or pass through sequentially a photo-ionization detector (PID) and the ITMS. The GC eluent gas could not be injected directly due to restricted performance of a portable ion pump. At this time, the membrane interface allowed an operation of the ITMS efficiently only with a mini-ion getter pump. The membrane interface also provided a concentrating effect because it has a higher permeability to VOCs than carrier gases such as N₂. We present two different configurations of two different ion detectors, and in addition, various advantages of a simultaneous detecting system for on-site VOC detection.

An emission model for cold electron ionization in portable ITMS

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

Efficient Enrichment of Phosphopeptides on Digital Microfluidics (DMF) Chip Using TiO₂-Magnetic Bead by MALDI-TOF MS.

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Phosphorylation is one of the most important post-translational modifications (PTMs) of proteins, which modulates a wide range of biological functions and activity of proteins. The analysis of phosphopeptides is still one of the most challenging tasks in proteomic research by mass spectrometry. In this study, phosphopeptide enrichment carried out on a digital microfluidic (DMF) chip was demonstrated by analyzing phosphopeptides in the tryptic digested β -casein (bovine) and ovalbumin (chicken). This approach was made using a magnetic bead (MB)-based titanium dioxide (TiO₂)-solid phase extraction (SPE) procedure. TiO₂-MB was employed to selectively enrich phosphopeptides from tryptic digests of β -casein and ovalbumin. The enriched phosphopeptides were detected using matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF MS). To evaluate the efficiency of the proposed enrichment method, the result is compared with the mass spectrometric data obtained from nano LC-ESI-MS analysis of the same phosphopeptides. This study shows that the phosphopeptide enrichment analysis can be automated and analyzed with a small sample volume on the DMF chip.

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

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

Mechanism Studies of FRIPS Mass Spectrometry

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

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

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

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

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Collision-induced dissociation (CID) of square-planar Na⁺-bound complexes of G-quartets with mixed ligands of guanine (G) and 9-methylguanine (9mG), [Na·G_n·9mG_m]⁺ ($n = 0 - 4$, $m = 0 - 4$; $n + m = 4$) were investigated using tandem mass spectrometry. The mass spectrum of [Na·G_n·9mG_m]⁺ produced by electrospray ionization (ESI) exhibited pronounced generation of mixed clusters of Na⁺-bound monomers, dimers, and G-quartets, wherein Na⁺-bound trimers were essentially missing. Similarly, CID of G-quartets hardly produced fragments of Na⁺-bound trimers from the square-planar complexes. Those suggest that a great stability is gained by forming a complete hydrogen bonding network in G-quartets, which agrees well with a large predicted stepwise enthalpy of formation by complexation with the fourth ligand to be as large as 55 kcal/mol. The stability gained by hydrogen bonding between G moieties in G-quartets further suggests that Na⁺-bound dimeric fragments may be formed from neighboring, hydrogen-bonded ligands; which in other words suggests preferential neutral loss of hydrogen-bonded G dimers in CID. It further allowed to address the stereochemistry of G-quartets, of which population for *cis*- and *trans*-conformers of [Na·G₂·9mG₂]⁺ can be assessed to be 50:50 in the gas phase. The observed ratio of 50:50 agrees well that the G-quartets were likely to be formed in the solution and produced according to thermochemical stability rather than in the course of electrospray ionization via kinetic trapping.

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

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

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

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

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

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

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

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

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

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

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

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

Herein, we applied metabolic isotope labeling strategy for glycan quantitation in yeast (*Saccharomyces cerevisiae*). We used the metabolic isotope labeling of polysaccharides with isotopic glucose (MILPIG) method to label the light (^{12}C) or heavy ($^{13}\text{C}_1$) glucose on glycan of yeast. As a result, the isotope cluster distribution of the heavy labeled glycan was optimized with glucose concentration and incubation times. We report the conditions to reduce the broaden isotope cluster distribution for accurate quantitative analysis.

Key words: Glycan, Yeast, MILPIG, Mass Spectrometry

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

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N-glycosylation is one of the most important post-translational modifications occurring in living animals and fungi. Animal N-linked glycans and fungi N-linked glycans differ in structure, amount, and role. In the case of animals, N-linked glycans have heterogeneous structures and have specific functions involved in cell-cell recognition, cell division, cell development, cell transport, cell differentiation, immune response and other many important biological phenomena depending on their structures. On the other hand, in the case of fungi, N-linked glycan mediated biological functions remain obscure. In this work, the structure of the fungal N-linked glycan was confirmed by mass spectrometry. In addition, the identified glycans were labeled using the MILPIG (Metabolic Isotope Labeling of Polysaccharides with Isotopic Glucose) method. The MILPIG method is *in-vivo* labeling method that allows fungi to produce heavy-labeled glycans by using carbon source as heavy isotope glucose ($^{13}\text{C}_1$ -glucose).

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

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

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

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

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

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

GC-MS-based metabolic signatures of Cushing's syndrome in serum cholesterol

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

Plasma lipid metabolites profiling for internet gaming disorder in korean males

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

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

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

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

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

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

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

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Glycosylation is a major posttranslational modification of proteins and plays various roles in biological activities. In N-linked glycoproteins, fucosylation is important and closely relevant to diseases such as cancer. For example, core type fucosylated N-glycoproteins in hepatocellular carcinoma has been well reported¹. Tandem mass spectrometry (MS/MS) with liquid chromatography (LC) is a powerful tool for characterization of N-glycoproteins and its fucosylation. Because manual analysis of N-glycoproteins is time consuming, we have developed GlycoProteome Analyzer (IQ-GPA)² software for automated analysis. Nevertheless, assignment of fucosylation in N-glycoprotein is not good enough to decide their core and/or outer positions. It is still remained challenge to classify the fucosylation types of N-glycoproteins.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Validation of Analytical Methods Using LC-MS to Characterize Bevacizumab

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

Validation of Analytical Methods Using LC-MS to Characterize Trastuzumab

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

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

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

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

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

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

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

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

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

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

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

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

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

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Adipocytes in human body play a role in regulating the fat storage and energy homeostasis. Excessive accumulation of adipocytes can lead to obesity, type II diabetes, and inflammation-related diseases via both hypertrophy and hyperplasia. In general, the cellular proteomics of adipocytes has been carried out by means of which the cellular proteome from adipocyte cell is obtained through a two dimensional (2D)-cultured strategy and followed by shotgun proteomics, thereby excavating a key protein that regulates metabolic mechanism in adipocyte cells. However, 2D-cultured cellular proteomics is still insufficient to exactly represent that of real tissue in living body. In order to deeply understand the metabolic mechanism of adipocytes, there is necessary to make the environment that is similar to real tissue. In this study, we developed 3D *in vitro* system for 3T3-L1 cell lines and co-cultured ones with macrophage and investigated on the difference of cellular proteome between 2D- and 3D-cultured systems. To do this, each protein sample was isobarically labeled using an iTRAQ-8plex, pooled equally, and performed tandem mass spectrometric analysis. As the results, we quantified a total of 4052 proteins in duplicate runs and find out proteins having a different quantities between 2D- and 3D-cultured adipocytes. In 3D-cultured adipocyte cells, the levels of proteins involving in glucose and fatty acid metabolisms, such as glucose transporter member 4, fatty acid binding protein, and acetyl-CoA carboxylase, were up-regulated, compared to that of 2D cultured-ones. Consequentially, 3D *in vitro* model offers to the alternative of 2D *in vitro* and *in vivo* models for the assessment of new medical products associated with metabolic disorder.

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

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

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

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In Korea and neighboring China, airborne particulate matter (PM_{2.5}) is very serious environment problems, having primary organic pollutants directly released from emission sources and secondary organic pollutants generated from atmosphere chemical reaction. Thus, the complex organic compounds extracted from PM_{2.5} collected day after day during one month in each country were analyzed to compare their identifications, relative quantities and emission sources. Samples of PM_{2.5} were simultaneously collected day after day for 28 days (4-31 January 2018) in Gwangju and Beijing using a high volume air sampler. The two days of extracts were combined, filtered and concentrated under N₂ gas. Comprehensive two-dimensional gas chromatography/high resolution time-of-flight mass spectrometry (GCxGC/HRMS) was utilized to analyze the organic extracts. Approximately, 460 compounds were separated on the polar and sequential nonpolar GC columns and identified based on the mass spectral data from NIST and Wiley libraries, and exact mass accuracy (<1 ppm) of molecular ion from high resolution data, including alkanes, carboxylic acids, hopanes, PAHs, substituted aromatics and steranes, so on. A variety of PAHs were identified in Beijing samples such as benzo[ghi]fluoranthene, benzo[a]anthracene, acepyrene, pyrene and benzo[A]yrene. Their concentrations in Beijing were more 49 to 3 times according to PAHs compounds than those in Gwangju for 16/17 days PM_{2.5}. Thus, it is anticipated that the issues between two countries related about the emission sources will be discussed, based on these objective results obtained for PM_{2.5} collected in Korea and China.

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

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

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

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

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

Environmental product for reference material

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

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

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

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

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

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

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

ICP MS Analyses of deciduous teeth for exposomics research

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

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

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

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

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

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

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

Proteomic analysis of exosomal proteins from rat Schwann cell

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

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

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

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

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

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

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

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

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

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

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

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

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

Performance evaluation of ICP-MS for Ra-226 determination

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

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

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

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Selection of functional metabolites of *Torreya nucifera* by comparison of metabolites

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

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

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

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

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

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

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

This work was supported by the Industrial Core Technology Development Program (10051129, Development of the system for ADME assessment using radiolabeled compounds) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea), and Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (NRF-2017R1A6A3A11035184).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Optimization of analysis conditions for native disulfide bond using mass spectrometry

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

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

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

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

Detection of Neu5Gc in Human Serum via MRM-MS

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

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

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

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

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

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

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

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

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

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

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

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

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

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Miscarriage is a pregnancy loss before 20 gestational weeks. Preterm birth (PTB), a birth before 37 gestational weeks, causes a high rate of perinatal morbidity and mortality. Despite the threats, there is a lack of diagnostic biomarker that can identify PTB or miscarriage in the early stage of pregnancy. Herein, we presented an analytical platform for the discovery of lipidomic PTB and miscarriage markers in mouse serum by metabolic heavy water ($^2\text{H}_2\text{O}$) labeling. Four replicates of two mouse models (CBA/J $\times$ DBA/2 and CBA/J $\times$ BALB/c) were used for PTB/miscarriage and control groups, respectively. In the control group, the female CBA/J mice were administrated with 8% $^2\text{H}_2\text{O}$ enriched drinking water for four days prior to mating with BALB/c male mice. In case of PTB/miscarriage group, normal drinking water was provided for female CBA/J mice. Serum was collected from CBA/J mice in both control and PTB/miscarriage group after 16 days of mating. Serum lipid extracts from control and PTB/miscarriage groups were mixed in 1:1 ratio based on the serum volume and then analyzed by LC-MS for the relative quantification. As a result, more than 440 lipids from fatty acyl, glycerophospholipid, glycerolipid, and sphingolipid were identified in each biological replicate. Statistical analysis confirmed 11 PTB or miscarriage biomarker candidates including triacylglycerols, phosphatidylethanolamine, and phosphatidylinositol.

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

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

Quantitative analysis method for metabolic markers of Preterm births and miscarriage

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

Development of Screening Software for Illicit Drugs and Analogues

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

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

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

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

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

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

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

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

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

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

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

Global identification of proteins in Korean Whole Saliva

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

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

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

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

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

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

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

Lectin affinity selection for plasma glycoprotein analysis of healthy elderly groups

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The sample was treated with saponification and conducted liquid-liquid extraction with hexane. The separation was carried out isocratic condition with 100% methanol (10 mmol/L ammonium acetate) and Cadenza C₁₈ (3 μ m, 4.6 mm x 250 mm) column. Mass spectrometry analysis was conducted in the negative mode of electrospray ionization and selected reaction monitoring mode was applied.

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

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

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

The aim of this study is developing the analysis method using isotope dilution(ID)-GC/MS as a higher-order reference method for the accurate measurement of four PAHs (Benzo(a)anthracene, Chrysene, Benzo(b)fluoranthene, Benzo(a)pyrene) in olive oil. Sample preparation procedure includes liquid-liquid extraction (LLE) and solid phase extraction (SPE). To optimize the sample clean-up process, we tested the clean-up performance of various cartridges for SPE such as florisil, C₁₈, silica, EZ-POP-NP dual-layer, and NH₂ cartridges. In addition, we compared the results when using deuterium and ¹³C labeled isotopic analogues as internal standards. PAHs were quantitated by SIM mode in GC-MS (Agilent 7890 GC/Jeol JMS 800D-UF MS). The ID-GC/MS method was validated by accuracy, repeatability, reproducibility, LODs, LOQs, assessment of uncertainty, and comparison with other reference method. The developed ID-GC/MS method can also be applied to other edible oils.

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

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

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

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

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

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

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

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

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

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

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

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

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

Comparison of aroma components by coffee producer using GC-MS

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

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

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

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

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

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

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

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

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

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

Detection of small molecules using MALDI-ToF mass spectrometry with TiO₂ nanowire solid matrix

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MALDI-TOF MS has been widely applied for the analysis of biomolecules with high molecular weights, such as proteins and peptides, because of its advantages on soft ionization, easy sample preparation, sensitive detection, and clinical field such as bacterial identification, newborn screening and drug monitoring. However, the conventional organic matrices are ionized themselves to produce their own peaks are called matrix noise at low mass-to-charge (m/z) ratio range (<500) while the sample analytes are ionized by pulsed laser. Moreover, the organic matrices formed non-uniform co-crystals with samples while drying on the surface of target. So, MALDI-TOF MS in the low mass range molecules is so hard. This reasons small molecular weight molecules detection so the other kinds of matrices are required. In this work, TiO₂ nanowire arrays such as solid matrix was synthesized in other to use matrix and applied to MALDI-TOF MS. TiO₂ nanowire arrays was synthesized to detect several amino acid and some small peptides by MALDI-TOF MS. TiO₂ nanowire arrays were synthesized by top-down hydrothermal process. characterizing their morphology and structures by X-ray diffraction (XRD), atomic force microscopy (AFM), scanning electron microscopy (SEM), Raman spectrometry and photo luminescence spectrometry. As a result, interference was significantly reduced and quantitative detections of several amino acid and small peptides were feasible using TiO₂ nanowire arrays.

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Keywords: TiO₂, Nanowires, Solid matrix, Mass spectrometry

Trace element analysis of optical fiber

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

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

As a result, significant results were obtained.

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

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

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

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

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

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

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

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

Biomarker discovery of coronary artery disease : serum proteomic profiling

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

Biomarker discovery of large artery atherosclerosis stroke: serum proteomic profiling

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

Biomarker discovery of rheumatoid arthritis: serum proteomic profiling

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

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

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

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

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

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

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

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

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

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

Development of extraction method for dried blood spot

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

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

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

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

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

Intense signal problem on TDC based LC/qTOF system

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Characterization of polymer additives by high resolution-GC/MS

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

Structure determination of Zn phthalocyanine compounds based on demetallization reaction

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

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

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Introduction

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

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

Methods

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

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

Preliminary data

The performance of separation was evaluated with different mobile phases (acidic and neutral), gradient conditions, and column types. Results indicate that most of isomeric compounds were fully resolved with neutral Buffer A and a 10-min linear gradient using the phenyl-hexyl column. Analyte retention time (RT) was a critical element for accurate identification of each forensic analyte using this screening method, the following RT reproducibility tests were conducted for each compound to evaluate the robustness of the LC condition in this method: (1) reproducibility on 3 separate columns; (2) the inter-day (n=3) reproducibility; (3) the reproducibility in neat versus matrix samples. The reproducibility tests indicated that the RTs generated from the optimized LC conditions are consistent and reproducible. RTs measured on three separated analytical columns all have %CVs of less than 5% for each of the 664 compounds. RT inter-day reproducibility (tested on 80 compounds) resulted in %CVs less than 5% over 3 days. Lastly, RT variability in human whole blood and urine samples (tested on 80 compounds) indicated that the %CV for 3 individual lots is less than 5%.

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

Novel Aspect

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

Poster Session: Toxicology

Development of protein characterization analytical method for antibody drug fragments

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

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

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

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

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

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

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

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

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