



Vanquish HPLC and UHPLC Bibliography

LC that takes your productivity to new heights

Introduction

The release of the Thermo Scientific™ Vanquish™ Horizon UHPLC system in 2014 marked the beginning of the Thermo Scientific™ Vanquish™ HPLC and UHPLC platform. Since then, the Vanquish platform has grown into the most advanced and dynamic product line of HPLC and UHPLC systems available. Built on innovation and ease-of-use, Vanquish LC systems push chromatographic boundaries while continually delivering robust results. Through combination with a variety of detectors from optical and charged aerosol to mass spectrometry, Vanquish HPLC and UHPLC systems have been utilized to address a broad range of analytical challenges from food analysis to large biomolecule characterization.

This bibliography is designed as a guide to the scope of Vanquish HPLC and UHPLC usage in the literature. Publications have been categorized based on either target analyte or field of application. Each publication has been hyperlinked to allow fast navigation to article content. A brief overview of the Vanquish portfolio, Vanquish LC detectors, and Vanquish-compatible mass spectrometers is supplied in the following introductory pages.



Vanquish system overview

Dependability



**Thermo Scientific™ Vanquish™
Core HPLC Systems**

Providing uninterrupted analysis and seamless method transfer. The Vanquish Core HPLC system is designed to continually deliver exceptional results. Ideal for use by analytical scientists performing HPLC analyses where highest dependability is crucial to success.

Flexibility



**Thermo Scientific™ Vanquish™
Flex UHPLC Systems**

Expanding the utility of the Vanquish platform for method development within a variety of both HPLC and UHPLC applications. The Vanquish Flex systems excel at accommodating diverse mobile phase and analyte requirements, made possible through both low and high pressure solvent blending, full system biocompatibility, and various alternative detection principles.

Performance



**Thermo Scientific™ Vanquish™
Horizon UHPLC System**

Offering unrivaled performance and throughput for the most demanding separations with no trade-offs in robustness or ease-of-use. The Vanquish Horizon UHPLC system delivers unsurpassed retention time and peak area precision as well as the highest detector sensitivity. The best choice for applications requiring high-end UHPLC.

Vanquish system overview

Confidence



**Thermo Scientific™ Vanquish™
Online 2D-LC Systems**

Improving analysis of complex samples by enabling separation of difficult-to-resolve analytes. Configurations exist for online SPE and various heart-cutting 2D workflows in order to maximize flexibility while ensuring confidence in your most difficult separations. The Vanquish Simple Switch 2D-LC system is even configured to deliver both 2D and dual LC without re-plumbing.

Productivity









**Thermo Scientific™ Vanquish™
Duo UHPLC Systems**

Providing increased productivity and sample knowledge by utilizing two distinct flow paths. The Vanquish Duo HPLC and UHPLC systems save time, cost per sample, and bench space without sacrificing performance, robustness, or ease-of-use. Ideal for increasing detector utilization, throughput, sample knowledge, or analyte quantification accuracy.

Detectors

Thermo Scientific Vanquish HPLC and UHPLC systems offer a wide range of detection capabilities for seamless integration into new and existing workflows.

Various detectors may also be combined for enhanced sample knowledge.

Thermo Scientific™ Vanquish HPLC and UHPLC Detectors				
Diode Array Detectors		Acquisition of spectra or multiple UV-Vis channels in parallel and a wide dynamic range		
		Sensitive Vanquish Diode Array Detector HL	Flexible Vanquish Diode Array Detector FG	Dependable Vanquish Diode Array Detector CG
Variable Wavelength Detectors		Simple operation with outstanding signal-to-noise and linearity and a wide flow cell portfolio		
		Flexible Vanquish Variable Wavelength Detector F	Dependable Vanquish Variable Wavelength Detector C	
Charged Aerosol Detectors		Sensitive, universal detection		
		Flexible Vanquish Charged Aerosol Detector H	Robust Vanquish Charged Aerosol Detector F	
Fluorescence Detectors		High selectivity and 10–1000 times more sensitivity than UV detectors where applicable		
		Flexible Vanquish Fluorescence Detector F	Dependable Vanquish Fluorescence Detector C	
Mass Spectrometers		Resolve co-eluting peaks and gain analyte mass confirmation		
		Flexible Thermo Scientific™ ISQ™ EM Single Quadrupole Mass Spectrometer	Simple Thermo Scientific™ ISQ™ EC Single Quadrupole Mass Spectrometer	Powerful Plus the full range of Thermo Scientific triple quadrupole and Orbitrap mass spectrometers
Additional Detectors		Universal detection for isocratic gradients		
		Cost effective RefractoMax 521 Refractive Index Detector		

Liquid chromatography-mass spectrometry

Orbitrap LC-MS

For high-resolution, accurate-mass analysis of both known and unknown compounds including small molecules, peptides, and intact proteins.

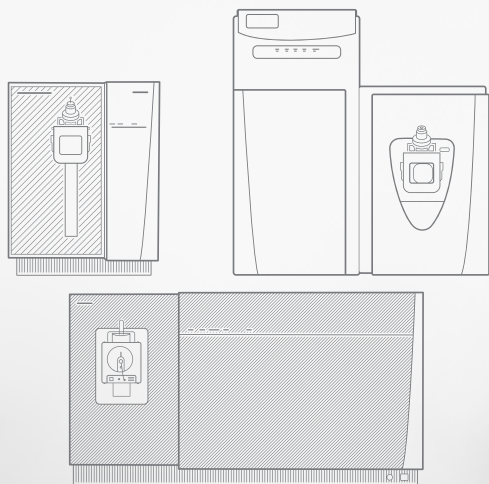
Orbitrap Hybrids

Thermo Scientific™ Orbitrap Exploris™ Series—ranging from small molecule analysis to record setting performance coupled with ease of use and robustness.

Thermo Scientific™ Exactive™ Series—For BioPharma applications and Native MS analysis.

Orbitrap Tribrids

Thermo Scientific™ Orbitrap Tribrid™ Series—Three mass analyzers enable multiple sophisticated modes of analysis using intelligent data acquisition and everyday experimental flexibility.



Triple Quadrupole LC-MS

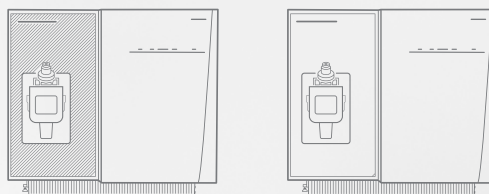
For ultimate sensitivity, robustness, and speed in routine, targeted quantitation.

Thermo Scientific™ TSQ Fortis™—Increase productivity in targeted workflows.

Thermo Scientific™ TSQ Endura™—Develop in vitro diagnostic tests that leverage sensitivity, confidence, and quantitative accuracy.

Thermo Scientific™ TSQ Quantis™—Excellent sensitivity and robustness for challenging quantitation workflows.

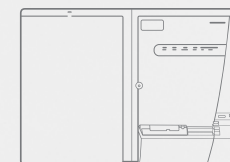
Thermo Scientific™ Altis™—For addressing the most stringent analytical challenges in targeted quantitation. Unprecedented sensitivity without sacrificing robustness.



Ion Trap LC-MS

For high sensitivity full scan MS along with in-depth MSⁿ (CRM) capabilities.

Thermo Scientific™ LTQ XL™—cost-effective, general-purpose instrument enabling all users to be more confident in their results and operation skills. Full scan and MSⁿ operating modes provide flexibility from running your application to teaching students the fundamentals of mass spectrometry.



Survey of applications

A total of 647 peer-reviewed publications and 76 Thermo Fisher Scientific collateral documents published from 2014 and 2020 are included in this bibliography. References are divided into 14 categories (including miscellaneous) best representing each article's focus or application—over 65% of studies targeted biomolecules, followed by combined 15% applied to the food and pharmaceutical industries. Hyphenation with mass spectrometry was mentioned in over 70% of articles, with the Thermo Scientific™ Exactive Orbitrap™ Mass Spectrometer product line utilized for 58% of all studies. The Vanquish DAD was the second most popular type of detector with 37 total citations.

This bibliography provides a survey demonstrating the breadth of the literature applications of Vanquish HPLC and UHPLC platforms. The range of analyte separation capabilities and Vanquish-compatible detectors help to make the Vanquish portfolio the premier chromatographic systems.

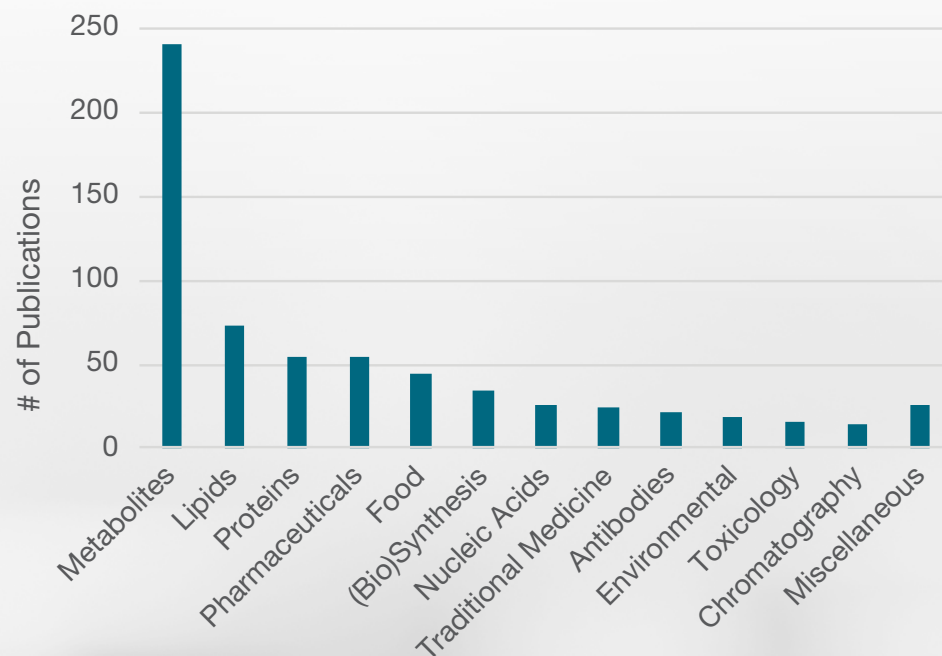
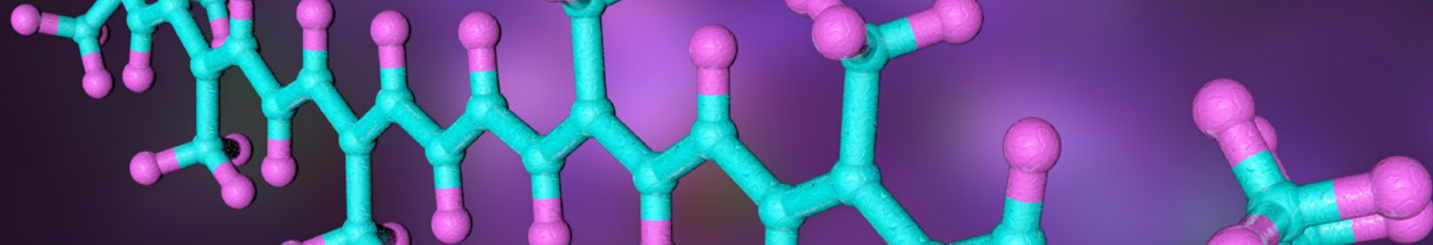


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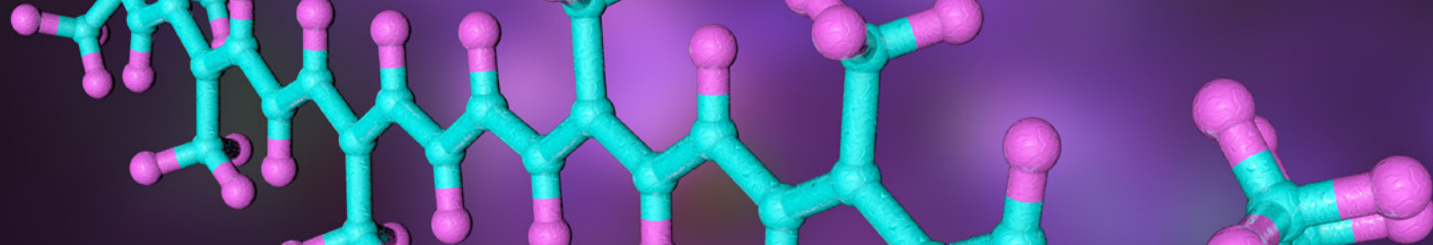
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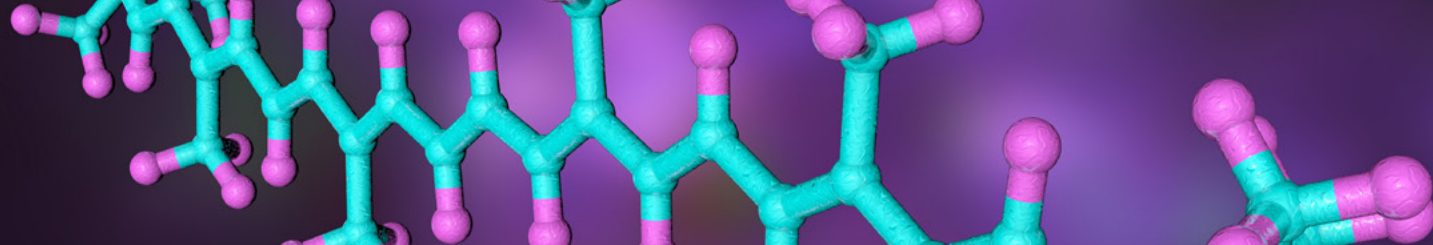
Metabolites

Title	Authors	Journal	Date
Oxidative modifications of glyceraldehyde 3-phosphate dehydrogenase regulate metabolic reprogramming of stored red blood cells	JA Reisz, MJ Wither, M Dzieciatkowska, T Nemkov, A Issaian, T Yoshida, AJ Dunham, RC Hill, KC Hansen, A D'Alessandro	Blood	2016
Biomarkers defining the metabolic age of red blood cells during cold storage	G Paglia, A D'Alessandro, Óttar Rolfsson, ÓE Sigurjónsson, A Bordbar, S Palsson, T Nemkov, KC Hansen, S Gudmundsson, BO Palsson	Blood	2016
From sample to multi-omics conclusions in under 48 Hours	RA Quinn, JA Navas-Molina, ER Hyde, SJ Song, Y Vázquez-Baeza, G Humphrey, J Gaffney, JJ Minich, AV Melnik, J Herschend, J DeReus, A Durant, RJ Dutton, M Khosroheidari, C Green, R da Silva, PC Dorrestein, R Knight	mSystems	2016
Glutamine metabolism drives succinate accumulation in plasma and the lung during hemorrhagic shock	AL Slaughter, A D'Alessandro, EE Moore, A Banerjee, CC Silliman, KC Hansen, JA Reisz, M Fragoso, MJ Wither, A Bacon, HB Moore, ED Peltz	The Journal of Trauma and Acute Care Surgery	2017
Characterization of rapid extraction protocols for high-throughput metabolomics	S Gehrke, JA Reisz, T Nemkov, KC Hansen, A D'Alessandro	Rapid Communications in Mass Spectrometry	2017
Methanol generates numerous artifacts during sample extraction and storage of extracts in metabolomics research	C Saurchnig, M Doppler, C Bueschl, R Schuhmacher	Metabolites	2017
Red blood cells in hemorrhagic shock: a critical role for glutaminolysis in fueling alanine transamination in rats	JA Reisz, AL Slaughter, R Culp-Hill, EE Moore, CC Silliman, M Fragoso, ED Peltz, KC Hansen, A Banerjee, A D'Alessandro	Blood Advances	2017
Red blood cell proteomics update: is there more to discover?	A D'Alessandro, M Dzieciatkowska, T Nemkov, KC Hansen	Blood Transfusion	2017
Estimation of flux ratios without uptake or release data: Application to serine and methionine metabolism	R Nilsson, I Roci, J Watrous, M Jain	Metabolic Engineering	2017
Structural and functional insight of sphingosine 1-phosphate-mediated pathogenic metabolic reprogramming in sickle cell disease	K Sun, A D'Alessandro, MH Ahmed, Y Zhang, A Song, TP Ko, T Nemkov, JA Reisz, H Wu, M Adebisi, Z Peng, J Gong, H Liu, A Huang, YE Wen, AQ Wen, V Berka, MV Bogdanov, O Abdulmalik, L Han, A Tsai, M Idowu, HS Juneja, RE Kellems, W Dowhan, KC Hansen, MK Safo, Y Xai	Scientific Reports	2017
The metabolic and proliferative state of vascular adventitial fibroblasts in pulmonary hypertension is regulated through a MiR-124/PTBP1/PKM axis	H Zhang, D Wang, M Li, L Plecítá-Hlavatá, A D'Alessandro, J Tauber, S Riddle, S Kumar, A Flockton, BA McKeon, MG Frid, JA Reisz, P Caruso, KC El Kasmi, P Ježek, NW Morrell, C Hu, KR Stenmark	Circulation	2017
A comparative study of biological and metabolic biomarkers between healthy individuals and patients with acne vulgaris	K Kim, I Ha, E Kim, K Kim	Medicine	2017
Metabolism of citrate and other carboxylic acids in erythrocytes as a function of oxygen saturation and refrigerated storage	T Nemkov, K Sun, JA Reisz, T Yoshida, A Dunham, EY Wen, AQ Wen, RC Roach, KC Hansen, Y Xia, A D'Alessandro	Frontiers in Medicine	2017



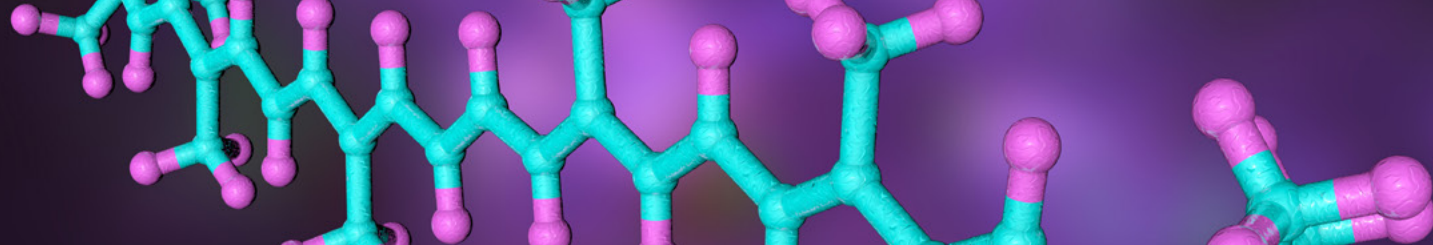
Metabolites

Title	Authors	Journal	Date
Inhibition of IKKε and TBK1 improves glucose control in a subset of patients with type 2 diabetes	EA Oral, SM Reilly, AV Gomez, R Meral, L Butz, N Ajiluni, TL Chenevert, E Korytnaya, A Neidert, R Hench, D Rus, J Horowitz, BA Poirier, P Zhao, K Lehmann, M Jain, R Yu, C Liddle, M Ahmadian, M Downes, RM Evans, AR Saltiel	Cell Metabolism	2017
Fine mapping and functional analysis reveal a role of SLC22A1 in acylcarnitine transport	HI Kim, J Raffler, W Lu, JJ Lee, D Abbey, D Saleheen, JD Rabinowitz, MJ Bennett, NJ Hand, C Brown, DJ Rader	American Journal of Human Genetics	2017
Evaluation of column length and particle size effect on the untargeted profiling of a phytochemical mixture by using UHPLC coupled to high-resolution mass spectrometry	RZ Chiozzi, AL Capriotti, C Cavaliere, F Ferraris, G La Barbera, S Piovesana, Aldo Leganà	Journal of Separation Science	2017
The glutamate/cystine xCT antiporter antagonizes glutamine metabolism and reduces nutrient flexibility	CS Shin, P Mishra, JD Watrous, V Carelli, M D'Aurelio, M Jain, DC Chan	Nature Communications	2017
Lifelong exposure to PCBs in the remote norwegian arctic disrupts the plasma stress metabolome in arctic charr	PT Gauthier, A Evenset, GN Christensen, EH Jorgensen, MM Vijayan	Environmental Science & Technology	2017
Revitalization of a forward genetic screen identifies three new regulators of fungal secondary metabolism in the genus Aspergillus	BT Pfannenstiel, X Zhao, J Wortman, P Wiemann, K Throckmorton, JE Spraker, AA Soukup, X Luo, DL Lindner, FY Lim, BP Knox, B Haas, GJ Fischer, T Choera, RAE Butchko, JW Bok, KJ Affeldt, NP Keller, JM Palmer	mBio	2017
Plasma succinate is a predictor of mortality in critically injured patients	A D'Alessandro, HB Moore, EE Moore, JA Reisz, MJ Wither, A Ghasabyan, J Chandler, CC Silliman, KC Hansen, A Banerjee	Journal of Trauma and Acute Care Surgery	2017
Unambiguous identification and characterization of a long-term human metabolite of dehydrochloromethyltestosterone	G Forsdahl, T Geisendorfer, L Göschl, S Pfeffer, P Gärtner, M Thevis, G Gmeiner	Drug Testing and Analysis	2017
Metabolomics analysis of human vitreous in diabetic retinopathy and rhegmatogenous retinal detachment	NR Haines, N Manoharan, JL Olson, A D'Alessandro, JA Reisz	Jouranl of Proteome Research	2018
Metabolomics reveals the molecular mechanisms of copper induced cucumber leaf (cucumis sativus) senescence	L Zhao, Y Huang, K Paglia, A Vaniya, B Wancewicz, A Keller	Environmental Science & Technology	2018
Profiling the metabolism of human cells by deep ¹³ C labeling	N Grankvist, JD Watrous, KA Lehmann, Y Lutvinskiy, M Jain, R Nilsson	Cell Chemical Biology	2018
Metabolic effect of alkaline additives and guanosine/gluconate in storage solutions for red blood cells	A D'Alessandro, JA Reisz, R Culp-Hill, H Korsten, R van Bruggen, D d Korte	Transfusion	2018
Metabolomics evaluation of early-storage red blood cell rejuvenation at 4° C and 37° C	S Gehrke, AJ Srinivasan, R Culp-Hill, JA Reisz, A Ansari, A Gray, M Landrigan, I Welsby, A D'Alessandro	Transfusion	2018
Quantitative metabolomics comparison of traditional blood draws and TAP capillary blood collection	A Catala, R Culp-Hill, T Nemkov, A D'Alessandro	Metabolomics	2018



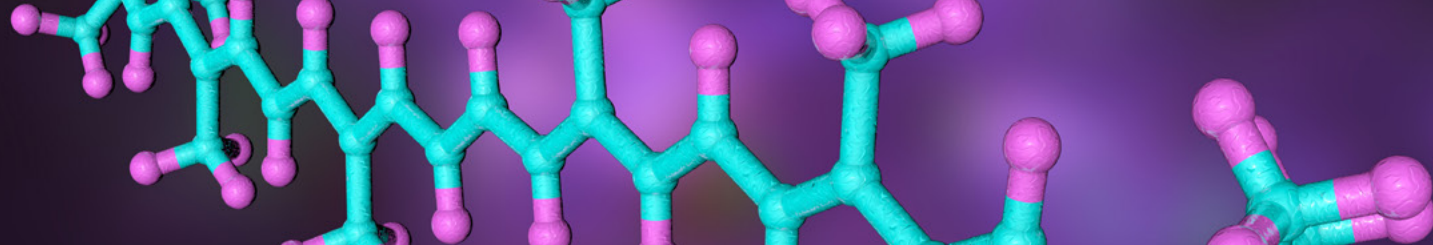
Metabolites

Title	Authors	Journal	Date
Peak annotation and verification engine for untargeted LC-MS metabolomics	L Wang, X Xing, L Chen, L Yang, X Su, H Rabitz, W Lu, JD Rabinowitz	Analytical Chemistry	2018
All animals are equal but some animals are more equal than others: Plasma lactate and succinate in hemorrhagic shock: A comparison in rodents, swine, non-human primates and injured patients	JA Reisz, MJ Wither, MJ Wither, EE Moore, AL Slaughter, HB Moore, A Ghasabyan, J Chandler, LJ Schaub, M Fragoso, G Nunns, CC Silliman, KC Hansen, A Banerjee, FR Sheppard, A D'Alessandro	Journal of Trauma and Acute Care Surgery	2018
A three-minute method for high-throughput quantitative metabolomics and quantitative tracing experiments of central carbon and nitrogen pathways	T Nemkov, KC Hansen, A D'Alessandro	Rapid Communications in Mass Spectrometry	2018
Distinctive patterns of flavonoid biosynthesis in roots and nodules of <i>Datisca glomerata</i> and <i>medicago</i> spp. revealed by metabolomic and gene expression profiles	I Gifford, K Battenberg, A Vaniya, A Wilson, L Tian, O Fiehn, AM Berry	Frontiers in Plant Science	2018
Regulation of human adipose tissue activation, gallbladder size, and bile acid metabolism by a β 3-adrenergic receptor agonist	AS Baskin, JD Linderman, RJ Brychta, S McGegee, E Anflück-Chames, C Cero, JW Johnson, AE O'Mara, LA Fletcher, BP Leitner, CJ Duckworth, S Huang, H Cai, HM Gerrafo, CM Millo, W Dieckmann, V Tolstikov, EY Chen, F Gao, NR Narain, MA Kiebish, PJ Walter, P Herscovitch, KT Chen, AM Cypess	Diabetes	2018
The epigenetic reader SntB regulates secondary metabolism, development and global histone modifications in <i>Aspergillus flavus</i>	BT Pfannenstiel, AT Sikowaty, NP Keller	Fungal Genetics and Biology	2018
Identification and metabolite profiling of alkaloids in aerial parts of <i>Papaver rhoeas</i> by liquid chromatography coupled with quadrupole time-of-flight tandem mass spectrometry	JH Oh, IJ Ha, MY Lee, EO Kim, D Park, JH Lee, SG Lee, DW Kim, TH Lee, EJ Lee, CK Kim	Journal of Separation Science	2018
^{13}C -labelled yeast as internal standard for LC-MS/MS and LC high resolution MS based amino acid quantification in human plasma	G Hermann, M Schwaiger, P Volejnik, G Koellensperger	Journal of Pharmaceutical and Biomedical Analysis	2018
Genetic modification of asexual <i>Epichloë</i> endophytes with the <i>perA</i> gene for peramine biosynthesis	IK Hettiarachchige, AC Elkins, P Reddy, RC Mann, KM Guthridge, TI Sawbridge, JW Forster GC Spangenberg	Molecular Genetics and Genomics	2018
Extraction of urinary metabolite-derived biomarker candidate for breast cancer	M Sakairi, M Abe, N Tanaka	Bulletin of the Chemical Society of Japan	2018
Restoring mitochondrial calcium uniporter expression in diabetic mouse heart improves mitochondrial calcium handling and cardiac function	J Suarez, F Cividini, BT Scott, K Lehmann, J Diaz-Juarez, T Diemer, A Dai, JA Suarez, M Jain, WH Dillman	Journal of Biological Chemistry	2018
Deep scanning lysine metabolism in <i>Escherichia coli</i>	MC Bassalo, AD Garst, A Choudhury, WC Grau, EJ Oh, E Spindler, T Lipscomb, RT Gill	Molecular Systems Biology	2018
Electrophilic properties of itaconate and derivatives regulate the $\text{I}\kappa\text{B}\zeta$ -ATF3 inflammatory axis	M Bambouskova, L Gorvel, Vicky Lampropoulou, A Surgushichev, E Loginicheva, K Johnson, D Korenfeld, ME Mathyer, H Kim, LH Huang, D Duncan, H Bregman, A Keskin, A Santeford, RS Apte, R Sehgal, B Johnson, GK Amarisinghe, MP Soares, T Satoh, S Akira, T Hai, CG Strong, K Auclair, TP Roddy, SA Biller, M Jovanovic, E Klechevsky, KM Stewart, GJ Randolph, MN Artymov	Nature Letters	2018



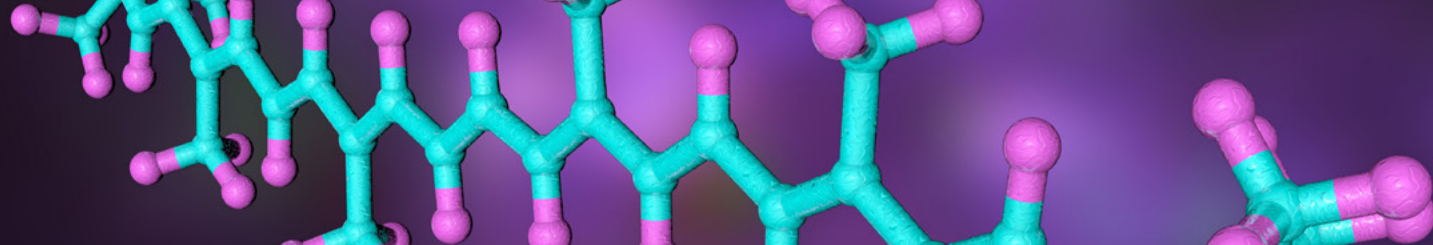
Metabolites

Title	Authors	Journal	Date
Macrophage-derived IL-1 β /NF- κ B signaling mediates parenteral nutrition-associated cholestasis	KC El Kasmi, PM Vue, AL Anderson, MW Devereaux, S Ghosh, N Balasubramanian, SA Fillon, C Dahrenmoeller, A Allawzi, C Woods, S McKenna, CJ Wright, L Johnson, A D'Alessandro, JA Reisz, E Nozik-Grayck, FJ Suchy, RJ Sokol	Nature Communications	2018
Cell-intrinsic glycogen metabolism supports early glycolytic reprogramming required for dendritic cell immune responses	P Thwe, L Pelgrom, R Cooper, S Beauchamp, JA Reisz, A D'Alessandro, B Everts, E Amiel	Cell Metabolism	2018
Conserved responses in a war of small molecules between a plant-pathogenic bacterium and fungi	JE Spraker, P Wiemann, JA Baccile, N Vankatesh, J Schumacher, FC Schroeder, LM Sanchez, NP Keller	mBio	2018
Male lifespan extension with 17- α estradiol is linked to a sex-specific metabolomic response modulated by gonadal hormones in mice	M Garratt, KA Lagerborg, YM Tsai, A Galecki, M Jain, RA Miller	Aging Cell	2018
Autophagy maintains tumour growth through circulating arginine	L Poillet-Perez, X Xie, Le Zhan, Y Yang, DW Sharp, ZS Hu, X Su, A Maganti, C Jiang, W Lu, H Zheng, MW Bosenberg, JM Mehnert, JY Guo, E Lattime, JD Rabinowitz, E White	Nature	2018
Chromatographic column evaluation for the untargeted profiling of glucosinolates in cauliflower by means of ultra-high performance liquid chromatography coupled to high resolution mass spectrometry	AL Capriotti, C Cavaliere, GL Barbera, CM Montone, S Piovesana, RZ Chiozzi, A Laganà	Talanta	2018
Early behavioral and metabolomic change after mild to moderate traumatic brain injury in the developing brain	J Chitturi, Y Li, V Santhakumar, SS Kannurpatti	Neurochemistry International	2018
IRE1 α -XBP1 controls T cell function in ovarian cancer by regulating mitochondrial activity	M Song, TA Sandoval, CS Chae, S Chopra, C Tan, MR Rutkowski, M Raundhal, RA Chaurio, KK Payne, Csaba Konrad, SE Bettigole, HR Shin, MJP Crowley, JP Cerliani, AV Kossenkov, I Motorykin, S Zhang, G Manfredi, D Zamarin, K Holcomb, PC Rodriguez, GA Rabinovich, JR Conejo-Garcia, LH Glimcher, JR Cubillos-Ruiz	Nature	2018
The gut microbiota in infants of obese mothers increases inflammation and susceptibility to NAFLD	TK Soderborg, SE Clark, CE Mulligan, RC Janssen, L Babcock, D Ir, B Young, N Krebs, DJ Lemas, LK Johnson, T Weir, LL Lenz, DN Frank, TL Hernandez, KA Kuhn, A D'Alessandro, LA Barbour, KC El Kasmi, JE Friedman	Nature Communications	2018
Antibacterial prenylated stilbenoids from peanut (<i>Arachis hypogaea</i>)	WJC de Bruijn, C Araya-Cloutier, J Bijlsma, A de Swart, MG Sanders, P de Waard, H Gruppen, JP Vincken	Phytochemistry Letters	2018
Identification of a metabolic disposal route for the oncometabolite S-(2-succino)cysteine in <i>Bacillus subtilis</i>	TD Niehaus, J Folz, DR McCarty, AJL Cooper, DM Amador, O Fiehn, AD Hanson	Journal of Biological Chemistry	2018
Investigation of the effects of storage and freezing on mixes of heavy-labeled metabolite and amino acid standards	R Culp-Hill, JA Reisz, KC Hansen, A D'Alessandro	Rapid Communications in Mass Spectrometry	2018
Fenofibrate prevents skeletal muscle loss in mice with lung cancer	MD Goncalves, SK Hwang, C Pauli, CJ Murphy, Z Cheng, BD Hopkins, D Wu, RM Loughran, BM Emerling, G Zhang, DT Fearon, LC Cantley	PNAS	2018



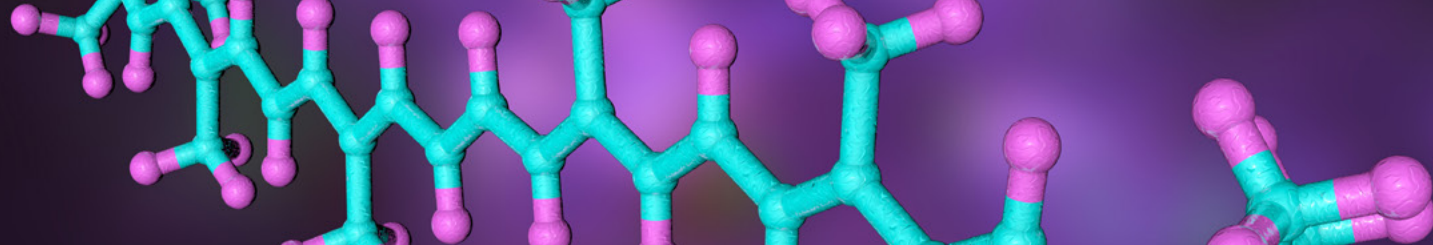
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Male lifespan extension with 17- α estradiol is linked to a sex-specific metabolomic response modulated by gonadal hormones in mice	M Garratt, KA Lagerborg, YM Tsai, A Galecki, M Jain, RA Miller	Aging Cell	2018
Adaptive remodeling of skeletal muscle energy metabolism in high-altitude hypoxia: Lessons from AltitudeOmics	AJ Chicco, CH Le, E Gnaiger, HC Dreyer, JB Muyskens, A D'Alessandro, T Nemkov, AD Hocker, JE Prenni, LM Wolfe, NM Sindt, AT Lovering, AW Subudhi, RC Roach	Journal of Biological Chemistry	2018
A Bcl-2 associated athanogene (bagA) modulates sexual development and secondary metabolism in the filamentous fungus <i>Aspergillus nidulans</i>	S Jain, P Wiemann, E Thill, B Williams, NP Keller, M Kabbage	Frontiers in Microbiology	2018
Inhibition of amino acid metabolism selectively targets human leukemia stem cells	CL Jones, BM Stevens, A D'Alessandro, JA Reisz, R Culp-Hill, T Nemkov, S Pei, N Khan, B Adane, H Ye, A Krug D Reinhold, C Smith, J DeGregori, CT Jordan	Cancer Cell	2018
Extraction and quantitation of nicotinamide adenine dinucleotide redox cofactors	W Lu, L Wang, S Hui, JD Rabinowitz	Antioxidant and Redox Signaling	2018
Mitochondrial one-carbon pathway supports cytosolic folate integrity in cancer cells	Y Zheng, TY Lin, G Lee, MN Paddock, J Momb, Z Cheng, Q Li, DL Fei, BD Stein, S Ramsamooj, G Zhang, J Blenis, LC Cantley	Cell	2018
Quantitative analysis of 4 β - and 4 α -hydroxycholesterol in human plasma and serum by UHPLC/ESI-HR-MS	H Hautajärvi, J Hukkanen, M Turpeinen, S Mattila, A Tolonen	Journal of Chromatography B	2018
Metabolic impact of red blood cell exchange with rejuvenated red blood cells in sickle cell patients	S Gehrke, N Shah, F Gamboni, R Kamyszek, AJ Srinivasan, A Gray, M Landrigan, I Welsby, A D'Alessandro	Transfusion	2019
Edible nuts deliver polyphenols and their transformation products to the large intestine: An in vitro fermentation model combining targeted/untargeted metabolomics	G Rocchetti, SR Bhumireddy, G Giuberti, R Mandal, L Lucini, DS Wishart	Food Research International	2019
Microbial transformations of organically fermented foods	R Raghuvanshi, AG Grayson, I Schena, O Amanze, K Suwintono, RA Quinn	Metabolites	2019
A comprehensive plasma metabolomics dataset for a cohort of mouse knockouts within the International Mouse Phenotyping Consortium	DK Barupal, Y Zhang, T Shen, S Fan, BS Roberts, P Fitzgerald, B Wancewicz, L Valdiviez, G Wohlgemuth, G Byram, YY Choy, B Haffner, MR Showalter, A Vaniya, CS Bloszies, JS Folz, T Kind, AM Flenniken, C McKerlie, LMJ Nutter, KC Lloyd, O Fiehn	Metabolites	2019
Predicting response to lisinopril in treating hypertension: a pilot study	BJ Sonn, JL Saben, G McWilliams, Sk Shelton, HK Flaten, A D'Allesandro, AA Monte	Metabolomics	2019
Functional analysis of isoprenoid precursors biosynthesis by quantitative metabolomics and isotopologue profiling	S Castaño-Cerezo, H Kulyk-Barbier, P Millard, JC Portais, S Heux, G Truan, F Bellvert	Metabolomics	2019
Heterogeneous pulmonary response after tracheal occlusion: clues to fetal lung growth	E Dobrinskikh, SI Al-Juboori, U Shabeka, J Reisz, C Zheng, AI Marwan	Journal of Surgical Research	2019
LC-MS-based metabolomic approach revealed the significantly different metabolic profiles of five commercial truffle species	X Li, X Zhang, L Ye, Z Kang, D Jia, L Yang, B Zhang	Frontiers in Microbiology	2019



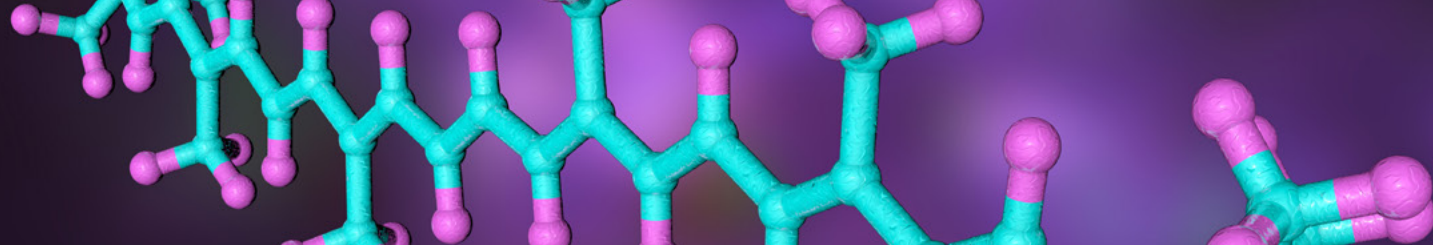
Metabolites

Title	Authors	Journal	Date
Metabolic alterations in the outer membrane vesicles of patients with Alzheimer's disease: An LC-MS/MS-based metabolomics analysis	SC Wei, W Wei, WJ Peng, Z Liu, ZY Cai, B Zhao	Current Alzheimer Research	2019
Preclinical studies on metal based anticancer drugs as enabled by integrated metallomics and metabolomics	L Galvez, M Rusz, M Schwaiger-Haber, Y El Abiead, G Hermann, Y Jungwirth, W Berger, BK Keppler, MA Jukapec, G Koellensperger	Metallomics	2019
Cysteine depletion targets leukemia stem cells through inhibition of electron transport complex II	CL Jones, BM Stevens, A D'Alessandro, E Culp-Hill, JA Reisz, S Pei, A Gustafson, N Khan, J DeGregori, DA Pollyea, CT Jordan	Blood	2019
The anti-algal mechanism of luteolin-7-O-glucuronide on <i>Phaeocystis globosa</i> by metabolomics analysis	J Zhu, Y Yang, S Duan, D Sun	International Journal of Environmental Research and Public Health	2019
Serine and 1-carbon metabolism are required for HIF-mediated protection against retinopathy of prematurity	C Singh, G Hoppe, V Tran, L McCollum, Y Bolok, W Song, A Sharma, H Brunengraber, JE Sears	Journal of Clinical Investigation	2019
Single spheroid metabolomics: optimizing sample preparation of three-dimensional multicellular tumor spheroids	M Rusz, E Rampler, BK Keppler, MA Jukapec, G Koellensperger	Metabolites	2019
Comparative metabolomics unravel the effect of magnesium oversupply on tomato fruit quality and associated plant metabolism	MC Kwon, YX Kim, S Lee, ES Jung, D Singh, J Sung, CH Lee	Metabolites	2019
Tremorgenic effects and functional metabolomics analysis of lolitrem B and its biosynthetic intermediates	P Reddy, S Rochfort, E Read, M Deseo, E Jaehne, M Van Den Buuse, K Guthridge, M Combs, G Spangenberg, J Quinn	Scientific Reports	2019
Quality variation and standardization of black pepper (<i>Piper nigrum</i>): A comparative geographical evaluation based on instrumental and metabolomics analysis	R Ahmad, N Ahmad, M Amir, F Aljishi, MH Alamer, HR Al-Shaban, ZA Alsadah, BM Alsultan, NA Aldawood, S Chathoth, SA Almofty	Biomedical Chromatography	2019
Urinary metabolic signature of primary aldosteronism: Gender and subtype-specific alterations	A Lana, K Alexander, A Castagna, A D'Alessandro, F Morandini, F Pizzolo, F Zorzi, P Mulatero, L Zolla, O Olivieri	Proteomics - Clinical Applications	2019
The metabolic time line of pancreatic cancer: Opportunities to improve early detection of adenocarcinoma	HB Moore, R Culp-Hill, JA Reisz, EE More, KC Hansen, A D'Alessandro	The American Journal of Surgery	2019
A single visualization technique for displaying multiple metabolite-phenotype associations	M Henglin, T Niiranen, JD Watrous, KA Lagerborg, J Antonelli, BL Claggett, EJ Demosthenes, B von Jeinsen, O Demler, RS Vasan, MG Larson, M Jain, S Cheng	Metabolites	2019
Characterization and tentative identification of new flunitrazepam metabolites in authentic human urine specimens using liquid chromatography-Q exactive-HF hybrid quadrupole-Orbitrap-mass spectrometry (LC-QE-HF-MS)	S Quin, G Xin, Y Wang, J Qiao, W Zhang, D Xu, Z Xu, Y Liu, Y Zhang, J Lu	Journal of Mass Spectrometry	2019
Urea cycle sustains cellular energetics upon EGFR inhibition in EGFR-mutant NSCLC	C Pham-Danis, S Gehrke, E Danis, AI Rozhok, MW Daniels, D Gao, C Collins, JT Di Paolam A D'Alessandro, J DeGregori	Molecular Cancer Research	2019
A strategy for identification and structural characterization of oplopane- and bisabolane-type sesquiterpenoids from <i>Tussilago farfara</i> L. by multiple scan modes of mass spectrometry	K Song, IJ Ha, YS Kim	Journal of Chromatography A	2019



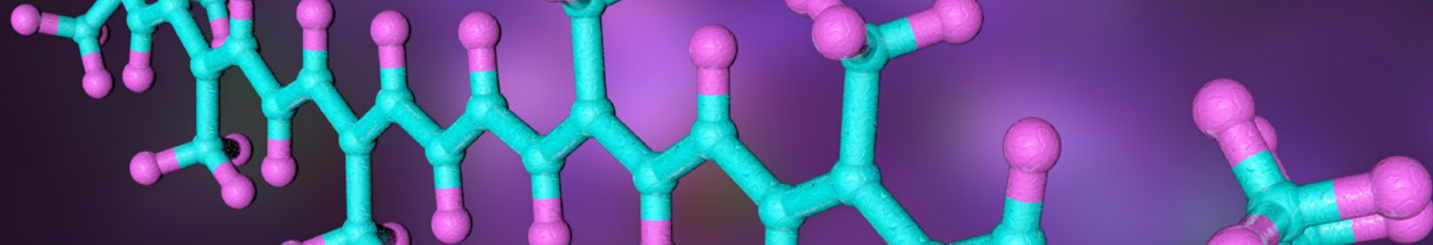
Metabolites

Title	Authors	Journal	Date
Identification of metabolites of peptide-derived drugs using an isotope-labeled reporter ion screening strategy	A Thomas, M Thevis	Clinical Chemistry and Laboratory Medicine	2019
Mapping metabolic events in the cancer cell cycle reveals arginine catabolism in the committed SG ₂ M phase	I Roci, JD Watrous, KA Lagerborg, L Lafranchi, A Lindqvist, M Jain, R Nilsson	Cell Reports	2019
Unique heterogeneous topological pattern of the metabolic landscape in rabbit fetal lungs following tracheal occlusion	Al Marwan, U Shabeka, JA Reisz, C Zheng, NJ Serkova, E Dobrinskikh	Fetal Diagnosis and Therapy	2019
Red blood cell metabolic responses to torpor and arousal in the hibernator arctic ground squirrel	S Gehrke, S Rice, D Stefanoni, RB Wilkerson, T Nemkov, JA Reisz, KC Hansen, A Lucas, P Cabrales, K Drew, A D'Alessandro	Journal of Proteome Research	2019
Metabolomic stability of exercise-induced sweat	SW Harshman, RL Pitsch, NM Schaeublin, ZK Smith, KE Strayer, MS Phelps, AV Qualley, DW Cowan, SD Rose, ML O'Connor, JJ Eckerle, T Das, AK Barbey, AJ Strang, JA Martin	Journal of Chromatography B	2019
Differential effects of coral-giant clam assemblages on biofouling formation	I Guibert, I Bonnard, X Pochon, M Zubia, C Sidobre, G Lecellier, V Berteaux-Lecellier	Scientific Reports	2019
Parabiosis incompletely reverses aging-induced metabolic changes and oxidant stress in mouse red blood cells	EJ Morrison, DP Champagne, M Dzieciatkowska, T Nemkov, JC Nimring, KC Hansen, F Guan, DM Huffman, L Santambrogio, A D'Alessandro	Nutrients	2019
Microbial bile acid metabolites modulate gut ROR γ ⁺ regulatory T cell homeostasis	X Song, X Sun, SF Oh, M Wu, Y Zhang, W Zheng, N Geva-Zatorsky, R Jupp, D Mathis, C Benoist, DL Kasper	Nature	2019
Metabolic profiling using stable isotope tracing reveals distinct patterns of glucose utilization by physiologically activated CD8 ⁺ T cells	EH Ma, MJ Verway, RM Johnson, DG Roy, M Steadman, S Hayes, KS Williams, RD Sheldon, B Samborska, PA Kosinski, H Kim, T Griss, B Faubert, SA Condotta, CM Krawczyk, RJ DeBarardinis, KM Stewart, MJ Richer, V Chubukov, TP Roddy, RG Jones	Immunity	2019
Mitochondrial stress causes neuronal dysfunction via an ATF4-dependent increase in L-2-hydroxyglutarate	RJ Hunt, L Granat, GS McElroy, R Ranganathan, NS Chandel, JM Bateman	Journal of Cell Biology	2019
Proposing a validation scheme for ¹³ C metabolite tracer studies in high-resolution mass spectrometry	M Schwaiger-Haber, G Hermann, YE Abiead, E Rampler, S Wernisch, K Sas, S Pennathur, G Koellensperger	Analytical and Bioanalytical Chemistry	2019
The plasma metabolome as a predictor of biological aging in humans	LC Johnson, K Parker, BF Aguirre, TG Nemkov, A D'Alessandro, SA Johnson, DR Seals, CR Martens	Geroscience	2019
Selective organ ischaemia/reperfusion identifies liver as the key driver of the post-injury plasma metabolome derangements	N Clendenen, GR Nunns, EE Moore, E Gonzalez, M Chapman, JA Reisz, E Peltz, M Fragoso, T Nemkov, MJ Wither, A Sauaia, CC Silliman, K Hansen, A Banerjee, A D'Alessandro, HB Moore	Blood Transfusion	2019
Merged targeted quantification and untargeted profiling for comprehensive assessment of acylcarnitine and amino acid metabolism	T Teav, H Gallart-Ayala, V van der Velpen, F Mehl, H Henry, J Ivanisevic	Analytical Chemistry	2019
Transfusional iron overload and intravenous iron infusions modify the mouse gut microbiota similarly to dietary iron	F La Carpia, B S Wojczyk, MK Annavajhala, A Rebbaa, R Culp-Hill, A D'Alessandro, DE Freedberg, AC Uhlemann, EA Hod	Biofilms and Microbiomes	2019



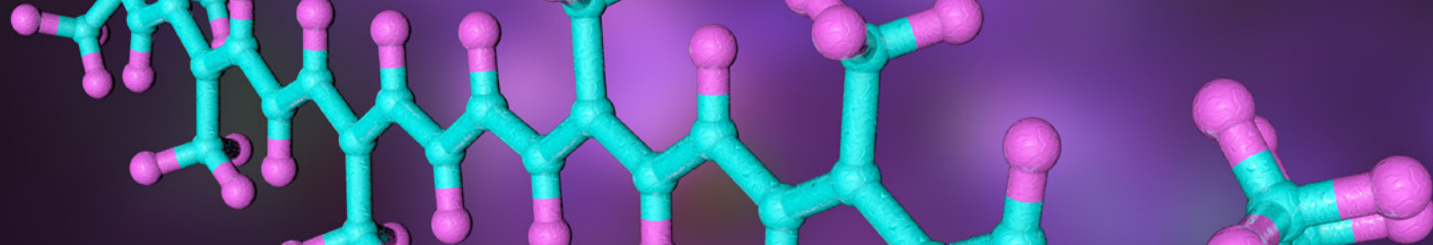
Metabolites

Title	Authors	Journal	Date
Loss of the glucocorticoid receptor in zebrafish improves muscle glucose availability and increases growth	E Fought, MM Vijayan	American Journal of Physiology Endocrinology Metabolism	2019
Metabolic analysis reveals evidence for branched chain amino acid catabolism crosstalk and the potential for improved treatment of organic acidurias	S McCally, D Pirman, M Clasquin, K Johnson, S Jin, J Vockley	Molecular Genetics and Metabolism	2019
Comparison of data acquisition modes with Orbitrap high-resolution mass spectrometry for targeted and non-targeted residue screening in aquacultured eel	IL Wu, SB Turnipseed, JM Storey, WC Andersen, MR Madson	Rapid Communications in Mass Spectrometry	2019
Simultaneous determination of urinary 31 metabolites of VOCs, 8-hydroxy-2'-deoxyguanosine, and trans-3 -hydroxycotinine by UPLC-MS/MS: ¹³ C- and ¹⁵ N-labeled isotoped internal standards are more effective on reduction of matrix effect	H Kuang, Y Li, W Jiang, P Wu, J Tan, H Zhang, O Pang, S Ma, T An, R Fan	Analytical and Bioanalytical Chemistry	2019
A triple quadrupole and a hybrid quadrupole Orbitrap mass spectrometer in comparison for polyphenol quantitation	C Cavaliere, M Antonelli, AL Capriotti, G La Barbera, CM Montone, S Piovesana, Aldo Laganà	Journal of Agricultural and Food Chemistry	2019
Analysis of the indole diterpene gene cluster for biosynthesis of the epoxy-janthitrems in <i>Epichloë endophytes</i>	EJ Ludlow, S Vassiliadis, PN Ekanayake, IK Hettiarachchige, P Reddy, TI Sawbridge, SJ Rochfort, GC Spangenberg, KM Guthridge	Microorganisms	2019
Pharmacokinetic profile of amoxicillin and its glucuronide-like metabolite when administered subcutaneously to koalas (<i>Phascolarctos cinereus</i>)	B Kimble, L Vogelnest, S Gharibi, AM Izes, M Govendir	Journal of Veterinary Pharmacology and Therapeutics	2019
Effects of aged stored autologous red blood cells on human plasma metabolome	A D'Alessandro, JA Reisz, Y Zhang, S Gehrke, K Alexander, T Kaniias, DJ Triulzi, C Donadee, S Barge, J Badlam, S Jain, MG Risbano, MT Gladwin	Blood Advances	2019
Comparison of the acute postprandial circulating B-vitamin and vitamer responses to single breakfast meals in young and older individuals: Preliminary secondary outcomes of a randomized controlled trial	P Sharma, N Gillies, S Pundir, CA Pileggi, JF Markworth, EB Thorstensen, D Cameron-Smith, AM Milan	Nutrients	2019
Biotransformation of myricetin: A novel metabolic pathway to produce aminated products in mice	S Zhang, R Wang, Y Zhao, FS Tareq, S Sang	Molecular Nutrition and Food Research	2019
Myc-mediated transcriptional regulation of the mitochondrial chaperone TRAP1 controls primary and metastatic tumor growth	E Agarwal, BJ Altman, JH Seo, JC Ghosh, AV Kossenkov, HY Tang, SR Krishn, LR Languino, DI Gabilovich, DW Speicher, CV Dang, DC Altieri	Journal of Biological Chemistry	2019
Disrupting mitochondrial pyruvate uptake directs glutamine into the TCA cycle away from glutathione synthesis and impairs hepatocellular tumorigenesis	SC Tompkins, RD Sheldon, RJ Rauckhorst, MF Noterman, SR Solst, JL Buchanan, KA Mapuskar, AD Pawa, LR Gray, L Oonthonpan, A Sharma, DA Scerbo, AJ Dupuy, DR Spitz, EB Taylor	Cell Reports	2019
Increase in post-reperfusion sensitivity to tissue plasminogen activator-mediated fibrinolysis during liver transplantation is associated with abnormal metabolic changes and increased blood product utilisation	HB Moore, A D'Alessandro, EE Moore, M Whither, PJ Lawson, BR Huebner, K Hansen, R Choudhury, TL Nydam	Blood Transfusion	2019



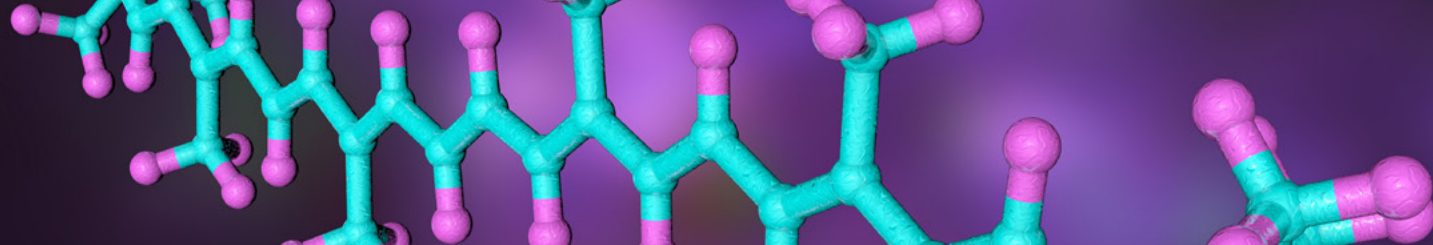
Metabolites

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Skeletal muscle amino acid uptake is lower and alanine production is greater in late gestation intrauterine growth-restricted fetal sheep hindlimb	EI Chang, SR Wesolowski, EA Gilje, PR Baker II, JA Reisz, A D'Alessandro, WW Hay Jr, PJ Rozance, LD Brown	American Journal of Physiology: Regulatory, Integrative, and Comparative Physiology	2019
Pharmacokinetics of hydroxyzine and cetirizine following oral administration of hydroxyzine to exercised Thoroughbred horses	JHK Knych, D Weiner, S Steinmetz, K Flynn, DS McKemie	Journal of Veterinary Pharmacology and Therapeutics	2019
Integrated multiomic analysis reveals comprehensive tumour heterogeneity and novel immunophenotypic classification in hepatocellular carcinomas	Q Zhang, Y Lou, J Yang, J Wang, J Feng, Y Zhao, L Wang, X Huang, Q Fu, M Ye, X Zhang, Y Chen, C Ma, H Ge, J Wang, J Wu, T Wei, Q Chen, J Wu, C Yu, C Yu, Y Xiao, X Feng, G Guo, Y Liang, X Bai	Gut	2019
Reactive metabolite production is a targetable liability of glycolytic metabolism in lung cancer	A Luengo, KL Abbott, SM Davidson, AM Hosios, B Faubert, SH Chan, E Freinkman, LG Zacharias, TP Mathews, CB Clish, RJ DeBerardinis, CA Lewis, MGV Heiden	Nature Communications	2019
Acyl ethanolamides in Diabetes and Diabetic Nephropathy: Novel targets from untargeted plasma metabolomic profiles of South Asian Indian men	S Devi, B Nongkhaw, M Limesh, RM Pasanna, T Thomas, R Kuriyan, AV Kurpad, A Mukhopadhyay	Scientific Reports	2019
Beneficial effects of kaempferol after developmental traumatic brain injury is through protection of mitochondrial function, oxidative metabolism, and neural viability	J Chitturi, V Santhakumar, SS Kannurpatti	Journal of Neurotrauma	2019
In vivo imaging of mitochondrial membrane potential in non-small-cell lung cancer	M Momcilovic, A Jones, ST Bailey, CM Waldmann, R Li, JT Lee, G Abdelhady, A Gomez, T Holloway, E Schmid D Stout, MC Fishbein, L Stiles, DV Dabir, SM Dubinett, H Christofk, O Shirihai, CM Koehler, S Sadeghi, DB Shackelford	Nature	2019
SPARC dependent collagen deposition and gemcitabine delivery in a genetically engineered mouse model of pancreas cancer	I Ramu, SM Buchholz, MS Patzak, RG Goetze, SK Singh, FM Richards, DI Jodrell, B Sipos, P Ströbel, V Ellenrieder, E Hessmann, A Neesse	EBioMedicine	2019
Consolidated biochemical profile of subacute stage traumatic brain injury in early development	J Chitturi, Y Li, V Santhakumar, SS Kannurpatti	Frontiers in Neuroscience	2019
Rac-mediated macropinocytosis of extracellular protein promotes glucose independence in non-small cell lung cancer	C Hodakoski, BD Hopkins, G Zhang, T Su, Z Cheng, R Morris, KY Rhee, MD Goncalves, LW Cantley	Cancers	2019
Intense light-mediated circadian cardioprotection via transcriptional reprogramming of the endothelium	Y Oyama, CM Bartman, S Bonney, JS Lee, LA Walker, J Han, CH Borchers, PM Buttrick, CM Aherne, N Clendenen, SP Colgan, T Eckle	Cell Reports	2019
EGFR-phosphorylated platelet isoform of phosphofructokinase 1 promotes PI3K activation	JH Lee, R Liu, J Li, Y Wang, L Tan, XJ Li, X Qian, C Zhang, Y Xia, D Xu, W Guo, Z Ding, L Du, Y Zheng, Q Chen, PL Lorenzi, GB Mills, T Jiang, Z Lu	Molecular Cell Press	2019
A simple LC-MS method for the quantitation of alkaloids in endophyte-infected perennial ryegrass	S Vassiliadis, AC Elkins, P Reddy, KM Guthridge, GC Spangenberg, SJ Rochfort	Toxins	2019



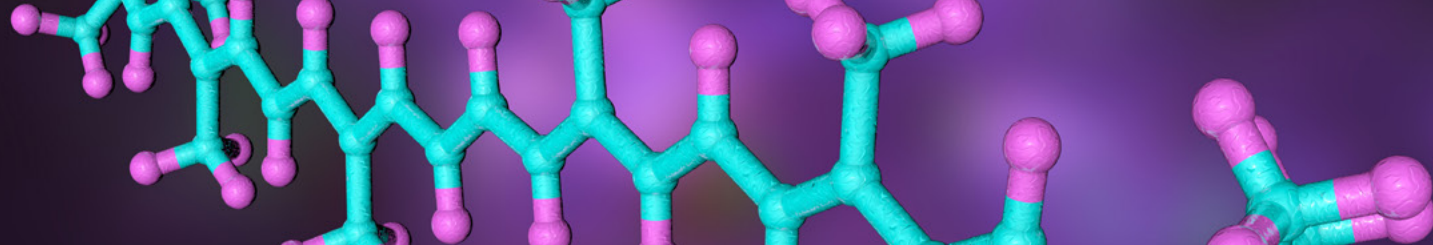
Metabolites

Title	Authors	Journal	Date
Effect of fermented corn-soybean meal on serum immunity, the expression of genes related to gut immunity, gut microbiota, and bacterial metabolites in grower-finisher pigs	J Lu, X Zhang, Y Liu, H Cao, Q Han, B Xie, L Fan, X Li, J Hu, G Yang, X Shi	Frontiers in Microbiology	2019
Metabolic profiling of dialysate at sensitized acupoints in knee osteoarthritis patients	S Li, XN Chai, CY Zou, P Lv, Y Tang, HJ Tan, LZ Liu, HY Yin, SG Yu	Medicine	2019
Ferredoxin5 deletion affects metabolism of algae during the different phases of sulfur deprivation	V Subramanian, MSA Wecker, A Gerritsen, M Boehm, W Xiong, B Wachter, A Dubini, D González-Ballester, RV Antonio, ML Ghirardi	Plant Physiology	2019
Type I interferon signaling disrupts the hepatic urea cycle and alters systemic metabolism to suppress T cell function	A Lercher, A Bhattacharya, AM Popa, M Caldera, MF Schlapansky, H Baazim, B Agerer, B Gürtl, L Kosack, P Májek, JS Brunner, D Vitko, T Pinter, JW Genger, A Orlova, K Pikor, D Reil, M Ozsvár-Kozma, U Kalinke, B Ludewig, R Moriggl, KL Bennett, J Menche, PN Cheng, G Schabbauer, M Trauner, K Klavins, A Bergthaler	Immunity	2019
Identification of potential biomarkers for soybean meal-induced enteritis in juvenile pearl gentian grouper, <i>Epinephelus lanceolatus</i> ♂ × <i>Epinephelus fuscoguttatus</i> ♀	W Zhang, B Tan, G Ye, J Wang, X Dong, Q Yang, S Chi, H Liu, S Zhang, H Zhang	Aquaculture	2019
Coordinate regulation of cholesterol and bile acid metabolism by the clock modifier nobiletin in metabolically challenged old mice	K Nohara, T Nemkov, A D'Alessandro, SH Yoo, Z Chen	International Journal of Molecular Sciences	2019
Metabonomic variation of exopolysaccharide from <i>Rhizopus nigricans</i> on AOM/DSS-induced colorectal cancer in mice	Y Lu, J Wang, Y Ji, K Chen	OncoTargets and Therapy	2019
Antibacterial isoquinoline alkaloids from the fungus <i>Penicillium spathulatum</i> Em19	C Nord, JJ Levenfors, J Bjerketorp, C Sahlberg, B Guss, B Öberg, A Broberg	Molecules	2019
Adult stem cell deficits drive <i>Slc29a3</i> disorders in mice	S Nair, AM Strohecker, AK Persaud, B Bissa, S Muruganandan, C McElroy, R Pathek, M Williams, R Raj, A Kaddoumi, A Sparreboom, AM Beedle, R Govindarajan	Nature Communications	2019
The pentose phosphate pathway of cellulolytic clostridia relies on 6-phosphofructokinase instead of transaldolase	JG Koendjibharie, S Hon, M Pabst, R Hooftman, DM Stevenson, J Cui, D Amador-Noguez, LR Lynd, DG Olson, R van Kranenburg	The Journal of Biological Chemistry	2019
Vancomycin relieves mycophenolate mofetil-induced gastrointestinal toxicity by eliminating gut bacterial β -glucuronidase activity	MR Taylor, KL Flannigan, H Rahim, A Mohamud, IA Lewis, SA Hirota, SC Greenway	Science Advances	2019
Biliopancreatic diversion induces greater metabolic improvement than Roux-en-Y gastric bypass	LA Harris, BD Kayser, C Cefalo, L Marini, JD Watrous, J Ding, M Jain, JG McDonald, BM Thompson, E Fabbrini, JC Eagon, BW Patterson, B Mittendorfer, G Mingrone, S Klein	Cell Metabolism	2019
Bacterial analogs of plant tetrahydropyridine alkaloids mediate microbial interactions in a rhizosphere model system	GL Lozano, HB Park, JI Bravo, EA Armstrong, JM Denu, EV Stabb, NA Broderick, JM Crawford, J Handelsman	Applied and Environmental Biology	2019



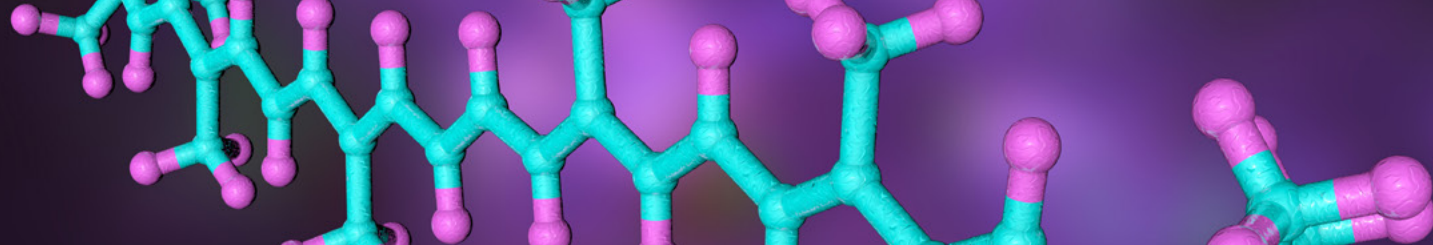
Metabolites

Title	Authors	Journal	Date
CD9 identifies pancreatic cancer stem cells and modulates glutamine metabolism to fuel tumour growth	VMY Wang, RMM Ferreira, J Almagro, T Evan, N Legrave, MZ Thin, D Frith, J Carvalho, DJ Barry, AP Snijders, E Herbert, EL Nye, JI MacRae, A Behrens	Nature Cell Biology	2019
p53 represses the mevalonate pathway to mediate tumor suppression	SH Moon, CH Huang, SL Houlihan, K Regunath, WA Freed-Pastor, JP Morris IV, DF Tschaharganeh, ER Kastenhuber, AM Barsotti, R Culp-Hill, W Xue, YJ Ho, T Baslan, X Li, A Mayle, E de Stanchina, L Zender, DR Tong, A D'Alessandro, SW Lowe, C Prives	Cell	2019
Determination of online quenching efficiency for an automated cellular microfluidic metabolomic platform using mass spectrometry based ATP degradation analysis	LA Filla, KL Sanders, JB Coulton, RT Filla, JL Edwards	Analytical and Bioanalytical Chemistry	2019
Loss of genomic integrity induced by lysosphingolipid imbalance drives ageing in the heart	G Ahuja, D Bartsch, W Yao, S Geissen, S Frank, A Aguirre, N Russ, JE Messling, J Dodzian, KA Lager, NE Vargas, JS Muck, S Brodesser, S Baldus, A Sachinidis, J Hescheler, C Dieterich, A Trifunovic, A Papantonis, M Petrascheck, A Klinke, M Jain, DR Valenzano, L Kurian	Embryo Reports	2019
Regulation of folate and methionine metabolism by multisite phosphorylation of human methylenetetrahydrofolate reductase	Y Zheng, S Ramsamooj, Q Li, JL Johnson, TM Yaron, K Sharra, LC Cantley	Scientific Reports	2019
Functional characterization of the cytochrome P450 monooxygenase CYP71AU87 indicates a role in marrubiin biosynthesis in the medicinal plant Marrubium vulgare	PS Karunanithi, P Dhanota, JB Addison, S Tong, O Fiehn, P Zerbe	BMC Plant Biology	2019
GPD1 specifically marks dormant glioma stem cells with a distinct metabolic profile	P Rusu, C Shao, A Neuerburg, AA Acikgöz, Y Wu, P Zou, P Phapale, TS Shankar, K Döring, S Dettling, H Körkel-Qu, G Bekki, B Costa, T Guo, O Friesen, M Schlotter, M Heikenwalder, DF Tschaharganeh, B Bukau, G Kramer, P Angel, C Herold-Mende, B Radlwimmer, HK Liu	Cell Stem Cell	2019
Analysis of amino acids in human tears by hydrophilic interaction liquid chromatography and quadrupole Orbitrap mass spectrometry	CX Du, Z Huang	RSC Advances	2019
The carbamate aldicarb altered the gut microbiome, metabolome, and lipidome of C57BL/6J mice	B Gao, L Chi, P Tu, N Gao, K Lu	Chemical Research in Toxicology	2019
Profiling glucosinolate metabolites in human urine and plasma after broccoli consumption using non-targeted and targeted metabolomic analyses	J Sun, CS Charron, JA Novotny, B Peng, L Yu, P Chen	Food Chemistry	2020
Lipid-lowering effects and intestinal transport of polyphenol extract from digested buckwheat in Caco-2/HepG2 coculture models	Y Yao, F Xu, X Ju, Z Li, L Wang	Journal of Agricultural and Food Chemistry	2020
Dietary genistein reduces methylglyoxal and advanced glycation end product accumulation in obese mice treated with high-fat diet	Y Zhao, Y Zhu, P Wang, S Sang	Journal of Agricultural and Food Chemistry	2020
Pectin and inulin stimulated the mucus formation at a similar level: An omics-based comparative analysis	J Xie, R Yu, J Qi, G Zhang, X Peng, J Luo	Journal of Food Science	2020



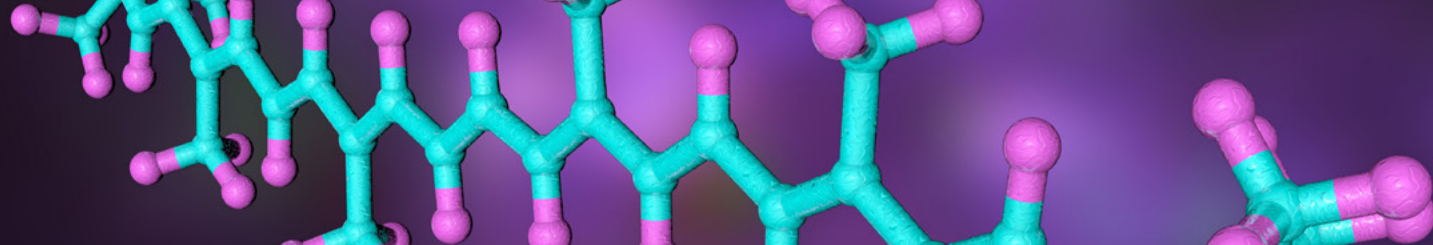
Metabolites

Title	Authors	Journal	Date
Integration of transcriptomics and metabolomics profiling reveals the metabolic pathways affected in dictamnine-induced hepatotoxicity in mice	ZQ Li, LL Wang, J Zhou, X Zheng, Y Jiang, P Li, HJ Li	Journal of Proteomics	2020
Heterogeneous response in rabbit fetal diaphragmatic hernia lungs after tracheal occlusion	E Dobrinskikh, SI Al-Juboori, M Oria, J Reisz, C Zheng, JL Peiro, Al Marwan	Journal of Surgical Research	2020
Large-scale profiling of cellular metabolic activities using deep ¹³C labeling medium	N Grankvist, JD Watrous, M Jain, R Nilsson	Methods in Molecular Biology	2020
Nicotine exposure increases markers of oxidant stress in stored red blood cells from healthy donor volunteers	D Stefanoni, X Fu, JA Reisz, T Kaniyas, T Nemkov, GP Page, L Dumont, N Roubinian, M Stone, S Kleinman, M Busch, JC Zimring, A D'Alessandro	Transfusion	2020
Metabolomics of endurance capacity in World Tour professional cyclists	I San-Millan, D Stefanoni, JL Martinez, KC Hansem, A D'Alessandro, T Nemkov	Frontiers in Physiology	2020
Toxicology of paraquat and pharmacology of the protective effect of 5-hydroxy-1-methylhydantoin on lung injury caused by paraquat based on metabolomics	L Gao, H Yuan, E Xu, J Liu	Scientific Reports	2020
Metabolic phenotypes of standard and cold-stored platelets	A D'Alessandro, KA Thomas, D Stefanoni, F Gamboni, SM Shea, JA Reisz, PC Spinella	Transfusion	2020
Integration of transcriptomic and metabolomic data reveals metabolic pathway alteration in mouse spermatogonia with the effect of copper exposure	S Lin, N Qiao, H Chen, Z Tang, Q Han, K Mehmood, SA Fazlani, S Hameed, Y Li, H Zhang	Chemosphere	2020
Integrative transcriptomics and metabolomics data exploring the effect of chitosan on postharvest grape resistance to Botrytis cinerea	Z Zhang, P Zhao, P Zhang, L Su, H Jia, Z Wei, J Fang, H Jia	Postharvest Biology and Technology	2020
Metabolomics response for drought stress tolerance in Chinese wheat genotypes (Triticum aestivum)	Z Guo, Z Xin, T Yang, X Ma, Y Zhang, Z Wang, Y Ren, T Lin	Plants	2020
Integrating RNA-sequencing and untargeted LC-MS metabolomics to evaluate the effect of lysine deficiency on hepatic functions in holstein calves	F Kong, Y Bi, B Wang, K Cui, T Fu, Q Diao, Y Tu	Amino Acids	2020
Drosha-independent miR-6778-5p strengthens gastric cancer stem cell stemness via regulation of cytosolic one-carbon folate metabolism	M Zhao, Y Hou, Y Du, L Yang, Y Qin, M Peng, S Liu, X Wan, Y Qiao, H Zeng, Z Cui, Y Teng, M Liu	Cancer Letters	2020
Improved annotation of untargeted metabolomics data through buffer modifications that shift adduct mass and intensity	W Lu, X Xing, L Wang, L Chen, S Zhang, MR McReynolds, JD Rabinowitz	Analytical Chemistry	2020
In-source CID ramping and covariant ion analysis of hydrophilic interaction chromatography metabolomics	X Su, E Chiles, S Maimouni, FE Wondisford, WX Zong, C Song	Analytical Chemistry	2020
Stable isotope metabolomics of pulmonary artery smooth muscle and endothelial cells in pulmonary hypertension and with TGF-beta treatment	D Hernandez-Saavedra, L Sanders, s Freeman, JA Reisz, MH Lee, C Mickael, R Kumar, B Kassa, S Gu, A D'Alessandro, KR Stenmark, RM Tuder, BB Graham	Scientific Reports	2020
Hypoxic storage of red blood cells improves metabolism and post-transfusion recovery	A D'Alessandro, T Yoshida, S Nestheide, T Nemkov, S Stocker, D Stefanoni, F Mohmoud, N Rugg, A Dunham, JA Cancelas	Transfusion	2020



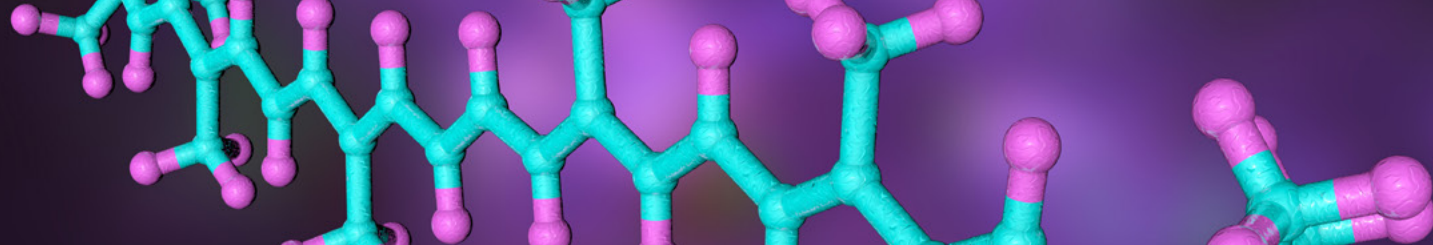
Metabolites

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Stored RBC metabolism as a function of caffeine levels	A D'Alessandro, X Fu, JA Reisz, T Kaniyas, GP Page, M Stone, S Kleinman, JC Zimring, M Busch	Transfusion Medicine	2020
A solution to antifolate resistance in group B streptococcus: Untargeted metabolomics identifies human milk oligosaccharide-induced perturbations that result in potentiation of trimethoprim	SA Chambers, RE Moore, KM Craft, HC Thomas, R Das, SD Manning, SG Codreanu, SD Sherrod, DM Aronoff, JA McLean, JA Gaddy, SD Townsend	Therapeutics and Prevention	2020
Development of a plasma pseudotargeted metabolomics method based on ultra-high-performance liquid chromatography–mass spectrometry	F Zheng, X Zhao, Z Zeng, L Wang, W Lv, Q Wang, G Xu	Nature Protocols	2020
Spatial metabolomics of in situ host–microbe interactions at the micrometre scale	B Geier, EM Sogin, D Michellod, M Janda, M Kompauer, B Spengler, N Dubilier, M Liebeke	Nature Microbiology	2020
Identification of a Small-Molecule Inhibitor That Disrupts the SIX1/EYA2 Complex, EMT, and Metastasis	H Zhou, MA Blevins, JY Hsu, D Kong, MD Galbraith, A Goodspeed, R Cul-Hill, MUJ Oliphant, D Ramirez, L Zhang, J Trinidad-Pineiro, LM Griner, R King, E Barnaeva, X Hu, NT Southall, M Ferrer, DL Gustafson, DP Regan, A D'Alessandro, JC Costello, S Patnaik, J Marugan, R Zhao, HL Ford	Cancer Research	2020
Metabolic reprogramming of mouse bone marrow derived macrophages following erythrophagocytosis	A Catala, LA Youssef, JA Reisz, M Dzieciatkowska, NE Powers, C Marchetti, M Karafin, JC Zimring, KE Hudson, KC Hansen, SL Spitalnik, A D'Alessandro	Frontiers in Physiology	2020
Rapid identification of MDMB-CHMINACA metabolites using zebrafish and human liver microsomes as the biotransformation system by LC-QE-HF-MS	Q Xu, Y Dai, W Zhang, J Wang, Y Wang, Y Zhang, Guobin-xin, Q Zhao, X Li	Journal of Analytical Toxicology	2020
Stevia metabolites in biosamples ranging from fetal life to adulthood	B Halasa, P Walter, H Cai, M Gonzales, M Walter, E Shouppe, P Kosa, B Bielekova, L Hui, K Rother	Current Developments in Nutrition	2020
In vitro hepatic metabolism of mefloquine using microsomes from cats, dogs and the common brush-tailed possum (<i>Trichosurus vulpecula</i>)	AM Izes, B Kimble, JM Norris, M Govendir	PLOS One	2020
Biosynthesis-inspired mining and identification of untapped alkaloids in <i>Camptotheca acuminata</i> for enzyme discovery using ultra-high performance liquid chromatography coupled with quadrupole-time of flight-mass spectrometry	X Pu, CR Zhang, HC Gao, YH Gao, L Huang, L Zhu, Y Rao, S Zhang, YY Jiang, L Zhang, QM Huang	Journal of Chromatography A	2020
Glucose metabolic characterization of human aqueous humor in relation to wet age-related macular degeneration	G Han, P Wei, M He, H Teng	Investigative Ophthalmology & Visual Science	2020
Synthesis of cyclophosphamide metabolites by a peroxygenase from <i>Marasmius rotula</i> for toxicological studies on human cancer cells	S Steinbrecht, J Kiebist, R König, M Thiessen, KU Schmidtke, S Kammerer, JH Küpper, K Scheibner	AMB Express	2020
Immune-responsive gene 1/itaconate activates nuclear factor erythroid 2–related factor 2 in hepatocytes to protect against liver ischemia–reperfusion injury	Z Yi, M Deng, MJ Scott, G Fu, PA Loughran, Z Lei, S Li, P Sun, C Yang, W Li, H Xu, F Huang, TR Billiar	Hepatology	2020



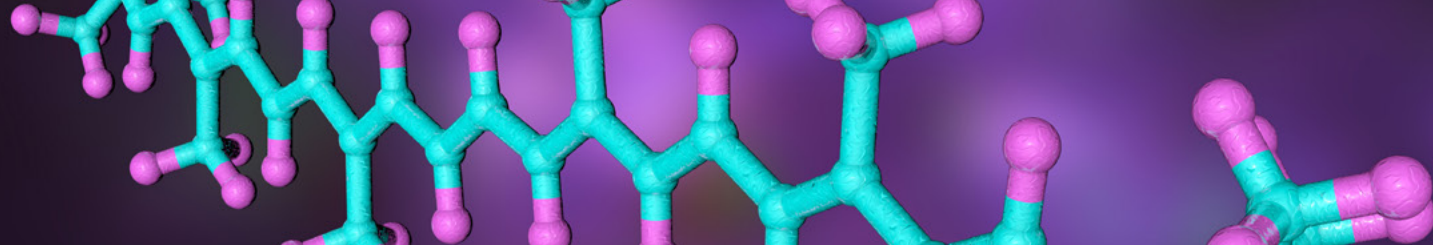
Metabolites

Title	Authors	Journal	Date
Intrinsic clearance rate of O-desmethyltramadol (M1) by glucuronide conjugation and phase I metabolism by feline, canine and common brush-tailed possum microsomes	AM Izes, B Kimble, Merran Govendir	Xenobiotica	2020
Local phenomena shape backyard soil metabolite composition	TD Nguyen, M Lesani, I Forrest, Y Lan, DA Dean, QMR Gibaut, Y Guo, E Hossain, M Olvera, H Panlilio, AR Parab, C Wu, JA Bernatchez, RH Cichewicz, LI McCall	Metabolites	2020
Antibacterial pyrrolidinyl and piperidinyl substituted 2,4-diacetylphloroglucinols from <i>Pseudomonas protegens</i> UP46	JJ Levenfors, C Nord, J Bjerketorp, J Ståhlberg, R Larsson, B Guss, B Öberg, A Broberg	The Journal of Antibiotics	2020
Mass spectrometry-based stable-isotope tracing uncovers metabolic alterations in pyruvate kinase-deficient <i>Aedes aegypti</i> mosquitoes	N Petchampai, J Isoe, TD Horvath, S Dagan, L Tan, PL Lorenzi, DH Hawke, PY Scaraffia	Insect Biochemistry and Molecular Biology	2020
Maternal erythrocyte ENT1-mediated AMPK activation counteracts placental hypoxia and supports fetal growth	S Sayama, A Song, BC Brown, J Couturier, X Cai, P Xu, C Chen, Y Zheng, T Iriyama, B Sibai, M Longo, RE Kellems, A D'Alessandro, Y Xia	JCI Insight	2020
IL-37 ameliorating allergic inflammation in atopic dermatitis through regulating microbiota and AMPK-mTOR signaling pathway-modulated autophagy mechanism	T Hou, X Sun, J Zhu, KL Hon, P Jiang, IMT Chu, MSM Tsang, CWK Lam, H Zeng, CK Wong	Frontiers in Immunology	2020
Quantitative analysis of metabolites in glucose metabolism in the aqueous humor of patients with central retinal vein occlusion	P Wei, M He, H Teng, G Han	Experimental Eye Research	2020
Simultaneous production of psilocybin and a cocktail of β -carboline monoamine oxidase inhibitors in "magic" mushrooms	F Blei, S Dorner, J Fricke, F Baldeweg, F Trottmann, A Komor, F Meyer, C Hertweck, D Hoffmeister	Chemistry	2020
Optimized serial expansion of human induced pluripotent stem cells using low-density inoculation to generate clinically relevant quantities in vertical-wheel bioreactors	BS Borys, T So, J Colter, T Dang, EL Roberts, T Revay, L Larijani, R Krawetz, I Lewis, B Argiropoulos, DE Rancourt, Jung, Y Hashimura, B Lee, MS Kallos	Stem Cells Translational Medicine	2020
A new software-assisted analytical workflow based on high-resolution mass spectrometry for the systematic study of phenolic compounds in complex matrices	A Cerrato, G Cannazza, AL Capriotti,	Talanta	2020
Paroxetine administration affects microbiota and bile acid levels in mice	F Dethloff, F Vargas, E Elijah, R Quinn, DI Park, DP Herzog, MB Müller, EC Gentry, R Knight, A Gonzalez, PC Dorrestein, CW Turck	Frontiers in Psychiatry	2020
Decoding the metabolic landscape of pathophysiological stress-induced cell death in anucleate red blood cells	T Nemkov, SM Qadri, WP Sheffield, A D'Alessandro	Blood Transfusion	2020
Gut microbiome and serum metabolome analyses identify unsaturated fatty acids and butanoate metabolism induced by gut microbiota in patients with chronic spontaneous urticaria	D Wang, S Guo, H He, L Gong, H Cui	Frontiers in Cellular and Infection Microbiology	2020
Levodocarnitine does not impair chemotherapy cytotoxicity against acute lymphoblastic leukemia	JL Sea, E Orgel, T Chen, RL Paszkiewicz, AS Krall, MJ Oberley, L Stiles, SD Mittelman	Leukemia and Lymphoma	2020



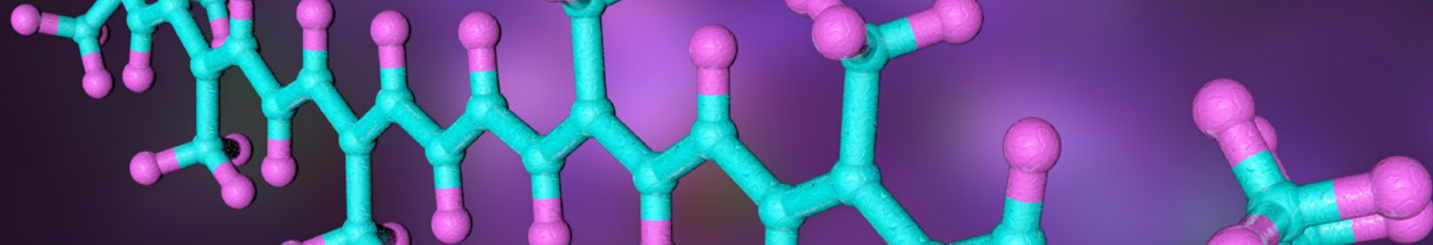
Metabolites

Title	Authors	Journal	Date
Identification of trenbolone metabolites using hydrogen isotope ratio mass spectrometry and liquid chromatography/high accuracy/high resolution mass spectrometry for doping control analysis	M Putz, T Piper, M Thevis	Frontiers in Chemistry	2020
A new phenolic compound from <i>Phedimus middendorffianus</i> with antiproliferative activity	J Lee, S Woo, SH Sung, H Yang	Natural Product Research	2020
Facile preparation of a magnetic porous organic frameworks for highly sensitive determination of eight alkaloids in urine samples based UHPLC-MS/MS	K Hu, T Pang, Y Shi, J Cheng, Y Huang	Microchemical Journal	2020
Gut microbiota compositional profile and serum metabolic phenotype in patients with primary open-angle glaucoma	H Gong, S Zhang, Q Li, C Zuo, X Gao, B Zheng, M Lin	Experimental Eye Research	2020
Germinal center B cells selectively oxidize fatty acids for energy while conducting minimal glycolysis	FJ Weisel, SJ Mullet, RB Elsner, AV Menk, N Trivedi, W Luo, D Wikenheiser, WF Hawse, M Chikina, S Smita, LJ Conter, SM Joachim, SG Wendell, MJ Jurczak, TH Winkler, GM Delgoffe, MJ Shlomchik	Nature Immunology	2020
A role for tryptophan-2,3-dioxygenase in CD8 T cell suppression and evidence of tryptophan catabolism in breast cancer patient plasma	LI Greene, TC Bruno, JL Christenson, A D'Alessandro, R Culp-Hill, K Torkko, VF Borges, JE Slansky, JK Richer	Molecular Cancer Research	2020
Leucinoastatins from <i>Ophiocordyceps</i> spp. and <i>Purpureocillium</i> spp. demonstrate selective antiproliferative effects in cells representing the luminal androgen receptor subtype of triple negative breast cancer	YS Kil, AL Risinger, CL Petersen, SL Mooberry, RH Cichewicz	Journal of Natural Products	2020
Strain-dependent inhibition of <i>Clostridioides difficile</i> by commensal clostridia carrying the bile acid-inducible (bai) operon	AD Reed, NA Stewart, R Barrangou, CM Theriot	Journal of Bacteriology	2020
Lipokine 5-PAHSA is regulated by adipose triglyceride lipase and primes adipocytes for de novo lipogenesis in mice	V Paluchova, M Oseeva, M Brezinova, T Cajka, K Bardova, K Adamcova, P Zacek, K Brejchova, L Balas, H Chodounska, E Kidova, R Schreiber, R Zechner, T Durand, M Rossmeisl, NA Abumrad, J Kopecky, O Kuda	Diabetes	2020
Reversal of triple-negative breast cancer EMT by miR-200c decreases tryptophan catabolism and a program of immune-suppression	TJ Rogers, JL Christenson, LI Greene, KI O'Neill, MM Williams, MA Gordon, T Nemkov, A D'Alessandro, GD Degala, J Shin, AC Tan, DM Cittelly, JR Lambert, JK Richer	Molecular Cancer Research	2020
Data highlighting phenotypic diversity of urine-associated <i>Escherichia coli</i> isolates	AR Eberly, CJ Beebout, CMC Tong, GT Van Horn, HD Green, MJ Fitzgerald, S De, EK Apple, AC Schrimpe-Rutledge, SG Codreanu, SD Sherrod, JA McLean, DB Clayton, CW Stratton, JE Schmitz, M Hadjifrangiskou	Data Brief	2020
Siderophore and indolic acid production by <i>Paenibacillus triticisoli</i> BJ-18 and their plant growth-promoting and antimicrobe abilities	Y Zhang, J Ren, W Wang, B Chen, E Li, S Chen	PeerJ	2020
Investigation on the influence of isolated environment on human psychological and physiological health	Meng, W Wang, Z Hao, H Liu	Science of the Total Environment	2020
Low-concentration of dichloroacetonitrile (DCAN) in drinking water perturbs the health-associated gut microbiome and metabolic profile in rats	B Xue, K Dai, X Zhang, S Wang, C Li, C Zhao, X Yang, Z Xi, Z Qiu, Z Shen, J Wang	Chemosphere	2020



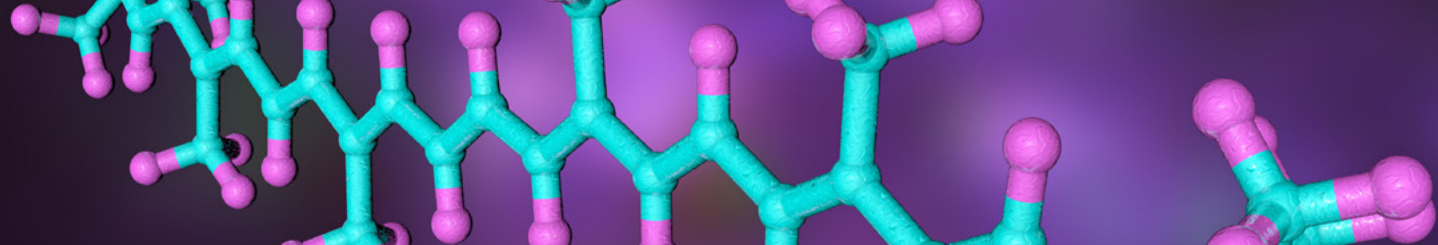
Metabolites

Title	Authors	Journal	Date
Streptomyces spp. from the marine sponge Antho dichotoma: Analyses of secondary metabolite biosynthesis gene clusters and some of their products	JF Guerrero-Garzón, M Zehl, O Schneider, C Rücker, T Busche, J Kalinowski, H Bredholt, SB Zotchev	Frontiers in Microbiology	2020
A wealth of genotype-specific proteoforms fine-tunes hemoglobin scavenging by haptoglobin	S Tamara, V Franc, AJR Heck	PNAS	2020
Huntington's disease genotype suppresses global manganese-responsive processes in pre-manifest and manifest YAC128 mice	AC Pfalzer, JM Wilcox, SG Codreanu, M Totten, TJV Bichell, T Halbesma, P Umashanker, KL Yang, NL Parmalee, SD Sherrod, KM Erikson, FE Harrison, JA McLean, M Aschner, AB Bowman	Metallomics	2020
Elevated choline kinase α -mediated choline metabolism supports the prolonged survival of TRAF3-deficient B lymphocytes	S Gokhale, W Lu, S Zhu, Y Liu, RP Hart, JD Rabinowitz, P Xie	The Journal of Immunology	2020
Dietary prebiotics alter novel microbial dependent fecal metabolites that improve sleep	RS Thompson, F Vargas, PC Dorrestein, M Chichlowski, BM Berg, M Fleshner	Scientific Reports	2020
Simultaneous measurement of urinary trimethylamine (TMA) and trimethylamine n-oxide (TMAO) by liquid chromatography–mass spectrometry	X Jia, LJ Osborn, Z Wang	Molecules	2020
A combination of inhibiting microglia activity and remodeling gut microenvironment suppresses the development and progression of experimental autoimmune uveitis	J Zhou, J Yang, M Dai, D Lin, R Zhang, H Liu, A Yu, S Vakal, Y Wang, X Li	Biochemical Pharmacology	2020
Insights into the natural defenses of a coral reef fish against gill ectoparasites: Integrated metabolome and microbiome approach	M Reverter, P Sasal, MT Suzuki, D Raviglione, N Inguibert, A Pare, B Banaigs, SN Voisin, P Bulet, N Tapissier-Bontemps	Metabolites	2020
Venetoclax with azacitidine disrupts energy metabolism and targets leukemia stem cells in acute myeloid leukemia patients	DA Pollyea, BM Stevens, CL Jones, A Winters, S Pei, M Minhajuddin, A D'Alessandro, R Culp-Hill, KA Riemondy, AE Gillen, JR Hesselberth, D Abbott, D Schatz, JA Gutman, E Purev, C Smith, CT Jordan	Nature Medicine	2020
Kynurenic acid protects against ischemia/reperfusion-induced retinal ganglion cell death in mice	RB Nahomi, MH Nam, J Rankenberg, S Rakete, JA Houck, GC Johnson, DL Stankowska, MB Pantcheva, PS MacLean, RH Nagaraj	International Journal of Molecular Sciences	2020
Androgen-induced expression of DRP1 regulates mitochondrial metabolic reprogramming in prostate cancer	YG Lee, Y Nam, KJ Shin, S Yoon, WS Park, JY Joung, JK Seo, J Jang, S Lee, D Nam, MC Caino, PG Suh, YC Chae	Cancer Letters	2020
A high-resolution mass spectrometry-based quantitative metabolomic workflow highlights defects in 5-fluorouracil metabolism in cancer cells with acquired chemoresistance	S Shahi, CS Ang, S Mathivanan	Biology	2020
Novel antifungal activity of lolium-associated Epichloë endophytes	K Fernando, P Reddy, IK Hettiarachchige, GC Spangenberg, SJ Rochfort, KM Guthridge	Microorganisms	2020
Red blood cell metabolism in Rhesus macaques and humans: comparative biology of blood storage	D Stefanoni, HKH Shin, JH Baek, DP Champagne, T Nemkov, T Thomas, RO Francis, JC Zimring, T Yoshida, JA Reisz, SL Spitalnik, PW Buehler, A D'Alessandro	Haematologica	2020



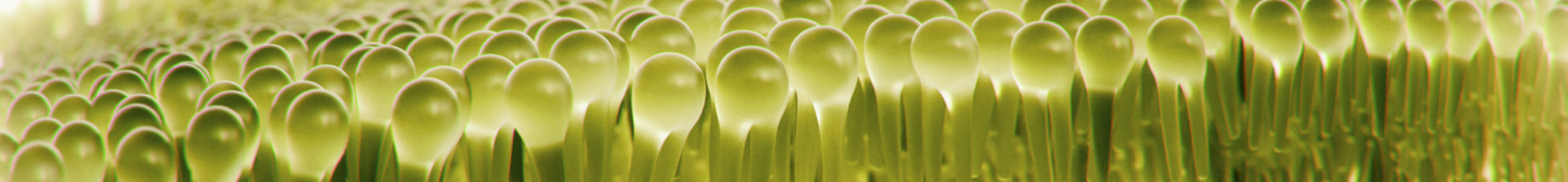
Metabolites

Title	Authors	Journal	Date
Environmental arginine controls multinuclear giant cell metabolism and formation	JS Brunner, L Vulliard, M Hofmann, M Kieler, A Lercher, A Vogel, M Russier, JB Brüggenthies, M Kerndl, V Saferding, B Niederreiter, A Junza, A Frauenstein, C Scholtyssek, Y Mikami, K Klavins, G Krönke, A Berghaler, JJ O'Shea, T Weichhart, F Meissner, JS SMolen, P Cheng, O Yanes, J Menche, PJ Murray, O Sharif, S Blüml, G Schabbauer	Nature Communications	2020
Spiking and homogenization of biological matrices for production of reference materials using cryogenic processes	DL Ellisor, WC Davis, RS Pugh	Analytical and Bioanalytical Chemistry	2020
Leishmania encodes a bacterium-like 2,4-dienoyl-coenzyme A reductase that is required for fatty acid β -oxidation and intracellular parasite survival	G Semini, D Paape, M Blume, MF Sernee, D Peres-Alonso, S Calvignac-Spencer, J Döllinger, S Jehle, E Saunders, MC McConville, T Aebischer	mBio	2020
Metabolic interaction between smmonia and baicalein	S Zhang, R Wang, Y Zhao, FS Tareq, S Sang	Chemical Research in Toxicology	2020
Effects of acute versus recurrent insulin-induced hypoglycemia on ventromedial hypothalamic nucleus metabolic-sensory neuron AMPK activity: Impact of alpha1-adrenergic receptor signaling	KP Briski, SK Mandal, K Bheemanapally, MMH Ibrahim	Brain Research Bulletin	2020
Comparative evaluation of itaconate and its derivatives reveals divergent inflammasome and type I interferon regulation in macrophages	A Swain, M Bambouskova, H Kim, PS Andhey, D Duncan, K Auclair, V Chubukov, DM Simons, TP Roddy, KM Stewart, MN Artymov	Nature Metabolism	2020
Diversity of secondary metabolism in Aspergillus nidulans clinical isolates	MT Drott, RW Bastos, A Rokas, LNA Ries, T Gabaldón, GH Goldman, NP Keller, C Greco	mSphere	2020
Smart biomimetic nanocomposites mediate mitochondrial outcome through aerobic glycolysis reprogramming: A promising treatment for lymphoma	Q Zhao, J Li, B Wu, Y Shang, X Huang, H Dong, H Liu, W Chen, R Gui, X Nie	Applied Materials an Interfaces	2020
Metabolite profiling revealed that a gardening activity program improves cognitive ability correlated with BDNF levels and serotonin metabolism in the elderly	SA Park, DY Son, AY Lee, HG Park, WL Lee, CH Lee	International Journal of Environmental Research and Public Health	2020
Identification and distribution of novel metabolites of lolitrem B in mice by high-resolution mass spectrometry	P Reddy, A Elkins, J Hemsworth, K Guthridge, S Vassiliadis, E Read, G Spangenberg, S Rochfort	Molecules	2020
Physiological phenotypes and urinary metabolites associated with the psychological changes of healthy human: A study in "lunar palace 365"	Z Hao, S Feng, Y Zhu, J Yng, C Meng, D Hu, H Liu, H Liu	Acta Astronautica	2020
Bacteria boost mammalian host NAD metabolism by engaging the deamidated biosynthesis pathway	I Shats, JG Williams, J Liu, MV Makarov, X Wu, FB Lih, LJ Deterding, C Lim, X Xu, TA Randall, E Lee, W Li, W Fan, JL Li, M Sokolsky, AV Kabanov, L Li, ME Migaud, JW Locasale, X Li	Cell Metabolism	2020
Methyl-metabolite depletion elicits adaptive responses to support heterochromatin stability and epigenetic persistence	SA Haws, D Yu, C Ye, CK Wille, LC Nguyen, KA Krautkramer, JT Tomaszewicz, SE Yang, BR Miller, WH Liu, K Igarashi, R Sridharan, BP Tu, VL Cryns, DW Lamming, JM Denu	Molecular Cell	2020



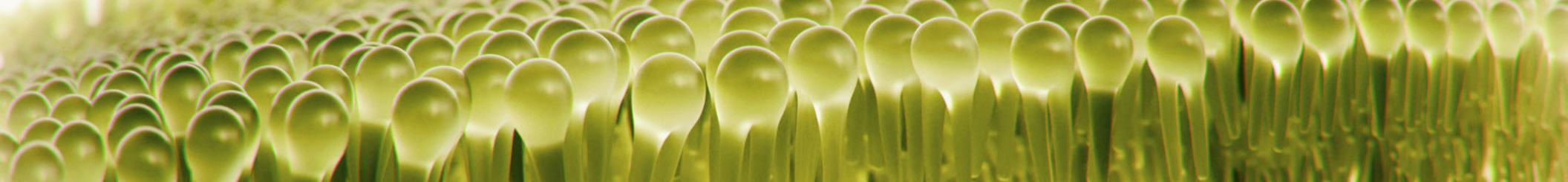
Metabolites

Title	Authors	Journal	Date
Combined transcriptomic and metabolomic analyses uncover rearranged gene expression and metabolite metabolism in tobacco during cold acclimation	J Xu, Z Chen, F Wang, W Jia, Z Xu	Scientific Reports	2020
Long-term high intake of 9-PAHPA or 9-OAHPA increases basal metabolism and insulin sensitivity but disrupts liver homeostasis in healthy mice	M Benlebna, L Balas, B Bonaños, L Pessemesse, C Vigor, J Grober, F Bernex, G Fouret, V Paluchova, S Gaillet, JF Landrier, O Kuda, T Durand, C Coudray, F Casas, C Feillet-Coudray	The Journal of Nutritional Biochemistry	2020
The small intestine shields the liver from fructose-induced steatosis	C Jang, S Wada, S Yang, B Gosis, X Feng, Z Zhang, Y Shen, G Lee, Z Arany, JD Rabinowitz	Nature Metabolism	2020
Single-cell RNA sequencing maps endothelial metabolic plasticity in pathological angiogenesis	K Rohlenova, J Goveia, M Garcíá-Caballero, A Subramanian, J Kalucka, L Treps, KD Falkenberg, LPMH de Rooij, Y Zheng, L Lin, L Sokol, LA Teuqen, V Geldhof, F Taverna, A Pircher, LC Conradi, S Khan, S Stegen, D Panovska, FD Smet, FJT Staal, RJ McLaughlin, S Vinckier, TV Bergen, N Ectors, PD Haes, J Wang, L Bolund, L Schoonjans, TK Karakach, H Yang, G Carmeliet, P Carmeliet	Cell Metabolism	2020
HDAC inhibitors elicit metabolic reprogramming by targeting super-enhancers in glioblastoma models	TTT Nguyen, Y Zhang, E Shang, C Shu, C Torrini, J Zhao, E Bianchetti, A Mela, N Humala, A Mahajan, AO Harmanci, Z Lei, M Maienschein-Cline, CM Quinzii, MA Westhoff, G Karpel-Massler, JN Bruce, P Canoll, MD Siegelin	The Journal of Clinical Investigation	2020
Effects of underfeeding and oral vancomycin on gut microbiome and nutrient absorption in humans	A Basolo, M Hohenadel, QY Ang, P Piaggi, S Heinitz, M Walter, P Walter, S Parrington, DD Trinidad, RJ von Schwartzenber, PJ Turnbaugh, J Krakoff	Nature Medicine	2020



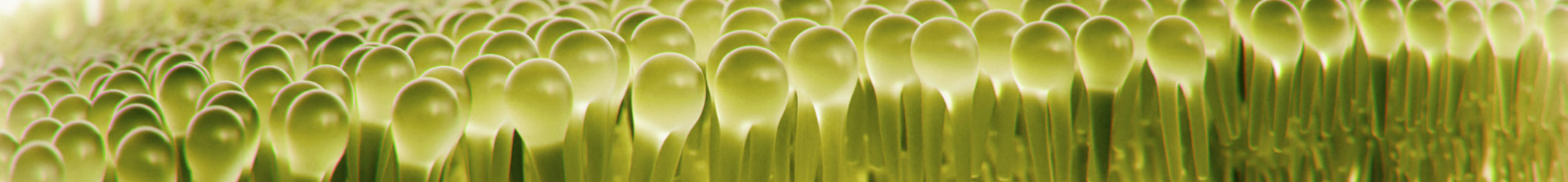
Lipids

Title	Authors	Journal	Date
Comprehensive untargeted lipidomic analysis using core-shell C30 particle column and high field Orbitrap mass spectrometer	M Narváez-Rivas, Q Zhang	Journal of Chromatography A	2016
Coupling targeted and untargeted mass spectrometry for Metabolome-microbiome-wide association studies of human fecal samples	AV Melnik, RR da Silva, ER Hyde, AA Aksenov, F Vargas, A Bouslimani, I Protsyuk, AK Jarmusch, A Tripathi, T Alexandrov, Rob Knight, PC Dorrestein	Analytical Chemistry	2017
LILY-lipidome isotope labeling of yeast: in vivo synthesis of ¹³ C labeled reference lipids for quantification by mass spectrometry	E Rampler, C Coman, G Hermann, A Sickmann, R Ahrends, G Koellensperger	Analyst	2017
Comparison of methylation methods for fatty acid analysis of milk fat	Z Liu, V Ezernieks, S Rochfort, B Cocks	Food Chemistry	2018
LipuDex: An integrated software package for high-confidence lipid identification	PD Hutchins, JD Russell, JJ Coon	Cell Systems	2018
Optimization of folch, bligh-dyer, and matyash sample-to-extraction solvent ratios for human plasma-based lipidomics studies	CZ Ulmer, CM Jones, CM Jones, RA Yost, TJ Garrett, JA Bowden	Analytica Chimica Acta	2018
Fumonisin B1 inhibits endoplasmic reticulum stress associated-apoptosis after FoscanPDT combined with C6-cyridinium ceramide or fenretinide	NB Boppana, JM Kraveka, M Rahmaniyan, L Li, A Bielawska, J Bielawski, JS Pierce, JS Delor, K Zhang, M Korbelik, D Separovic	Anticancer Research	2018
Endogenous fatty acids are essential signaling factors of pancreatic β -cells and insulin secretion	S Hauke, K Keutler, P Phapale, DA Yushchenko, C Schultz	Diabetes	2018
Comprehensive quantitative analysis of fatty-acyl-Coenzyme A species in biological samples by ultra-high performance liquid chromatography-tandem mass spectrometry harmonizing hydrophilic interaction and reversed phase chromatography	L Abrankó, G Williamson, S Gardner, A Kerimi	Journal of Chromatography A	2018
Simultaneous non-polar and polar lipid analysis by on-line combination of HILIC, RP and high resolution MS	E Rampler, H Schoeny, BM Mitic, YE Abiead, M Schwaiger, G Koellensperger	Analyst	2018
Delving into the polar lipidome by optimized chromatographic separation, high-resolution mass spectrometry, and comprehensive identification with Lipostar: Microalgae as case study	G La Barbera, M Antonelli, C Cavaliere, G Cruciani, L Goracci, CM Montone, S Piovesana, A Laganà, AL Capriotti	Analytical Chemistry	2018
Multi-omic mitoprotease profiling defines a role for Oct1p in coenzyme Q production	MT Veling, AG Reidenbach, EC Freiburger, NW Kwiecien, PD Hutchins, MJ Drahnak, A Jochem, A Ulbrich, MJP Rush, JD Russel, JJ Coon, DJ Pagliarini	Molecular Cell	2018
Isobaric labeling of intact gangliosides toward multiplexed LC-MS/MS-based quantitative analysis	RC Barrientos, Q Zhang	Analytical Chemistry	2018
Caspase-2 associates with FAN through direct interaction and overlapping functionality	J Forsberg, X Li, AV Zamaraev, T Panaretakis, B Zhivotovsky, M Olsson	Biochemical Biochemical Research Communications	2018



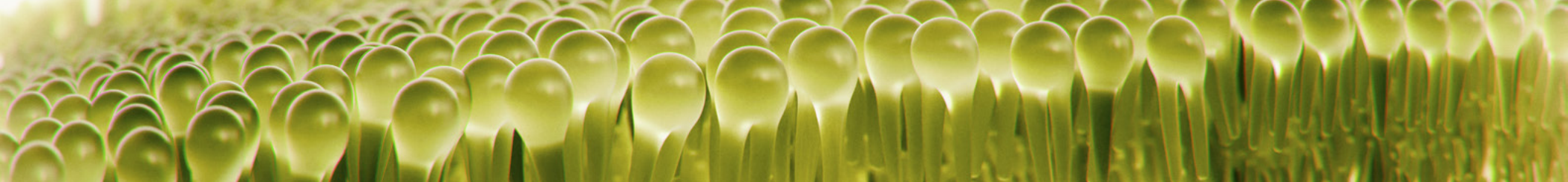
Lipids

Title	Authors	Journal	Date
Anti-inflammatory benefits of antibiotics: Tylvalosin induces apoptosis of porcine neutrophils and macrophages, promotes efferocytosis, and inhibits pro-inflammatory CXCL-8, IL1 α , and LTB4 production, while inducing the release of pro-resolving lipoxin A4 and resolvin D1	R Moges, DD De Lamache, S Sajedy, BS Renaux, MD Hollenberg, G Muench, EM Abbott, AG Buret	Frontiers in Veterinary Medicine	2018
A novel lipidomics workflow for improved human plasma identification and quantification using RPLC-MSn methods and isotope dilution strategies	E Rampler, A Criscuolo, M Zeller, Y El Abiead, H Schoeny, G Hermann, E Sokol, K Cook, DA Peake, B Delanghe, G Koellensperger	Analytical Chemistry	2018
Metabolic control over mTOR-dependent diapause-like state	AM Hussein, Y Wang, J Mathieu, L Margaretha, C Song, DC Jones, C Cavanaugh, JW Miklas, E Mahan, MR Showalter, WL Ruzzo, O Fiehn, CB Ware, CA Blau, H Ruohola-Baker	Developmental Cell	2018
Towards measuring growth rates of pathogens during infections by D ₂ O-labeling lipidomics	C Neubauer, AL Sessions, IR Booth, BP Bowen, SH Kopf, DK Newman, NF Dalleska	Rapid Communications in Mass Spectrometry	2018
Influence of charged aerosol detector instrument settings on the ultra-high-performance liquid chromatography analysis of fatty acids in polysorbate 80	K Schilling, R Pawellek, K Lovejoy, T Muellner, U Holzgrabe	Journal of Chromatography A	2018
Lipidomics for wildlife disease etiology and biomarker discovery: a case study of pansteatitis outbreak in South Africa	JP Koelmel, CZ Ulmer, S Fogelson, CM Jones, H Botha, JT Bangma, TC Guillette, WJ Luus-Powell, JR Sara, WJ Smit, K Albert, HA Miller, MP Guillette, BC Olsen, JA Cochran, TJ Garrett, RA Yost, JA Bowden	Metabolomics	2019
Merging metabolomics and lipidomics into one analytical run	M Schwaiger, H Schoeny, Y El Abiead, G Hermann, E Rampler, G Koellensperger	Analyst	2019
Shared reference materials harmonize lipidomics across MS-based detection platforms and laboratories	A Triebel, B Burla, J Selvalatchmanan, J Oh, SH Tan, MY Chan, NA Mellet, PJ Meikle, F Torta, MR Wenk	Journal of Lipid Research	2019
Alterations of gut microbiota and blood lipidome in gestational diabetes mellitus with hyperlipidemia	J Liu, LL Pan, S Lv, Q Yang, H Zhang, W Chen, Z Lv, J Sun	Frontiers in Physiology	2019
Accelerating lipidomic method development through in silico simulation	PD Hutchins, JD Russell, JJ Coon	Analytical Chemistry	2019
High-throughput measure of bioactive lipids using non-targeted mass spectrometry	KA Lagerborg, JD Watrous, S Cheng, M Jain	Methods in Molecular Biology	2019
Mapping lipid fragmentation for tailored mass spectral libraries	PD Hutchins, JD Russell, JJ Coon	Journal of the American Society for Mass Spectrometry	2019
The metabolite repair enzyme Nit1 is a dual-targeted amidase that disposes of damaged glutathione in Arabidopsis	TD Niehaus, JA Patterson, DC Alexander, JS Folz, M Pyc, BS MacTavish, SD Bruner, RT Mullen, O Fiehn, AD Hanson	Biochemical Journal	2019
Directed non-targeted mass spectrometry and chemical networking for discovery of eicosanoids and related oxylipins	JD Watrous, TJ Niiranen, KA Lagerborg, M Henglin, YJ XU, J Rong, S Sharma, RS Vasani, MG Larson, A Armando, S Mora, O Quehenberger, EA Dennis, S Cheng, M Jain	Cell Chemical Biology	2019
Treg cells promote the SREBP1-dependent metabolic fitness of tumor-promoting macrophages via repression of CD8 ⁺ T cell-derived interferon- γ	C Liu, M Chikina, R Deshpande, AV Menk, T Wang, T Tabib, EA Brunazzi, KM Vignali, M Sun, DB Stolz, RA Lafyatis, W Chen, GM Delgoffe, CJ Workman, SG Wendell, DAA Vignali	Immunity	2019



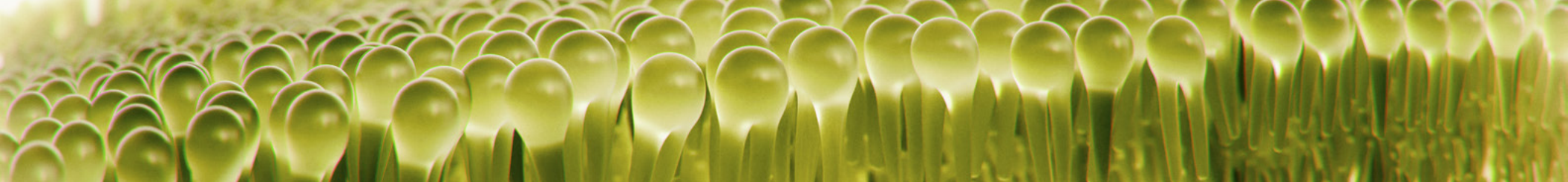
Lipids

Title	Authors	Journal	Date
Chronic arsenic exposure induces oxidative stress and perturbs serum lysolipids and fecal unsaturated fatty acid metabolism	I Chi, P Tu, CW Liu, Y Lai, J Xue, H Ru, K Lu	Chemical Research in Toxicology	2019
Perilipin 5 deletion in hepatocytes remodels lipid metabolism and causes hepatic insulin resistance in mice	SN Keenan, RC Meex, JCY Lo, A Ryan, S Nie, MK Montgomery, MJ Watt	Diabetes	2019
Enrichment procedure based on graphitized carbon black and liquid chromatography-high resolution mass spectrometry for elucidating sulfolipids composition of microalgae	M Antonelli, B Benedetti, C Cavaliere, A Cerrato, GL Barbera, CM Montone, S Piovesana A Laganà	Talanta	2019
Differential isotope labeling by permethylation and reversed-phase liquid chromatography-mass spectrometry for relative quantification of intact neutral glycolipids in mammalian cells	RC Barrientos, Q Zhang	Analytical Chemistry	2019
Electrophilic fatty acid nitroalkenes are systemically transported and distributed upon esterification to complex lipids	M Fazzari, DA Vitturi, SR Woodcock, SR Salvatore, BA Freeman, FJ Schopfer	Journal of Lipid Research	2019
An isoprene lipid-binding protein promotes eukaryotic coenzyme Q biosynthesis	DC Lohman, D Aydin, HC Von Bank, RW Smith, V Linke, E Weisenhorn, MT McDevitt, P Hutchins, EM Wilkerson, B Wancewicz, J Russell, MS Stefely, ET Beebe, A Jochem, JJ Coon, CA Bingman, M Dal Peraro	Molecular Cell	2019
The use of styrene-maleic acid copolymer (SMA) for studies on T cell membrane rafts	P Angelisová, O Ballek, J Sýkora, O Benada, T Čajka, J Pokorná, D Pinkas, V Hořejší	Biochimica et Biophysica Acta - Biomembranes	2019
A mitochondrial specific antioxidant reverses metabolic dysfunction and fatty liver induced by maternal cigarette smoke in mice	G Li, YL Chan, S Sukjamnong, AG Anwer, H Vindin, M Padula, R Zakarya, J George, BG Oliver, S Saad, H Chen	Nutrients	2019
Selective Ah receptor ligands mediate enhanced SREBP1 proteolysis to restrict lipogenesis in sebocytes	GE Muku, N Blazanin, F Dong, PB Smith, D Thiboutot, K Gowda, S Amin, IA Murray, GH Perdeu	Toxicological Sciences	2019
Generation of human fatty livers using custom-engineered induced pluripotent stem cells with modifiable SIRT1 metabolism	AC de L'Hortet, K Takeishi, J Guzman-Lepe, K Morita, A Achreja, B Popovic, Y Wang, K Handa, A Mittal, N Meurs, Z Zhu, F Weinberg, M Salomon, IJ Fox, CX Deng, D Nagrath, A Soto-Gutierrez	Cell Metabolism	2019
A role for the orphan human cytochrome P450 2S1 in polyunsaturated fatty acid ω -1 hydroxylation using an untargeted metabolomic approach	MI Fekry, Y Xiao, JZ Berg, FP Guengerich	Drug Metabolism and Disposition	2019
Coenzyme Q biosynthetic proteins assemble in a substrate-dependent manner into domains at ER-mitochondria contacts	K Subramanian, A Jochem, M Le Vasseur, S Lewis, BR Paulson, TR Reddy, JD Russell, JJ Coon, DJ Pagliarini, J Nunnari	Journal of Cell Biology	2019
Multi-omics reveal specific targets of the RNA-binding protein Puf3p and its orchestration of mitochondrial biogenesis	CP Lapointe, JA Stefely, A Jochem, PD Hutchins, GM Wilson, NW Kwiecien, JJ Coon, M Wickens, DJ Pagliarini	Cell Systems	2019
Multi-omics analyses detail metabolic reprogramming in lipids, carnitines, and use of glycolytic intermediates between prostate small cell neuroendocrine carcinoma and prostate adenocarcinoma	B Gao, HW Lue, J Podolak, S Fan, Y Zhang, A Serawat, JJ Alumkal, O Fiehn, GV Thomas	Metabolites	2019
The power of LC-MS based multiomics: exploring adipogenic differentiation of human mesenchymal stem/stromal cells	E Rampler, D Egger, H Schoeny, M Ruzs, MP Pacheco, G Marino, C Kasper, T Naegele, G Koellensperger	Molecules	2019



Lipids

Title	Authors	Journal	Date
Overcoming iron deficiency of an Escherichia coli tonB mutant by increasing outer membrane permeability	N Qiu, R Misra	Journal of Bacteriology	2019
Accurate mass and retention time library of serum lipids for type 1 diabetes research	N Vu, M Narvaez-Rivas, GY Chen, MJ Rewers, Q Zhang	Analytical and Bioanalytical Chemistry	2019
A randomized 3-way crossover study indicates that high-protein feeding induces de novo lipogenesis in healthy humans	E Charidemou, T Ashmore, X Li, BD McNally, JA West, S Liggi, M Harvey, E Orford, JL Griffin	JCI Insight	2019
Phospholipidome of extra virgin olive oil: Development of a solid phase extraction protocol followed by liquid chromatography–high resolution mass spectrometry for its software-assisted identification	M Antonelli, B Benedetti, C Cavaliere, A Cerrato, CM Montone, S Piovesana, A Lagana, AL Cipriotti	Food Chemistry	2020
Comprehensive characterization of bovine milk lipids: Phospholipids, sphingolipids, glycolipids, and ceramides	Z Liu, C Li, J Pryce, S Rochfort	Journal of Agricultural and Food Chemistry	2020
Sacha inchi oil alleviates gut microbiota dysbiosis and improves hepatic lipid dysmetabolism in high-fat diet-fed rats	P Li, J Huang, N Xiao, X Cai, Y Yang, J Deng, LH Zhang, B Du	Food & Function	2020
First report on quality and purity evaluations of avocado oil sold in the US	HS Green, SC Wang	Food Control	2020
Neurotoxicity assessment of triazole fungicides on mitochondrial oxidative respiration and lipids in differentiated human SH-SY5Y neuroblastoma cells	CL Sanchez, CL Souders II, CJ Pena-Delgado, KT Nguyen, N Kroyter, N El Ahmadie, JJ Aristizabal-Henao, JA Bowden, CJ Martyniuk	Neurotoxicology	2020
MYC regulates fatty acid metabolism through a multigenic program in claudin-low triple negative breast cancer	JC Casciano, C Perry, AJ Cohen-Nowak, KD Miller, JV Voorde, Q Zhang, S Chalmers, ME Sandison, Q Lui, A Hedley, T McBryan, HY Tang, N Gorman, T Beer, DW Spreicher, PD Adams, Z Liu, R Schlegel, JG McCarron, MJO Wakelam, E Gottlieb, AV Kossenkov, ZT Schug	British Journal of Cancer	2020
Triacylglycerol-rich oils of marine origin are optimal nutrients for induction of polyunsaturated docosahexaenoic acid ester of hydroxy linoleic acid (13-DHAHLA) with anti-inflammatory properties in mice	V Paluchova, A Vik, T Cajka, M Brezinova, K Brejchova, V Bugajev, L Draberova, P Draber, J Buresova, P Kroupova, K Bardova, M Rossmesl, J Kopecky, TV Hansen O Kuda	Molecular Nutrition and Food Research	2020
Evaluation of lipid quantification accuracy using HILIC and RPLC MS on the example of NIST® SRM® 1950 metabolites in human plasma	M Lange, M Fedorova	Analytical and Bioanalytical Chemistry	2020
New insights in hemp chemical composition: a comprehensive polar lipidome characterization by combining solid phase enrichment, high-resolution mass spectrometry, and cheminformatics	M Antonelli, B Benedetti, G Cannazza, A Cerrato, C Citti, CM Montone, S Piovesana, A Lagana	Analytical and Bioanalytical Chemistry	2020
Comprehensive characterization of bovine milk lipids: Triglycerides	Z Liu, C Li, J Pryce, S Rochfort	ACS Omega	2020
The presence of active brown adipose tissue determines cold-induced energy expenditure and oxylipin profiles in humans	OC Kulterer, L Niederstaetter, CT Herz, AR Haug, A Bileck, D Pils, A Kautzky-Willer, C Gerner, FW Kiefer	The Journal of Endocrinology and Metabolism	2020
A comprehensive analysis of liposomal biomolecular corona upon human plasma incubation: The evolution towards the lipid corona	G La Barbera, AL Capriotti, G Caracciolo, C Cavaliere, A Cerrato, CM Montone, S Piovesana, D Pozzi, E Quagliarini, A Lagana	Talanta	2020



Lipids

Title	Authors	Journal	Date
mTORC1 restrains adipocyte lipolysis to prevent systemic hyperlipidemia	LM Paoletta, S Mukherjee, CM Tran, B Bellaver, M Hugo, TS Luongo, SV Shewale, W Lu, K Chellappa, JA Baur	Molecular Metabolism	2020
Dietary sphinganine is selectively assimilated by members of the mammalian gut microbiome	MT Lee, HH Le, EL Johnson	Journal of Lipid Research	2020
Lipidome-wide ¹³ C flux analysis: A novel tool to estimate the turnover of lipids in organisms and cultures	M Schlame, Y Xu, H Erdjument-Bromage, TA Neubert, M Ren	Journal of Lipid Research	2020
In vitro digestion of grape seed oil inhibits phospholipid-regulating effects of oxidized lipids	S Fruehwirth, S Zehentner, M Salim, S Sterneder, J Tiroch, B Lieder, M Zehl, V Somoza, M Pignitter	Biomolecules	2020
Human GDPD3 overexpression promotes liver steatosis by increasing lysophosphatidic acid production and fatty acid uptake	CCC Key, AC Bishop, X Wang, Q Zhao, GY Chen, MA Quinn, X Zhu, Q Zhang, JS Parks	Journal of Lipid Research	2020
Exercise training induces insulin-sensitizing PAHSAs in adipose tissue of elderly women	M Brezinova, T Cajka, M Oseeva, M Stepan, K Dadova, L Rossmeislova, M Matous, M Siklova, M Rossmeisl, O Kuda	Biochimica et Biophysica Acta - Molecular and Cell Biology of Lipids	2020
Increased ATP synthesis might counteract hepatic lipid accumulation in acromegaly	P Fellingner, P Wolf, L Pflieger, P Krumpolec, M Krssak, K Klavins, S Wolfsberger, A Micko, P Carey, B Gürtl, G Vila, W Raber, C Fürsinn, T Scherer, S Trattinig, A Kautzky-Willer, M Krebs, KY Winhofer	JCI Insight	2020
Structure of the neurotensin receptor 1 in complex with β -arrestin 1	W Huang, M Masureel, Q Qu, J Janetzko, A Inoue, HE Kato, MJ Robertson, KC Nguyen, JS Glenn, G Skiniotis, BK Kobilka	Nature	2020
Differential postprandial incorporation of 20:5n-3 and 22:6n-3 into individual plasma triacylglycerol and phosphatidylcholine molecular species in humans	AL West, LV Michaelson, EA Miles, RP Haslam, KA Lillycrop, R Georgescu, L Han, O Sayanova, JA Napier, PC Calder, GC Burdge	Biochimica et Biophysica Acta - Molecular and Cell Biology of Lipids	2020
Lipid composition and abundance in the reproductive and alimentary tracts of female <i>Haemonchus contortus</i>	T Wang, G Ma, S Nie, NA Williamson, GE Reid, RB Gasser	Parasites and Vectors	2020
Lipid landscape of the human retina and supporting tissues revealed by high-resolution imaging mass spectrometry	DMG Anderson, JD Messinger, NH Patterson, ES Rivera, A Kotnala, JM Spraggins, RM Caprioli, CA Curcio, KL Schey	Journal of American Society for Mass Spectrometry	2020
Gangliosides are essential endosomal receptors for quasi-enveloped and naked hepatitis A virus	A Das, R Barrientos, T Shiota, V Madigan, I Misumi, KL McKnight, L Sun, Z Li, RM Maganck, Y Li, E Kaluzna, A Asokan, JK Whitmire, M Kapustina, Q Zhang, SM Lemon	Nature Microbiology	2020
Discovering new lipidomic features Using cell type specific fluorophore expression to provide spatial and biological specificity in a multimodal workflow with MALDI imaging mass spectrometry	MA Jones, SH Cho, NH Patterson, RV de Plas, JM Spraggins, MR Boothby, RM Caprioli	Analytical Chemistry	2020
Changes in aged fibroblast lipid metabolism induce age-dependent melanoma cell resistance to targeted therapy via the fatty acid transporter FATP2	GM Alicea, VW Rebecca, AR Goldman, ME Fane, ST Douglass, R Behera, MR Webster, CH Kugel III, BL Ecker, MC Caino, AV Kossenkov, HY Tang, DT Frederick, KT Flaherty, X Xu, Q Liu, DI Gabrilovich, M Herlyn, IA Blair, ZT Schug, DW Speicher, AT Weeraratna	Cancer Discovery	2020



Pharmaceuticals

Title	Authors	Journal	Date
The suppressive effects of cinnamomi cortex and its phytochemical coumarin on oxaliplatin-induced neuropathic cold allodynia in rats	C Kim, JH Lee, W Kim, D Li, Y Kim, K Lee, SK Kim	Molecules	2016
Understanding the metabolism of the anticancer drug Triapine: Electrochemical oxidation, microsomal incubation and in vivo analysis using LC-HRMS	K Pelivan, L Frensemeier, U Karst, G Koellensperger, B Bielec, S Hager, P Heffeter, BK Keppler, CR Kowol	Analyst	2017
Identification of new process-related impurity in the key intermediate in the synthesis of TCV-116	A Testen, M Plevnik, B Štefane, IK Cigić	Acta Pharmaceutica	2018
Fentanyl delays the platelet inhibition effects of oral ticagrelor: Full report of the PACIFY randomized clinical trial	K Ibrahim, R Shah, RR Goli, TS Kickler, WA Clarke, RK Hasan, RS Blumenthal, DR Thiemann, JR Resar, SP Schulman, JW McEvoy	Thrombosis and Haemostasis	2018
Effect of intravenous fentanyl on ticagrelor absorption and platelet inhibition among patients undergoing percutaneous coronary intervention: Design, rationale, and sample characteristics of the PACIFY randomized trial	K Ibrahim, RR Goli, R Shah, JR Resar, SP Schulman, JW McEvoy	Contemporary Clinical Trials	2018
Comparison of pharmacokinetics of phytoecdysones and triterpenoid saponins of monomer, crude and processed Radix achyranthis bidentatae by UHPLC-MS/MS	L Yang, H Jiang, M Yan, X Xing, X Guo, W Man, A Hou, B Yang, Q Wang, H Kuang	Xenobiotica	2018
A 2D LC-MS/MS strategy for reliable detection of 10-ppm level residual host cell proteins in therapeutic antibodies	F Yang, DE Walker, J Schoenfelder, J Carver, A Zhang, R Harris, JT Stults, XC Yu, DA Michels	Analytical Chemistry	2018
Quantitation of the anticancer drug abiraterone and its metabolite $\Delta(4)$ -abiraterone in human plasma using high-resolution mass spectrometry	A Bhatnagar, MJ McKay, M Crumbaker, K Ahire, P Karuso, H Gurney, MP Molloy	Biomedical Analysis	2018
Using superficially porous particles and ultrahigh pressure liquid chromatography in pharmacopeial monograph modernization of common analgesics	GA Kresge, JMT Wong, MD Pra, F Steiner, JP Grinias	Chromatographia	2018
A general LC-MS/MS method for monitoring potential β -lactam contamination in drugs and drug-manufacturing surfaces	C Qiu, H Zhu, C Ruzicka, D Keire, H Ye	The AAPS Journal	2018
Esketamine counters opioid-induced respiratory depression	K Jonkman, E van Rijnsvoever, E Olofsen, L Aarts, E Sarton, M van Velzen, M Niesters, A Dahan	British Journal of Anesthesia	2018
Determination of epoxide impurity in sarpogrelate hydrochloride intermediate by UHPLC and column-switching liquid chromatography	R Wang, Z Zhu, X Qiu, L Bai, W Guo, L Zou, T Zhao, G Shan	Journal of Pharmaceutical and Biomedical Analysis	2019
Brain delivery of thyrotropin-releasing hormone via a novel prodrug approach	K Prokai-Tatrai, DL De La Cruz, V Nguyen, BP Ross, I Toth, L Prokai	Pharmaceutics	2019
Model-based drug development in pulmonary delivery: Pharmacokinetic analysis of novel drug candidates for treatment of Pseudomonas aeruginosa lung infection	T Sou, I Kukavica-Ibrulji, F Soukarieh, N Halliday, RC Levesque, P Williams, M Stocks, M Câmara, LE Fribert, CAS Bergström	Journal of Pharmaceutical Sciences	2019



Pharmaceuticals

Title	Authors	Journal	Date
A reliable LC–MS/MS method for the quantification of five bioactive saponins of crude and processed <i>Bupleurum scorzonerifolium</i> in rat plasma and its application to a pharmacokinetic study	Y Tao, S Huang, J Yan, B Cai	Biomedical Chromatography	2019
Pharmacokinetics of midazolam and its major metabolite 1-hydroxymidazolam in the ball python (<i>Python regius</i>) after intracardiac and intramuscular administrations	CB Larouche, R Johnson, F Beaudry, C Mosley, Y Gu, KA Zaman, H Beaufrère, C Dutton	Journal of Veterinary and Therapeutics	2019
Pharmacokinetic study of six triterpenoids of raw and processed <i>Alisma plantago-aquatica</i> in rat plasma by using ultra performance liquid chromatography-tandem mass spectrometry approach	Y Tao, S Huang, J Yan, B Cai	Journal of Chromatography B	2019
Development and validation of an analytical method for regorafenib and its metabolites in mouse plasma	Q Fu, M Chen, S Hu, A McElroy, RH Mathijssen, A Sparreboom, SD Baker	Journal of Chromatography B	2019
Dasatinib/HP- β -CD inclusion complex based aqueous formulation as a promising tool for the treatment of paediatric neuromuscular disorders	A Cutrignelli, F Sanarica, A Lopalco, A Lepedota, V Laquintana, M Franco, B Boccanegra, P Mantuano, A De Luca, N Denora	International Journal of Molecular Sciences	2019
Quantitation of a novel engineered anti-infective host defense peptide, ARV-1502: Pharmacokinetic study of different doses in rats and dogs	A Brakel, D Volke, CN Kraus, L Otvos, R Hoffman	Frontiers in Chemistry	2019
Bioactivation of napabucasin triggers reactive oxygen species-mediated cancer cell death	FEM Froeling, MM Swamynathan, A Deschênes, IIC Chio, E Brosnan, MA Yao, P Alagesan, M Lucito, J Li, AY Chang, LC Trotman, P Belleau, Y Park, HA Rogoff, JD Watson, DA Tuveson	Clinical Cancer Research	2019
Development and validation of a UPLC-MS/MS analytical method for dofetilide in mouse plasma and urine, and its application to pharmacokinetic study	ME Uddin, X Sun, KM Huang, S Hu, CA Carnes, A Sparreboom, Q Fu	Journal of Pharmaceutical and Biomedical Analysis	2019
Red-osier dogwood extracts prevent inflammatory responses in Caco-2 cells and a Caco-2 BBe1/EA.hy926 cell co-culture model	Q Jiang, H Zhang, R Yang, Q Hui, Y Chen, L Mats, R Tsao, C Yang	Antioxidants	2019
The occurrence of putative cognitive enhancing research peptides in seized pharmaceutical preparations: An incentive for controlling agencies to prepare for future encounters of the kind	C Vanhee, A Francotte, S Janvier, E Deconinck	Drug Testing and Analysis	2019
Fourier-transform infrared spectroscopy as a process analytical technology for near real time in-line estimation of the degree of PEGylation in chromatography	A Sanden, S Suhm, M Rüdtt, J Hubbuch	Journal of Chromatography A	2019
Pharmacodynamics of isavuconazole in a rabbit model of cryptococcal meningoencephalitis	LL Kovanda, C Giamberardino, L McEntee, DL Toffaletti, KS Franke, A Bartuska, G Smilnak, GC de Castro, K Ripple, WW Hope, JR Perfect	Antimicrobial Agents and Chemotherapy	2019
Identification of four amoebicidal nontoxic compounds by a molecular docking screen of <i>Naegleria fowleri</i> sterol $\Delta 8$ - $\Delta 7$ -isomerase and phenotypic assays	D Shi, KK Chahal, P Oto, LF Nothias, A Debnath, JH McKerrow, LM Podust, R Abagyan	Infectious Disease	2019



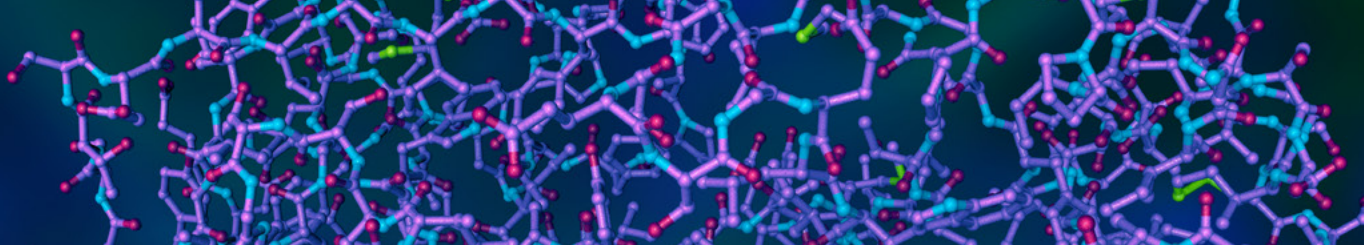
Pharmaceuticals

Title	Authors	Journal	Date
Interaction between sex and organic anion-transporting polypeptide 1b2 on the pharmacokinetics of regorafenib and its metabolites regorafenib-N-oxide and regorafenib-glucuronide in mice	Q Fu, M Chen, JT Anderson, X Sun, S Hu, A Sparreboom, SD Baker	Clinical and Translational Science	2019
Therapeutic suppression of pulmonary neutrophilia and allergic airway hyperresponsiveness by an ROR γ t inverse agonist	GS Whitehead, HS Kang, SY Thomas, A Medvedev, TP Karcz, G Izumi, K Nakano, SS Makarov, H Nakano, AM Jetten, DN Cook	JCI Insight	2019
Bioanalytical evaluation of dried plasma spots for monitoring of abiraterone and Δ (4)-abiraterone from cancer patients	A Bhatnager, MJ McKay, M Thaysen-Andersen, M Arasaratnam, M Crumbaker, H Gurney, MP Molloy	Journal of Chromatography B	2019
Proof-of-concept validation of the mechanism of action of Src tyrosine kinase inhibitors in dystrophic mdx mouse muscle: in vivo and in vitro studies	F Sanarica, P Mantuano, E Conte, A Cozzoli, RF Capogrosso, A Giustino, A Cutrignelli, O Cappellari, JF Rolland, M De Bellis, GM Camerino, A De Luca	Pharmacological Research	2019
Simple, fast and robust LC-MS/MS method for the simultaneous quantification of canagliflozin, dapagliflozin and empagliflozin in human plasma and urine	AB van der AB van der Art-van der Beek, AMA Wessels, HJL Heerspink, DJ Touw	Journal of Chromatography B	2020
ATI-2173, a novel liver-targeted non-chain terminating nucleotide for hepatitis B virus cure regimens	KE Squires, DL Mayers, GR Bluemling, AA Kolykhalov, DV Guthrie, P Reddy, DG Mitchell, MT Saindane, ZM Stitche, V Edpuganti, A De La Rosa	Antimicrobial Agents and Chemotherapy	2020
Impurity profiling of L-aspartic acid and glycine using high-performance liquid chromatography coupled with charged aerosol and ultraviolet detection	R Pawellek, K Schilling, U Holzgrabe	Journal of Pharmaceutical and Biomedical Analysis	2020
Model-informed drug development in pulmonary delivery: semimechanistic pharmacokinetic–pharmacodynamic modeling for evaluation of treatments against chronic Pseudomonas aeruginosa lung infections	T Sou, I Kukavica-Ibrulji, RC Levesque, LE Fribert, CAS Bergström	Molecular Pharmaceuticals	2020
A rapid UHPLC–MS/MS method for the quantification of ARQ531 in rat plasma: Validation and its application to a pharmacokinetic study	J Liu, M Ji, Z Li, X Xu, L Li, H Li, Y Tian, X Su	Biomedical Chromatography	2020
Simultaneous determination of a promising anti-brain tumor agent CAT3 and its two major metabolites in mouse plasma and brain by a LC-MS/MS method	S Zhao, RB Wang, J Bai, X Fan, M Hu, B Wang, J Hu, Y Li	Journal of Pharmaceutical and Biomedical Analysis	2020
Room-temperature preparation of MIL-88A as a heterogeneous photo-Fenton catalyst for degradation of rhodamine B and bisphenol a under visible light	H Fu, XX Song, L Wu, C Zhao, P Wang, CC Wang	Materials Research Bulletin	2020
In vivo modulation of cervicovaginal drug transporters and tissue distribution by film-released tenofovir and darunavir for topical prevention of HIV-1	K Hijazi, F Iannelli, AM Cuppone, D Desjardins, A Caldwell, N Dereuddre-Bosquet, C Scala, KA Smith, I Mukhopadya, B Frank, G Gwozdz, F Santoro, R Le Grand, G Pozzi, C Kelly	Molecular Pharmaceutics	2020
Role of OATP2B1 in drug absorption and drug-drug interactions	M Chen, S Hu, Y Li, AA Gibson, Q Fu, SD Baker, A Sparreboom	Drug Metabolism and Disposition	2020
Chronic mirabegron treatment increases human brown fat, HDL cholesterol, and insulin sensitivity	AE O'Mara, JW Johnson, JD Linderman, RJ Brychta, S McGehee, LA Fletcher, YA Fink, D Kapuria, TM Cassimatis, N Kelsey, C Cero, ZA Sater, F Piccinini, AS Baskin, BP Leitner, H Cai, CM Mollo, W Dieckmann, M Walter, NB Javitt, Y Rotman, PJ Walter, M Ader, RN Bergman, P Herscovitch, KY Chen, AM Cypess	The Journal of Clinical Investigation	2020



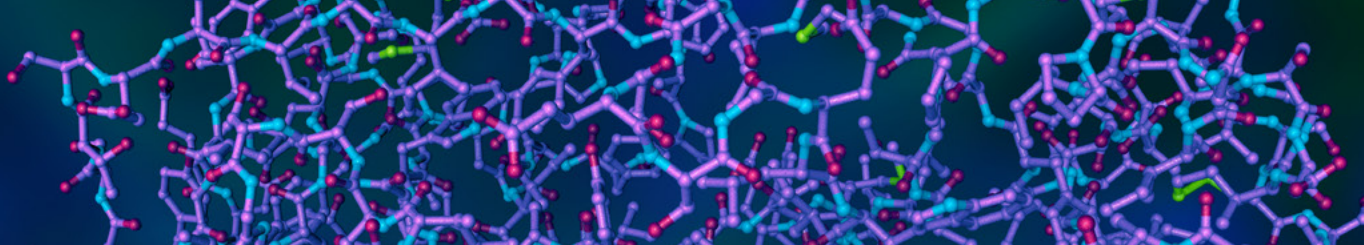
Pharmaceuticals

Title	Authors	Journal	Date
Cysteine aminoethylation enables the site-specific glycosylation analysis of recombinant human erythropoietin using trypsin	S Lippold, A Büttner, MSF Choo, M Hook, CJ de Jong, T Nguyen-Khuong, M Haberger, D Reusch, M Wuhrer, N de Haan	Analytical Chemistry	2020
Nitro-oleic acid, a ligand of CD36, reduces cholesterol accumulation by modulating oxidized-LDL uptake and cholesterol efflux in RAW264.7 macrophages	MM Vazquez, MV Gutierrez, SR Salvatore, M Puiattie, VA Dato, GA Chiabrando, BA Freeman, FJ Schopfer, G Bonacci	Redox Biology	2020
Physicochemical and biological evaluation of JR-131 as a biosimilar to a long-acting erythropoiesis-stimulating agent darbepoetin alfa	J Tani, Y Ito, S Tatemichi, M Yamakami, T Fukui, Y Hatano, S Kakimoto, A Kotani, A Sugimura, K Mihara, R Yamamoto, N Tanaka, K Minami, K Takahashi, T Hirato	PLOS One	2020
Strategies in developing high-throughput liquid chromatography protocols for method qualification of pharmacopeial monographs	GA Kresge, S Grosse, A Zimmer, KM Grinias, MD Pra, JMT Wong, F Steiner, JP Grinias	Journal of Separation Science	2020
Retina-targeted delivery of 17 β -estradiol by the topically applied DHED prodrug	K Prokai-Tatrai, Vien Nguyen, DL De La Cruz, R Guerra, K Zaman, F Rahlouni, L Prokai	Pharmaceutics	2020
A bioanalytical UHPLC based method used for the quantification of thymoquinone-loaded-PLGA-nanoparticles in the treatment of epilepsy	N Ahmad, R Ahmad, SA Qatifi, M Alessa, HA Hajji, M Sarafroz	BMC Chemistry	2020
Quantification of T cell binding polyclonal rabbit anti-thymocyte globulin in human plasma with liquid chromatography tandem-mass spectrometry	ME Amrani, R Admiraal, L Willaert, LJC Ebskamp-van Raaij, AM Lacna, CE Hack, ADR Huitema, S Nierkens, EM van Maarseveen	The AAPS Journal	2020
Evaluation of crystal zenith microtiter plates for high-throughput formulation screening	JA Floyd, JM Shaver, AJ Gillespie, U Park, RS Rogers, NS Nighlinger, Y Ogata, JJ James, BA Kerwin	Journal of Pharmaceutical Sciences	2020
Topical treatment of cutaneous leishmaniasis with novel amphotericin B-miltefosine co-incorporated second generation ultra-deformable liposomes	MJ Dar, S Khalid, CA McElroy, AR Satoskar, GM Khan	International Journal of Pharmaceutics	2020
Serum concentrations, pharmacokinetic/pharmacodynamic modeling, and effects of dexamethasone on inflammatory mediators following intravenous and oral administration to exercised horses	HK Knych, D Weiner, RM Arthur, R Baden, DS McKemie, PH Kass	Drug Testing and Analysis	2020
Development and validation of a sensitive UHPLC-MS/MS analytical method for venetoclax in mouse plasma, and its application to pharmacokinetic studies	ED Eisenmann, Y Jin, RH Weber, A Sparreboom, SD Baker	Journal of Chromatography B	2020
Chronic inhibition of CYP3A is temporarily reduced by each hemodialysis session in patients with end-stage renal disease	EJ Egeland, BJ Witczak, HK Zaré, H Christensen, A Åsberg, I Robertsen	Clinical Pharmacology, and Therapeutics	2020
Effects of titanium contamination caused by iron-free high-performance liquid chromatography systems on peak shape and retention of drugs with chelating properties	M De Pra, G Greco, MP Krajewski, M Martin, E George, N Bartsch, F Steiner	Journal of Chromatography A	2020



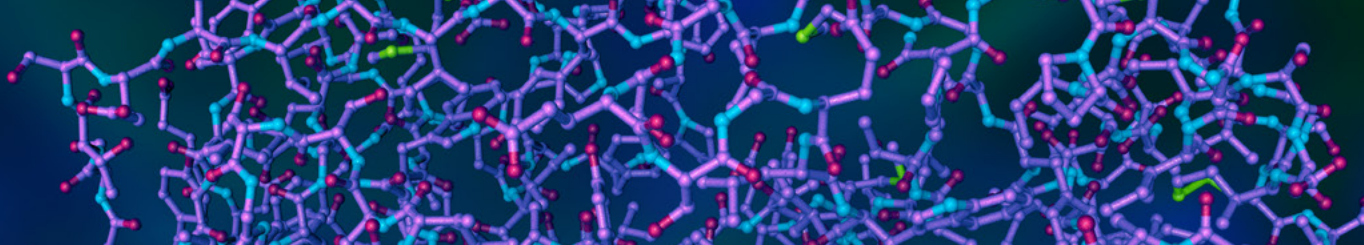
Proteins

Title	Authors	Journal	Date
Methylation of protein aspartates and deamidated asparagines as a function of blood bank storage and oxidative stress in human red blood cells	JA Reisz, T Nemkov, M Dzieciatkowska, R Culp-Hill, D Stefanoni, RC Hill, T Yoshida, A Dunham, T Kanias, LJ Dumont, M Busch, EZ Eisenmesser, JC Zimring, KC Hansen, A D'Alessandro	Transfusion	2018
Development and validation of a targeted affinity-enrichment and LC-MS/MS proteomics approach for the therapeutic monitoring of adalimumab	Y Yang, E Wysocki, K Antwi, E Niederkofler, EKY Leung, E Lazar-Molnar, KTJ Yeo	Clinica Chimica Acta	2018
Cell-free identification of <i>S. cerevisiae</i> strains by analysis of supernatant using LC-MS	C Muste, KG Owens	Journal of the American Society for Mass Spectrometry	2018
The use of in-strip digestion for fast proteomic analysis on tear fluid from dry eye patients	Z Huang, CX Du, XD Pan	PLOS One	2018
Generic workflow for mapping of complex disulfide bonds using in-source reduction and extracted ion chromatograms from data-dependent mass spectrometry	CN Cramer, CD Kelstrup, JV Olsen, KF Haselmann, PK Nielsen	Analytical Chemistry	2018
Assessing MS-based quantitation strategies for low-level impurities in peptide reference materials: application to angiotensin II	BB Stocks, MP Thibeault, J Meija, JE Melanson	Analytical and Bioanalytical Chemistry	2018
Dissecting ribosomal particles throughout the kingdoms of life using advanced hybrid mass spectrometry methods	M van de Waterbeemd, S Tamara, KL Fort, E Damoc, V Frac, P Bieri, M Itten, A Makarov, N Ban, AJR Heck	Nature Communications	2018
Molecular basis for the loss-of-function effects of the Alzheimer's disease-associated R47H variant of the immune receptor TREM2	A Sudom, S Talreja, J Danao, E Bragg, R Kegel, X Min, J Richardson, Z Zhang, N Sharkov, E Marcora, S Thibault, J Bradley, S Wood, AC Lim, H Chen, S Wang, IN Foltz, S Sambashivan, Z Wang	Journal of Biological Chemistry	2018
Analysis of insulin and insulin analogs from dried blood spots by means of liquid chromatography-high resolution mass spectrometry	A Thomas, M Thevis	Drug Testing and Analysis	2018
Deciphering the role of EGL-3 for neuropeptides processing in <i>Caenorhabditis elegans</i> using high-resolution quadrupole-Orbitrap mass spectrometry	JB Salem, B Nkambeu, DN Arvanitis, F Beaudry	Neurochemical Research	2018
Proteometabolomics of melphalan resistance in multiple myeloma	DC Koomen, JD Guingab-Cagmat, PS Oliveira, B Fang, M Liu, EA Welsch, MB Meads, T Nguyen, L Meke, SA Eschrich, KH Shain, TJ Garrett, JM Koomen	Methods in Molecular Biology	2019
The challenge of classifying metastatic cell properties by molecular profiling exemplified with cutaneous melanoma cells and their cerebral metastasis from patient derived mouse xenografts	B Neuditschko, L Janker, L Niederstaetter, J Brunmair, K Krivanek, S Izraely, O Sagi-Assif, T Meshel, BK Keppler, G Del Favero, IP Witz, C Gerner	Molecular & Cellular Proteomics	2019
Automating complex, multistep processes on a single robotic platform to generate reproducible phosphoproteomic data	BT Mullis, S Hwang, LA Lee, A Iliuk, R Woolsey, D Quilici, Q Wang	SLAS Discovery	2019
Exploiting the dynamic relationship between peptide separation quality and peptide coisolation in a multiple-peptide matches-per-spectrum approach offers a strategy to optimize bottom-up proteomics throughput and depth	MIV Solis, RJ Giannone, RL Hettich, PE Abraham	Analytical Chemistry	2019



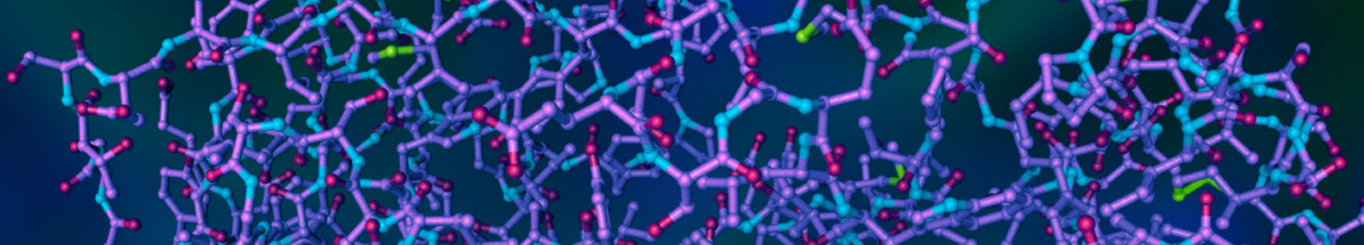
Proteins

Title	Authors	Journal	Date
EGL-3 and EGL-21 are required to trigger nocifensive response of <i>Caenorhabditis elegans</i> to noxious heat	B Nkambeu, JB Salem, S Leonelli, FA Marashi, F Beaudry	Neuropeptides	2019
Corona discharge electrospray ionization of formate-containing solutions enables in-source reduction of disulfide bonds	BB Stocks, JE Melanson	Analytical and Bioanalytical Chemistry	2019
Rapid characterization of chemical components in edible mushroom <i>Sparassis crispa</i> by UPLC-Orbitrap MS analysis and potential inhibitory effects on allergic rhinitis	Z Wang, J Liu, X Zhong, J Li, Z Wang, L Ji, Z Shang	Molecules	2019
Identificaion and CRISPR inactivation and CRISPR/Cas9 inactivation of the C1s protease responsible for proteolysis of recombinant proteins produced in CHO cells	SW Li, B Yu, G Byrne, M Wright, S O'Rourke, K Mesa, PW Berman	Biotechnology and Bioengineering	2019
Neuropeptidomics: Comparison of parallel reaction monitoring and data-independent acquisition for the analysis of neuropeptides using high-resolution mass spectrometry	M Saidi, S Kamali, F Beaudry	Biomedical Chromatography	2019
Cracking proteoform complexity of ovalbumin with anion-exchange chromatography–high-resolution mass spectrometry under native conditions	F Füssli, A Criscuolo, K Cook, K Scheffler, J Bones	Journal of Proteome Research	2019
Identification of bioactive short peptides in cow milk by high-performance liquid chromatography on C18 and porous graphitic carbon coupled to high-resolution mass spectrometry	CM Montone, AL Capriotti, A Cerrato, M Antonelli, G La Barbera, S Piovesana, A Laganà, C Cavaliere	Analytical and Bioanalytical Chemistry	2019
Sensitive untargeted identification of short hydrophilic peptides by high performance liquid chromatography on porous graphitic carbon coupled to high resolution mass spectrometry	S Piovesana, CM Montone, C Cavaliere, C Crescenzi, G La Barbera, A Laganà, AL Capriotti	Journal of Chromatography A	2019
Graphitized carbon black enrichment and UHPLC-MS/MS allow to meet the challenge of small chain peptidomics in urine	S Piovesana, AL Capriotti, A Cerrato, C Crescenzi, G La Barbera, A Laganà, CM Montone, C Cavaliere	Analytical Chemistry	2019
Identification and tracking of problematic host cell proteins removed by a synthetic, highly functionalized nonwoven media in downstream bioprocessing of monoclonal antibodies	S Gilgunn, H El-Sabbahy, S Albrecht, M Gaikwad, K Corrigan, L Deakin, G Jellum, J Bones	Journal of Chromatography A	2019
A colorful pallet of B-phycoerythrin proteoforms exposed by a multimodal mass spectrometry approach	S Tamara, M Hoek, RA Scheltema, AC Leney, AJR Heck	Chem	2019
Monitoring of on-column methionine oxidation as part of a system suitability test during UHPLC–MS/MS peptide mapping	B Mautz, M König, V Larraillet, M Mølhøj	LCGC	2019
Evaluation of peptide fractionation and native digestion as two novel sample preparation workflows to improve HCP characterization by LC–MS/MS	R Kufer, M Haindl, H Wegele, S Wohlrab	Analytical Chemistry	2019



Proteins

Title	Authors	Journal	Date
Quantification of coagulation factor VIII in human plasma with liquid chromatography tandem mass spectrometry using a selective sample purification with camelid nanobodies	M El Amrani, AAM Donners, G Graat, EG Lentjes, A Huisman, REA Musson, EM van Maarseveen		2019
The effects of exercise on pain and reproductive performance in female pregnant mice with neuropathic pain	M Parent-Vachon, F Beaudry, D Carrier, G Di Cristo, P Vachon	Biological Research for Nursing	2019
Proteomic modelling of gluten digestion from a physiologically relevant food system: A focus on the digestion of immunogenic peptides from wheat implicated in celiac disease	O Ogilvie, S Roberts, K Sutton, L Domigan, N Larsen, J Gerrard, N Demarais	Food Chemistry	2020
Peptide selection for accurate targeted protein quantification via a dimethylation high-resolution mass spectrum strategy with a peptide release kinetic model	Q Chen, Y Jiang, Y Ren, M Ying, B Lu	ACS Omega	2020
Monitoring modifications in biopharmaceuticals: Toolbox for a generic and robust high-throughput quantification method	LG Bauer, S Hoelterhoff, T Graf, C Bell, A Bathke	Journal of Chromatography B	2020
The tetrameric pheromone module SteC-MkkB-MpkB-SteD regulates asexual sporulation, sclerotia formation and aflatoxin production in <i>Aspergillus flavus</i>	D Frawley, C Greco, B Oakley, MM Alhussain, AB Fleming, NP Keller, Ö Bayram	Cellular Microbiology	2020
Outer membrane channel protein TolC regulates <i>Escherichia coli</i> K12 sensitivity to plantaricin BM-1 via the CpxR/CpxA two-component regulatory system	H Wang, H Zhang, H Zhang, J Jin, Y Xie	Probiotics and Antimicrobial Proteins	2020
Quantitative proteomic analysis reveals the influence of plantaricin BM-1 on metabolic pathways and peptidoglycan synthesis in <i>Escherichia coli</i> K12	H Wang, Y Xie, H Zhang, J Jin, H Zhang	PLOS One	2020
Comparative proteomic analysis reveals the molecular mechanisms underlying the accumulation difference of bioactive constituents in <i>Glycyrrhiza uralensis</i> fisch under salt stress	C Wang, L Chen, ZC Cai, C Chen, Z Liu, X Liu, L Zou, J Chen, M Tan, L Wei, Y Mei	Journal of Agricultural and Food Chemistry	2020
Structural similarity with cholesterol reveals crucial insights into mechanisms sustaining the immunomodulatory activity of the mycotoxin alternariol	G Del Favero, RM Mayer, L Dellaflora, L Janker, L Niederstaetter, C Dall'Asta, C Gerner, D Marko	Cells	2020
Measurement of surface protein antigens, PorA and PorB, in Bexsero vaccine using quantitative mass spectrometry	G Whiting, C Vipond, A Facchetti, H Chan, JX Wheeler	Vaccine	2020
Quantitative proteomic analysis reveals the mechanisms of polymyxin B toxicity to <i>Escherichia coli</i>	J Liu, Z Huang, B Ruan, H Wang, M Chen, S Rehman, P Wu	Chemosphere	2020
Quantification of total apolipoprotein E and its isoforms in cerebrospinal fluid from patients with neurodegenerative diseases	K Minta, G Brinkmalm, S Janelidze, S Sjödin, E Stomrud, H Zetterberg, K Blennow, O Hansson, U Andreasson	Alzheimer's Research and Therapy	2020
A clean-up strategy for identification of circulating endogenous short peptides in human plasma by zwitterionic hydrophilic liquid chromatography and untargeted peptidomics identification	S Piovesana, A Cerrato, M Antonelli, B Benedetti, AL Capriotti, C Cavaliere, CM Montone, A Laganà	Journal of Chromatography A	2020



Proteins

Title	Authors	Journal	Date
How presence of a signal peptide affects human galectins-1 and -4: Clues to explain common absence of a leader sequence among adhesion/growth-regulatory galectins	TJ Kutzner, AM Higuero, M Süßmair, J Kopitz, M Hingar, N Díez-Revuelta, GG Caballero, H Kaltner, I Lindner, J Abad-Rodríguez, D Reusch, HJ Gabius	Biochimica et Biophysica Acta - General Subjects	2020
Impaired EAT-4 vesicular glutamate transporter leads to defective nocifensive response of <i>Caenorhabditis elegans</i> to noxious heat	S Leonelli, B Nkambeu, F Beaudry	Neurochemical Research	2020
A new opening for the tricky untargeted investigation of natural and modified short peptides	A Cerrato, SE Aita, AL Capriotti, C Cavaliere, CM Montone, A Laganà, S Piovesana	Talanta	2020
Dietary choline supplementation attenuates high-fat-diet-induced hepatocellular carcinoma in mice	AL Brown, K Conrad, DS Allende, AD Gromovsky, R Zhang, CK Neumann, AP Owens III, M Tranter, RN Helsley	The Journal of Nutrition	2020
Structure-based design of prefusion-stabilized filovirus glycoprotein trimers	L Rutten, MSA Gilman, S Blokland, J Juraszek, JS McLellan, JPM Langedijk	Cell Reports	2020
How paired PSII-LHCII supercomplexes mediate the stacking of plant thylakoid membranes unveiled by structural mass-spectrometry	P Albanese, S Tamara, G Saracco, RA Scheltema, C Pagliano	Nature Communications	2020
Immunoaffinity microflow liquid chromatography/tandem mass spectrometry for the quantitation of PD1 and PD-L1 in human tumor tissues	Y Zhu, J Zalaznick, B Slecza, K Parrish, Z Yang, T Olah, P Shipkova	Rapid Communications in Mass Spectrometry	2020
Isomeric separation of N-glycopeptides derived from glycoproteins by porous graphitic carbon (PGC) LC-MS/MS	R Zhu, Y Huang, J Zhao, J Zhong, Y Mechref	Analytical Chemistry	2020
Proline behavior in model prebiotic peptides formed by wet-dry cycling	JN Ervin, M Bouza, FM Fernández, JG Forsythe	ACS Earth and Space Chemistry	2020
Cyclodepsipeptide biosynthesis in <i>Hypocreales</i> fungi and sequence divergence of The non-ribosomal peptide synthase genes	M Urbaniak, A Waśkiewicz, A Trzebny, G Koczyk, Ł Stępień	Pathogens	2020
Revealing dynamic protein acetylation across subcellular compartments	J Baeza, AJ Lawton, J Fan, MJ Smallegan, I Lienert, T Gandhi, OM Bernhardt, L Reiter, JM Denu	Journal of Proteome Research	2020
The pathways by which the marine diatom <i>Thalassiosira</i> sp. OUC2 biodegrades p-xylene, combined with a mechanistic analysis at the proteomic level	W Duan, S Du, F Meng, X Peng, L Peng, Y Lin, G Wang, J Wu	Ecotoxicology and Environmental Safety	2020
Simplified quantification of insulin, its synthetic analogs and C-peptide in human plasma by means of LC-HRMS	A Thomas, R Yang, S Petring, L Bally, M Thevis	Drug Testing and Analysis	2020
Concentration and chemical stability of commercially available insulins: A high-resolution mass spectrometry study	F Baechler, C Stettler, B Vogt, L Bally, M Groessl	Diabetes Technology and Therapeutics	2020



Food

Title	Authors	Journal	Date
Mass spectrometric characterization of benzoxazinoid glycosides from rhizopus-elicited wheat (<i>Triticum aestivum</i>) seedlings	WJC de Bruijn, JP Vincken, K Duran, H Gruppen	Journal of Agricultural and Food Chemistry	2016
Green and chamomile teas, but not acarbose, attenuate glucose and fructose transport via inhibition of GLUT2 and GLUT5	JA Villa-Rodriguez, E Aydin, JS Gauer, A Pyner, G Williamson, A Kerimi	Molecular Nutrition and Food Research	2017
Reduced ultraviolet light transmission increases insecticide longevity in protected culture raspberry production	H Leach, JC Wise, R Isaacs	Chemosphere	2017
Quantification of 16 β -lactams in chicken muscle by QuEChERS extraction and UPLC-Q-Orbitrap-MS with parallel reaction monitoring	Q Chen, XD Pan, BF Huang, JL Han	Journal of Pharmaceutical and Biomedical Analysis	2017
Validation of a rapid and sensitive HPLC/MS method for measuring sucrose, fructose and glucose in plant tissues	N Georgelis, K Fencil, CM Richael	Food Chemistry	2018
Toward a harmonized and standardized protocol for the determination of total hydroxytyrosol and tyrosol content in virgin olive oil (VOO). Extraction solvent	N Nenadis, A Mastralexi, MZ Tsimidou, S Vichi, B Quintanilla-Casas, J Donarski, V Bailey-Horne, B Butinar, M Miklavčič, DLG González, TG Toschi	European Journal of Lipid Science and Technology	2018
Effect of purslane (<i>Portulaca oleracea</i> L.) extract on anti-browning of fresh-cut potato slices during storage	X Liu, Q Yang, Y Lu, Y Li, T Li, B Zhou, L Qiao	Food Chemistry	2019
Mass spectrometric characterisation of avenanthramides and enhancing their production by germination of oat (<i>Avena sativa</i>)	WJC de Bruijn, S van Dinteren, H Gruppen, JP Vincken	Food Chemistry	2019
Quantitative analysis and anti-inflammatory activity evaluation of the A-type avenanthramides in commercial sprouted oat products	C Hu, Y Tang, Y Zhao, S Sang	Journal of Food Composition and Analysis	2019
Comparative evaluation of six traditional fermented soybean products in East Asia: A metabolomics approach	YS Kwon, S Lee, SH Lee, HJ Kim, CH Lee	Metabolites	2019
Solvent and temperature effects of accelerated solvent extraction (ASE) with Ultra-high pressure liquid chromatography (UHPLC-PDA) technique for determination of piperine and its ICP-MS analysis	R Ahmad, N Ahmad, A Shehzad	Industrial Crops and Products	2019
Extraction of methyl xanthines and their UHPLC–DAD determination in consumable beverages used in Eastern province of Saudi Arabia	R Ahmad, N Ahmad, F AIOthman, H Mohammad, F AlZahrani	Biomedical Chromatography	2019
Extraction and UHPLC–DAD detection of undeclared substances in market-available dietary supplements and slimming products in Eastern region, Saudi Arabia: An application of principal component analysis	R Ahmad, N Ahmad, N AlHudaithi, A AlHebshi, A Bukhari	Biomedical Chromatography	2019
Chemical composition of commercial cow's milk	A Foroutan, AC Guo, R Vazquez-Fresno, M Lipfert, L Zhang, J Zheng, H Badran, Z Budinski, R Mandal, BN Ametaj, DS Wishart	The Journal of Agricultural and Food Chemistry	2019



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Title	Authors	Journal	Date
Chemometrics coupled with UPLC-MS/MS for simultaneous analysis of markers in the raw and processed <i>Fructus Xanthii</i> , and application to optimization of processing method by BBD design	J Hai, Y Liu, X Xudong, Y Meiling, G Xinyue, Y Bingyou, W Qui-Hong, K Hai-Xue	Phytomedicine	2019
Screening of multi-class antibiotics in pork meat by LC-Orbitrap-MS with modified QuEChERS extraction	Q Chen, XD Pan, BF Huang, JL Han, B Zhou	RSC Advances	2019
Pyrrolizidine alkaloids of blue heliotrope (<i>Heliotropium amplexicaule</i>) and their presence in Australian honey	MC de Jesus, NL Hungerford, SJ Carter, SR Anuj, JT Blanchfield, JJ De Voss, MT Fletcher	Journal of Agricultural and Food Chemistry	2019
Allelopathic effects account for the inhibitory effect of field-pea (<i>Pisum sativum</i> L.) shoots on wheat growth in dense clay subsoils	X Wang, S Peter, Z Liu, R Armstrong, S Rochfort, C Tang,	Biology and Fertility of Soils	2019
Composition and safety evaluation of tea from New Zealand kawakawa (<i>Piper excelsum</i>)	CA Butts, JW van Klink, NI Joyce, G Paturi, DI Hedderley, S Martell, D Harvey	Journal of Ethnopharmacology	2019
Anti-inflammatory effect and cellular uptake mechanism of peptides from common bean (<i>Phaseolus vulga</i> L.) milk and yogurts in Caco-2 mono- and Caco-2/EA.hy926 co-culture models	Y Chen, H Zhang, L Mats, R Liu, Z Deng, Y Mine, R Tsao	Journal of Agricultural and Food Chemistry	2019
Solvent and temperature effects of accelerated solvent extraction (ASE) coupled with ultra-high pressure liquid chromatography (UHPLC-DAD) technique for determination of thymoquinone in commercial food samples of black seeds (<i>Nigella sativa</i>)	R Ahmad, N Ahmad, A Shehzad	Food Chemistry	2020
Solvent and temperature effect of accelerated solvent extraction (ASE) coupled with ultra-high-pressure liquid chromatography (UHPLC-PDA) for the determination of methyl xanthines in commercial tea and coffee	R Ahmad, N Ahmad, WS Al-Anaki, FA Ismail, F Al-Jishi	Food Chemistry	2020
Identification and absolute quantification of animal blood products by peptide markers using an UPLC-MS/MS method	Y Zhang, S Wang, Y Ma, H Li & Y Li	European Food and Research Technology	2020
A comparison of the phenolic composition of old and young tea leaves reveals a decrease in flavanols and phenolic acids and an increase in flavonols upon tea leaf maturation	Z Liu, ME Bruins, WJC de Bruijn, JP Vincken	Journal of Food Composition and Analysis	2020
The phenolic compounds, tocopherols, and phytosterols in the edible oil of guava (<i>Psidium guava</i>) seeds obtained by supercritical CO2 extraction	CE Narvaez-Cuenca, ML Inampues-Charfuegan, AM Hurtado-Benavides, F Parada-Alfonso, JP Vincken	Journal of Food Composition and Analysis	2020
Impact of <i>Lactobacillus plantarum</i> 423 fermentation on the antioxidant activity and flavor properties of rice bran and wheat bran	M Wang, M Lei, N Samina, LL Chen, CL Liu, TT Yin, XT Yan, C Wu, H He, CP Yi	Food Chemistry	2020
Protein digestion of different protein sources using the INFOGEST static digestion model	R Sousa, R Portmann, S Dubois, I Recio, L Egger	Food Research International	2020
A rapid protocol to distinguish between <i>Citri exocarpium rubrum</i> and <i>Citri reticulatae pericarpium</i> based on the characteristic fingerprint and UHPLC-Q-TOF MS methods	L Shi, R Wang, T Liu, J Wu, H Zhang, Z Liu, S Liu, Z Liu	Food & Function	2020



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Title	Authors	Journal	Date
Analysis of peptide antibiotic residues in milk using liquid chromatography-high resolution mass spectrometry (LC-HRMS)	IL Wu, SB Turnipseed, WC Andersen & MR Madson	Food Additives & Contaminants: Part A	2020
Quality changes in cold pressed juices after processing by high hydrostatic pressure, ultraviolet-c light and thermal treatment at commercial regimes	VR de Souza, V Popović, S Bissonnette, I Ros, L Mats, L Duizer, K Warriner, T Koutchma	Innovative Food Science & Emerging Technologies	2020
Effect of acid on glycoalkaloids and acrylamide in French fries	H Liu, J Roasa, L Mats, H Zhu & S Shao	Food Additives & Contaminants: Part A	2020
Effect of different combined mechanical and thermal treatments on the quality characteristics of garlic paste	B Zhang, Z Zheng, N Liu, P Liu, Z Qiu & X Qiao	Journal of Food Science and Technology	2020
Targeted characterization of acylated compounds from <i>Scrophulariae radix</i> using liquid chromatography coupled with Orbitrap mass spectrometry and diagnostic product ion-based data analysis	Z Shang, L Xu, H Wang, L Sun, T Bo, M Ye, X Qiao	Journal of Separation Science	2020
Optimization of extraction and quantification technique for phenolics content of garlic (<i>Allium sativum</i>): An application for comparative phytochemical evaluation based on cultivar origin	R Ahmad, N Ahmad, M Riaz, M Al-tarouti, F Aloufi, A AlDarwish, B Alalqa, B Alhanfoush, Z Khan	Biomedical Chromatography	2020
Optimizing the supercritical carbon dioxide extraction of sweet cherry (<i>Prunus avium</i> L.) leaves and UPLC-MS/MS analysis	H Zhang, Q Li, G Qiao, Z Qiu, Z Wen, X Wen	Analytical Methods	2020
Androgens modify therapeutic response to cabazitaxel in models of advanced prostate cancer	D Begemann, Y Wang, W Yang, N Kyprianou	The Prostate	2020
Effects of quercetin and cinnamaldehyde on the nutrient release from beef into soup during stewing process	Y Li, D Fan, Y Zhao, M Wang	Food Science and Technology	2020
Inhibitory effect of selected hydrocolloids on 2-amino-1-methyl-6-phenylimidazo [4,5-b]pyridine (PhIP) formation in chemical models and beef patties	H Yang, Z Ji, R Wang, D Fan, Y Zhao, M Wang	Journal of Hazardous Materials	2020
Endo-1,3(4)- β -glucanase-treatment of oat β -glucan enhances fermentability by infant fecal microbiota, stimulates dectin-1 activation and attenuates inflammatory responses in immature dendritic cells	R Akkerman, MJ Logtenberg, R An, MA Van Den Berg, BJ de Haan, MM Faas, E Zoetendal, P de Vos, HA Schols	Nutrients	2020
Terpinen-4-ol enhances disease resistance of postharvest strawberry fruit more effectively than tea tree oil by activating the phenylpropanoid metabolism pathway	Z Li, N Wang, Y Wei, X Zou, S Jiang, F Xu, H Wang, X Shao	Journal of Agricultural and Food Chemistry	2020
Pre-harvest treatment of kiwifruit trees with mixed culture fermentation broth of <i>Trichoderma pseudokoningii</i> and <i>Rhizopus nigricans</i> prolonged the shelf life and improved the quality of fruit	Q Ma, Y Cong, J Wang, C Liu, L Feng, K Chen	Postharvest Biology and Technology	2020



Food

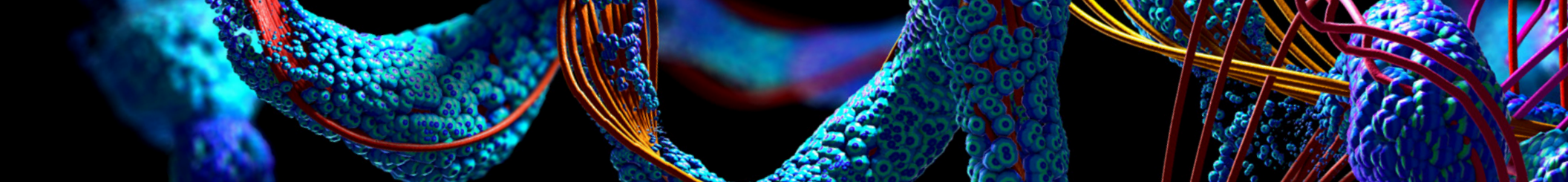
Title	Authors	Journal	Date
New insights into cheddar cheese microbiota-metabolome relationships revealed by integrative analysis of multi-omics data	R Afshari, CJ Pillidge, E Read, S Rochfort, DA Dias, AM Osborn, H Gill	Scientific Reports	2020
Determination of 400 pesticide residues in green tea leaves by UPLC-MS/MS and GC-MS/MS combined with QuEChERS extraction and mixed-mode SPE clean-up method	TK Ly, TD Ho, P Behra, TT Nhu-Trang	Food Chemistry	2020
Exogenous salicylic acid mitigates the accumulation of some pesticides in cucumber seedlings under different cultivation methods	T Liu, C Yuan, Y Gao, J Luo, S Yang, S Liu, R Zhang, N Zou	Ecotoxicology and Environmental Safety	2020
A rapid method for the detection of extra virgin olive oil adulteration using UHPLC-CAD profiling of triacylglycerols and PCA	HS Green, X Li, M De Pra, KS Lovejoy, F Steiner, IN Acworth, SC Wang	Food Control	2020

(Bio)Synthesis

Title	Authors	Journal	Date
Characterization of the functional variance in MbtH-like protein interactions with a nonribosomal peptide synthetase	RA Schomer, MG Thomas	Biochemistry	2017
Antibacterial 3,6-Disubstituted 4-Hydroxy-5,6-dihydro-2H-pyran-2-ones from <i>Serratia plymuthica</i> MF371-2	J Bjerketorp, JJ Levenfors, C Sahlberg, CL Nord, PF Andersson, B Guss, Bo Öberg, A Broberg	Journal of Natural Products	2017
The creatinase homolog MftE from <i>Mycobacterium smegmatis</i> catalyzes a peptide cleavage reaction in the biosynthesis of a novel ribosomally synthesized post-translationally modified peptide (RiPP)	NA Bruender, V Bandarian	Journal of Biological Chemistry	2017
Biochemical and structural characterization of a Schiff base in the radical-mediated biosynthesis of 4-demethylwyosine by TYW1	TAJ Grell, AP Young, CL Drennan, V Bandarian	Journal of the American Chemical Society	2018
A radical clock probe uncouples H atom abstraction from thioether cross-link formation by the radical s-adenosyl-l-methionine enzyme SkfB	WM Kincannon, NA Vruender, V Bandarian	Biochemistry	2018
Degradation of 4-chlorophenol in a batch electrochemical reactor using BDD electrodes	E Peralta, M Ruiz, G Martinez, J Mentado-Morales, LG Zárate, ME Cordero, M Garcia-Morales, R Natividad, A Regalado-Méndez	International Journal of Electrochemical Sciences	2018
Synthesis, purification, and mass spectrometric characterization of stable isotope-labeled amadori-glycated phospholipids	X He, Q Zhang	ACS Omega	2018
Green-light-sensitive BODIPY photoprotecting groups for amines	K Sitkowska, BL Feringa, W Szymański	The Journal of Organic Chemistry	2018
Total synthesis of tiacumicin A. Total synthesis, relay synthesis, and degradation studies of fidaxomicin (tiacumicin B, lipiarmycin A3)	H Hattori, E Kaufmann, H Miyatake-Ondozabal, R Berg, K Gademann	The Journal of Organic Chemistry	2018
Coupling of heterogeneous advanced oxidation processes and photocatalysis in efficient degradation of tetracycline hydrochloride by Fe-based MOFs: Synergistic effect and degradation pathway	Y Zhang, J Zhou, X Chen, L Wang, W Cai	Chemical Engineering Journal	2019
Taming the combinatorial explosion of the formose reaction via recursion within mineral environments	S Colón-Santos, GJT Cooper, L Cronin	ChemSystemsChem	2019
Palladium-catalyzed hydroxycarbonylation of (hetero)aryl halides for DNA-encoded chemical library synthesis	JY Li, G Miklossy, RK Modukuri, KM Bohren, Z Yu, M Palaniappan, JC Faver, K Riehle, MM Matzok, N Simmons	Bioconjugate Chemistry	2019
Selective production of dihydroxyacetone and glyceraldehyde by photo-assisted oxidation of glycerol	A Mendoza, R Romero, GP Gutiérrez-Cadillo, G López-Tellez, O Lorenzo-González, RM Gomez-Espinosa, R Natividad	Catalysis Today	2019
Rational design and optimization of a novel class of macrocyclic apoptosis signal-regulating kinase 1 inhibitors	MK Himmelbauer, Z Xin, JH Jones, I Enyedy, K King, DJ Marcotte, P Murugan, JC Santoro, T Hesson, K Spilker, JL Johnson, MJ Luzzio, R Gilfillan, FGL de Turiso	Journal of Medicinal Chemistry	2019
Replacement of an indole scaffold targeting human 15-lipoxygenase-1 using combinatorial chemistry	D Prismawan, R van der Vlag, H Guo, FJ Dekker, AKH Hirsch	Helvetica Chimica Acta	2019
Toward developing a yeast cell factory for the production of prenylated flavonoids	M Levisson, C Araya-Cloutier, WJC de Bruijn, M van der Heide, JMS Lopez, JM Daran, JP Vincken, J Beekwilder	Journal of Agricultural and Food Chemistry	2019

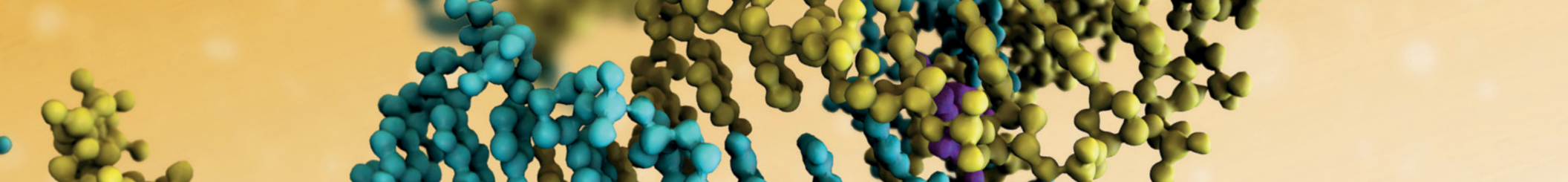
(Bio)Synthesis

Title	Authors	Journal	Date
Soft sensor-based monitoring and efficient control strategies of biomass concentration for continuous cultures of <i>Haloferax mediterranei</i> and their application to an industrial production chain	T Mainka, N Mahler, C Herwig, S Pflügl	Microorganisms	2019
Electro-oxidation of 2-chlorophenol with BDD electrodes in a continuous flow electrochemical reactor	E Peralta-Reyes, R Natividad, M Castellanos, J Mentado-Morales, ME Cordero, D Amado-Piña, A Regalado-Méndez	Journal of Flow Chemistry	2020
Room-temperature preparation of MIL-88A as a heterogeneous photo-Fenton catalyst for degradation of rhodamine B and bisphenol a under visible light	H Fu, XX Song, L Wu, C Zhao, P Wang, CC Wang	Materials Research Bulletin	2020
Protocol for community-created public MS/MS reference spectra within the Global Natural Products Social Molecular Networking infrastructure	F Vargas, KC Weldon, N Sikora, M Wang, Z Zhang, EC Gentry, MW Panitchpakdi, AM Caraballo-Rodríguez, PC Dorrestein, AK Jarmusch	Rapid Communications in Mass Spectrometry	2020
Rapid degradation of tetracycline hydrochloride by heterogeneous photocatalysis coupling persulfate oxidation with MIL-53(Fe) under visible light irradiation	Y Zhang, J Zhou, J Chen, X Feng, W Cai	Journal of Hazardous Materials	2020
In-situ construction of Co(OH) ₂ nanoparticles decorated urchin-like WO ₃ for highly efficient degradation of sulfachloropyridazine via peroxymonosulfate activation: Intermediates and DFT calculation	X Tao, P Pan, T Huang, L Chen, H Ji, J Qi, F Sun, W Liu	Chemical Engineering Journal	2020
A new carbazole-based colorimetric and ratiometric fluorescent probe for hypochlorite sensing in living cells and zebrafishes	A Feng, P Liu, Q Liang, X Zhang, L Huang, Y Jia, M Xie, Q Yan, C Li, S Wang	Dyes and Pigments	2020
Photocatalytic degradation of ofloxacin by perovskite-type NaNbO ₃ nanorods modified g-C ₃ N ₄ heterojunction under simulated solar light: Theoretical calculation, ofloxacin degradation pathways and toxicity evolution	D Zhang, J Qi, H Ji, S Li, T Huang, C Xu, X Chen, W Liu	Chemical Engineering Journal	2020
An investigation of the antileishmanial properties of semi-synthetic saponins	O Anderson, J Beckett, CC Briggs, LA Natrass, CF Cranston, EJ Wilkinson, JH Owen, RM Williams, A Loukaidis, ME Bouillon, D Pritchard, M Lahmann, MS Baird, PW Denny	RSC Medicinal Chemistry	2020
Facile enzymatic C _γ -acylation of lignin model compounds	R Hilgers, JP Vincken, MA Kabel	Catalysis Communications	2020
Controlling the competition: Boosting laccase/HBT-catalyzed cleavage of a β-O-4' linked lignin model	R Hilgers, A van Dam, H Zuilhof, JP Vincken, MA Kabel	ACS Catalysis	2020
Three-dimensional Co/Ni bimetallic organic frameworks for high-efficient catalytic ozonation of atrazine: Mechanism, effect parameters, and degradation pathways analysis	G Ye, Y Zhao, G Qiu, Y Hu, S Preis, C Wei	Chemosphere	2020
Oxidative release of thiol-conjugated forms of the mycotoxin 4-deoxynivalenol	S Uhlig, L Ivanova, CO Miles	Chemical Research in Toxicology	2020
Synthesis of molecularly imprinted polymer via emulsion polymerization for application in solanesol separation	G Zhao, J Liu, M Liu, X Han, Y Peng, X Tian, J Liu, S Zhang	Applied Sciences	2020



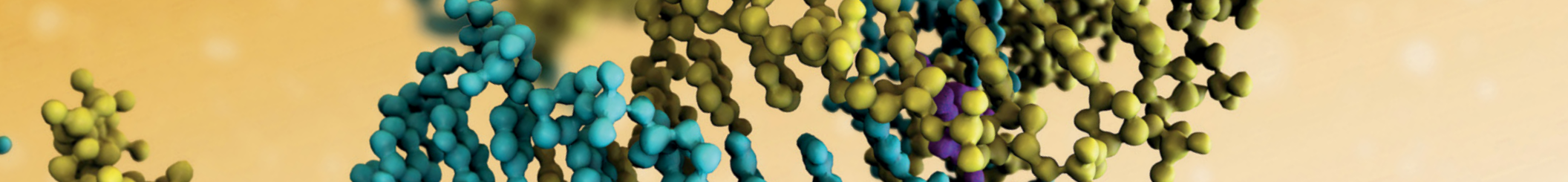
(Bio)Synthesis

Title	Authors	Journal	Date
Synthesis and investigation of novel chlorin sensitizers containing the myristic acid residue for antimicrobial photodynamic therapy	AV Kustov, TV Kustova, DV Belykh, IS Khudyaeva, DB Berezin	Dyes and Pigments	2020
Scale-up synthesis of IID572: A new β-lactamase inhibitor	M Furegati, S Nocito, F Reck, A Casarez, R Simmons, H Schuetz, G Koch	Organic Process Research and Development	2020
Directed evolution of adenine base editors with increased activity and therapeutic application	NM Gaudelli, DK Lam, HA Rees, NM Solá-Estevés, LA Barrera, DA Born, A Edwards, JM Gehrke, SJ Lee, AJ Liquori, R Murray, MS Packer, C Rinaldi, IM Slaymaker, J Yen, LE Young, G Ciaramella	Nature Biotechnology	2020
PelX is a UDP-N-acetylglucosamine C4-epimerase involved in Pel polysaccharide-dependent biofilm formation	LS Marmont, GB Whitfield, R Pfoh, RJ Williams, TE Randall, A Ostaszewski, E Razvi, RA Groves, H Robinson, M Nitz, MR Parsek, IA Lewis, JC Whitney, JJ Harrison, PL Howell	Journal of Biological Chemistry	2020



Nucleic Acids

Title	Authors	Journal	Date
Novel ribonuclease activity of cusativin from <i>Cucumis sativus</i> for mapping nucleoside modifications in RNA	B Addepalli, S Venus, P Thakur, PA Limbach	Analytical and Bioanalytical Chemistry	2017
Development of SPE method for the extraction of phosphorothioate oligonucleotides from serum samples	Łukasz Nuckowski, A Kaczmarkiewicz, S Studzińska	Bioanalysis	2018
Salmonella reprograms nucleotide metabolism in its adaptation to nitrosative stress	LF Fitzsimmons, L Liu, JS Kim, J Jones-Carson, A Vázquez-Torres	mBio	2018
Gene <i>ssfg_01967</i> (<i>miaB</i>) for tRNA modification influences morphogenesis and moenomycin biosynthesis in <i>Streptomyces ghanensis</i> ATCC14672	Y Sehlin, O Koshla, Y Dacyuk, R Zhao, R Ross, M Myronovskiy, PA Limbach, A Luzhetskyy, S Walker, V Fedorenko, B Ostash	Microbiology	2018
Differentiating positional isomers of nucleoside modifications by higher-energy collisional dissociation mass spectrometry (HCD MS)	M Jora, AP Burns, RL Ross, PA Lobue, R Zhao, CM Palumbo, PA Beal, B Addepalli, PA Limbach	Journal of the American Society for Mass Spectrometry	2018
Development of DNA-compatible Suzuki-Miyaura reaction in aqueous media	JY Li, H Huang	Bioconjugate Chemistry	2018
Directed evolution of heterologous tRNAs leads to reduced dependence on post-transcriptional modifications	KC Baldrige, M Jora, AC Maranhao, MM Quick, B Addepalli, JS Brodbelt, AD Ellington, PA Limbach, LM Contreras	ACS Synthetic Biology	2018
A new approach to preparation of antisense oligonucleotide samples with microextraction by packed sorbent	Łukasz Nuckowski, A Kaczmarkiewicz, S Studzińska, B Buszewski	Analyst	2019
Safety evaluation of 2'-deoxy-2'-fluoro nucleotides in GalNAc-siRNA conjugates	MM Janas, I Zlatev, J Liu, Y Jiang, SA Barros, JE Sutherland, WP Davis, J Liu, CR Brown, X Liu, MK Schlegel, L Blair, X Zhang, B Das, C Tran, K Aluri, J Li, S Agarwal, R Indrakanti, K Charisse, J Nair, S Matsuda, KG Rajeev, T Zimmermann, L Sepp-Lorenzino, Y Xu, A Akinc, K Fitzgerald, AK Vaishnav, PF Smith, M Manoharan, V Jadhav, JT Wu, MA Maier	Nucleic Acids Research	2019
Conversion of PRPS hexamer to monomer by AMPK-mediated phosphorylation inhibits nucleotide synthesis in response to energy stress	X Qian, X Li, L Tan, JH Lee, Y Xia, Q Cai, Y Zheng, H Wang, PL Lorenzi, Z Lu	Cancer Discovery	2019
Cyclic GMP-AMP signalling protects bacteria against viral infection	D Cohen, S Melamed, A Millman, G Shulman, Y Oppenheimer-Shaanan, A Kacen, S Doron, G Amitai, R Sorek	Nature	2019
TYW1: A radical SAM enzyme involved in the biosynthesis of wybutosine bases	AP Young, V Bandarian	Methods in Enzymology	2019
Pseudouridines on <i>Trypanosoma brucei</i> spliceosomal small nuclear RNAs and their implication for RNA and protein interactions	KS Rajan, T Doniger, S Cohen-Chalamish, D Chen, O Semo, S Aryal, EG Saar, V Chikne, D Gerber, R Unger, C Tschudi, S Michaeli	Nucleic Acids Research	2019
MTHFD1 interaction with BRD4 links folate metabolism to transcriptional regulation	S Sdelci, AF Rendeiro, P Rathert, W You, JMG Lin, A Ringler, G Hofstätter, HP Moll, B Gürtl, M Farlik, S Schick, F Klepsch, M Oldach, P Buphamalai, F Schischlik, P Májek, K Parapatics, C Schmid, M Schuster, T Penz, DL Buckley, O Hudecz, R Imre, SY Wang, HM Maric, R Kralovics, KL Bennett, AC Müller, K Mechtler, J Menche, JE Bradner, GE Winter, K Klavins, E Casanova, C Bock, J Uber, S Kubicek	Nature Genetics	2019



Nucleic Acids

Title	Authors	Journal	Date
Improved application of RNAModMapper – an RNA modification mapping software tool – for analysis of liquid chromatography tandem mass spectrometry (LC-MS/MS) data	PA Lobue, N Yu, M Jora, S Abernathy, PA Limbach	Methods	2019
Physiology and effects of nucleosides in mice lacking all four adenosine receptors	C Xiao, N Liu, KA Jacobson, O Gavrilova, ML Reitman	PLOS Biology	2019
Distinct substrate specificities of the human tRNA methyltransferases TRMT10A and TRMT10B	NH Howell, M Jora, BF Jepson, PA Limbach, JE Jackman	RNA	2019
Hydrophilic interaction in solid-phase extraction of antisense oligonucleotides	Łukasz Nuckowski, A Kilanowska, S Studzińska	Journal of Chromatographic Science	2020
Ultra-high-performance reversed-phase liquid chromatography hyphenated with ESI-Q-TOF-MS for the analysis of unmodified and antisense oligonucleotides	S Studzińska, Łukasz Nuckowski, A Kilanowska	Chromatographia	2020
Survey and validation of tRNA modifications and their corresponding genes in <i>Bacillus subtilis</i> sp Subtilis strain 168	V de Crécy-Lagard, RL Ross, M Jaroch, V Marchand, C Eisenhart, D Brégeon, Y Motorin, PA Limbach	Biomolecules	2020
Characterization of antisense oligonucleotide impurities by ion-pairing reversed-phase and anion exchange chromatography coupled to hydrophilic interaction liquid chromatography/mass spectrometry using a versatile two-dimensional liquid chromatography setup	A Goyon, K Zhang	Analytical Chemistry	2020
Attachment of hybridizable oligonucleotides to a silica support and its application for selective extraction of unmodified and antisense oligonucleotides from serum samples	S Studzińska, M Skoczylas, S Bocain, A Dembska, B Buszewski	RSC Advances	2020
Extracellular cGAMP is a cancer-cell-produced immunotransmitter involved in radiation-induced anticancer immunity	JA Carozza, V Böhnert, KC Nguyen, G Skariah, KE Shaw, JA Brown, M Rafat, R von Eyben, EE Graves, JS Glenn, M Smith, L Li	Nature Cancer	2020
CBASS immunity uses CARF-related effectors to sense 3'-5'- and 2'-5'-linked cyclic oligonucleotide signals and protect bacteria from phage infection	B Lowey, AT Whiteley, AFA Keszei, BR Morehouse, IT Mathews, SP Antine, VJ Cabrera, D Kashin, P Niemann, M Jain, F Schwede, JJ Mekalanos, S Shao, ASY Lee, PJ Kranzusch	Cell	2020
C-N coupling of DNA-conjugated (hetero)aryl bromides and chlorides for DNA-encoded chemical library synthesis	YC Chen, JC Faver, AF Ku, G Miklossy, K Riehle, KM Bohren, MN Ucisik, MM Matzuk, Z Yu, N Simmons	Bioconjugate Chemistry	2020



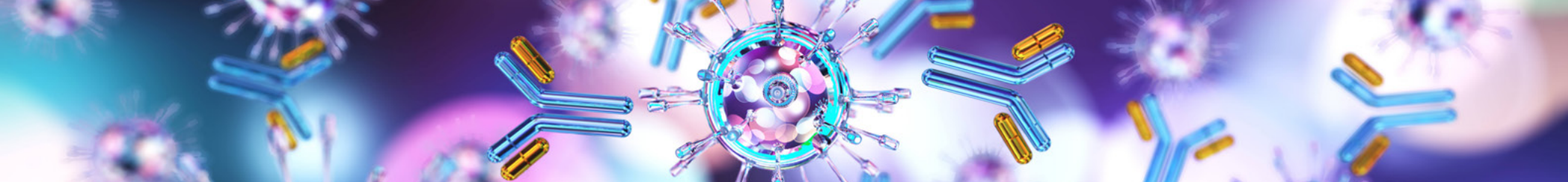
Traditional Medicine

Title	Authors	Journal	Date
Flavone glucosides from <i>Artemisia juncea</i>	BS Okhendedaev, M Bacher, RF Mukhamatkhanaev, IJ Shamyayov, G Zengin, S Böhmdorfer, NZ Mamadalieva, T Rosenau	Natural Product Research	2018
On-line comprehensive two-dimensional liquid chromatography tandem mass spectrometry for the analysis of <i>Curcuma kwangsiensis</i>	W Zhou, Z Guo, L Yu, H Zhou, A Shen, Y Jin, G Jin, J Yan, Y Liu, CR Wang, JT Feng, Y Liu, X Liang	Talanta	2018
UHPLC-MS/MS quantification combined with chemometrics for comparative analysis of different batches of raw, wine-processed, and salt-processed radix <i>Achyranthis bidentatae</i>	L Yang, H Jiang, M Yan, X Xing, X Guo, B Yang, Q Wang, H Kuang	Molecules	2018
Biflavones from <i>Ginkgo biloba</i> as inhibitors of human thrombin	TR Chen, LH Wei, XQ Guan, C Huang, Y Liu, FJ Wang, J Hou, Q Jin, YF Liu, PH Wen, SJ Zhang, GB Ge, WZ Guo	Bioorganic Chemistry	2019
Investigating the protective effect of gross saponins of <i>Tribulus terrestris</i> fruit against ischemic stroke in rat using metabolomics and network pharmacology	Y Wang, W Guo, Y Liu, J Wang, M Fan, H Zhao, S Xie, Y Xu	Metabolites	2019
Study on the antihypertensive mechanism of <i>Astragalus membranaceus</i> and <i>Salvia miltiorrhiza</i> based on intestinal flora-host metabolism	C Han, Y Jiang, W Li, Y Liu, Z Qi	Evidence-Based Complementary and Alternative Medicine	2019
Bioactivity-guided isolation and identification of antiadipogenic compounds in shiya tea (leaves of <i>Adinandra nitida</i>)	C Yuan, L Huang, JH Suh, Y Wang	Journal of Agricultural and Food Chemistry	2019
Taeumjowi-tang, a traditional Korean sasang remedy, improves obesity-atopic dermatitis comorbidity by regulating hypoxia-inducible factor 1 alpha	J Park, DH Youn, JW Kang, KS Ahn, HJ Kwak, JY Um	Frontiers in Pharmacology	2019
<i>Papaver nudicaule</i> (Iceland poppy) alleviates lipopolysaccharide-induced inflammation through inactivating NF- κ B and STAT3	JH Oh, M Yun, D Park, IJ Ha, CK Kim, DW Kim, EO Kim, SG Lee	BMC Complementary and Alternative Medicine	2019
Fermented dried <i>Citrus unshiu</i> peel extracts exert anti-inflammatory activities in LPS-induced RAW264.7 macrophages and improve skin moisturizing efficacy in immortalized human HaCaT keratinocytes	C Kim, J Ji, SH Baek, JH Lee, IJ Ha, SS Lim, HJ Yoon, YJ Nam, KS Ahn	Pharmaceutical Biology	2019
Rapid quantitation and identification of the chemical constituents in <i>Danhong Injection</i> by liquid chromatography coupled with Orbitrap mass spectrometry	L Xu, Shang, T Bo, L Sun, Q Guo, X Qiao, M Ye	Journal of Chromatography A	2019
Simultaneous determination of five iridoid glycosides and three flavonoid glycosides in <i>Hedyotis diffusa</i> wild by UPLC-UV with ultrasound-assisted extraction	X Huang, Y Wu, X Zhang, B Chen, H Luo, X Lin, P Shi, H Yao	Current Pharmaceutical Analysis	2019
Simultaneous determination of thirteen Q-markers in raw and processed <i>Tussilago farfara</i> L. by UPLC-QQQ-MS/MS coupled with chemometrics	L Yang, H Jiang, A Hou, X Guo, W Man, M Yan, X Xing, B Yang, Q Wang, H Kuang	Molecules	2019
A UPLC-MS/MS application for comparisons of the hepatotoxicity of raw and processed <i>Xanthii Fructus</i> by energy metabolites	H Jiang, L Yang, X Xing, M Yan, X Guo, A Hou, W Man, B Yang, Q Wang, H Kuang	RSC Advances	2019



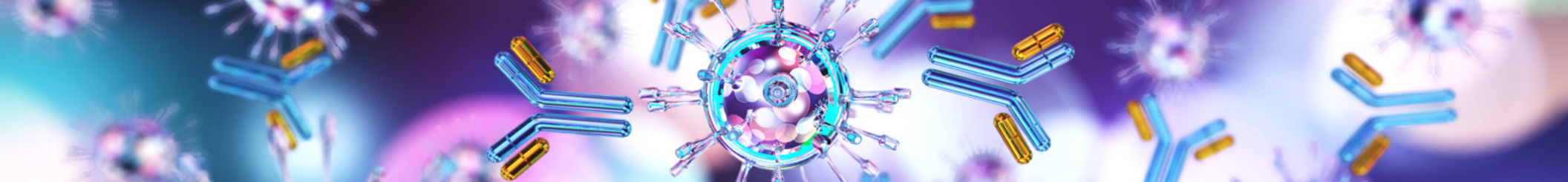
Traditional Medicine

Title	Authors	Journal	Date
Phytochemical analysis and biological evaluation of <i>Lagochilus</i> species from Uzbekistan	DK Akramov, M Bacher, S Böhmdorfer, T Rosenau, G Zengin, A Ptthast, L Nahar, SD Sarker, NZ Mamadalieva	Industrial Crops and Products	2020
An integrated microbiome and metabolomic analysis identifies immunoenhancing features of <i>Ganoderma lucidum</i> spores oil in mice	X Wu, J Cao, M Li, P Yao, H Li, W Xu, C Yuan, J Liu, S Wang, P Li, Y Wang	Pharmacological Research	2020
Pharmacokinetics and metabolism research of Shengkang injection in rats based on UHPLC-MS/MS and UHPLC-Q-Orbitrap HRMS	X Jiang, L Zhou, L Zou, X Wang, Y Shi, X Du, J Zhang, L Liu, L Xue, X Liu, Z Sun	Drug Design, Development and Theory	2020
Spleen and thymus metabolomics strategy to explore the immunoregulatory mechanism of total withanolides from the leaves of <i>Datura metel</i> L. on imiquimod-induced psoriatic skin dermatitis in mice	Y Cheng, Y Liu, J Tan, Y Sun, W Guan, Y Liu, B Yang, H Kuang	Biomedical Chromatography	2020
Integrated serum metabolomics and network pharmacology approach to reveal the potential mechanisms of withanolides from the leaves of <i>Datura metel</i> L. on immune thrombocytopenic purpura	Y Cheng, Y Liu, J Tan, Y Sun, W Guan, P Jiang, B Yang, H Kuang	Journal of Pharmaceutical and Biomedical Analysis	2020
Rapid characterizaition of chemical constituents of the tubers of <i>Gymnadenia conopsea</i> by UPLC-Orbitrap-MS/MS analysis	X Wang, XJ Zhong, N Zhou, N Cai, JH Xu, QB Wang, JJ Li, Q Liu, PC Lin, ZY Shang	Molecules	2020
Effects of <i>Hericium erinaceus</i> mycelium extracts on the functional activity of purinoceptors and neuropathic pain in mice with L5 spinal nerve ligation	PP Yang, SH Chueh, HL Shie, CC Chen, LY Lee, WP Chen, YW Chen, L Shiu, PS Liu	Evidence-Based Complementary and Alternative Medicine	2020
Pharmacokinetic comparisons of eight active components from raw <i>Farfarae flos</i> and honey-processed <i>Farfarae flos</i> after oral administration in rats by UHPLC-MS/MS approaches	L Yang, H Jiang, X Guo, A Hou, W Man, S Wang, J Zhang, B Yang, J Li, H Kuang	Journal of Analytical Methods in Chemistry	2020
Screening and quantification of TNF- α ligand from <i>Angelicae pubescentis radix</i> by biosensor and UPLC-MS/MS	L Yang, A Hou, S Wang, J Zhang, J Zhang, W Man, X Guo, B Yang, Q Wang, H Jiang, H Kuang	Analytical Biochemistry	2020
α -glucosidase inhibitory activity of the extracts and major phytochemical components of <i>Smilax glabra</i> Roxb	PTM Nguyen, QV Ngo, MTH Nguyen, AT Maccarone, SG Pyne	The Natural Products Journal	2020



Antibodies

Title	Authors	Journal	Date
Process-relevant concentrations of the leachable bDtbPP impact negatively on CHO cell production characteristics	PS Kelly, S McSweeney, O Coleman, S Carillo, M Henry, D Chandran, A Kellett, J Bones, M Clynes, P Meleady, N Barron	Biotechnology Progress	2016
Coformulation of broadly neutralizing antibodies 3BNC117 and PGT121: Analytical challenges during preformulation characterization and storage stability studies	A Patel, V Gupta, J Hickey, NS Nightlinger, RS Rogers, C Siska, SB Joshi, MS Seaman, DB Volkin, BA Kerwin	Journal of Pharmaceutical Sciences	2018
Development of two analytical methods bBased on reverse phase chromatographic and SDS-PAGE gel for assessment of deglycosylation yield in N-glycan mapping	AD Eckard, DR Dupont, JK Young	BioMed Research International	2018
Native mass spectrometry combined with enzymatic dissection unravels glycoform heterogeneity of biopharmaceuticals	T Wohlschlager, K Scheffler, IC Forstenlehner, W Skala, S Senn, E Damoc, J Holzmann, CG Huber	Nature Communications	2018
Charge variant analysis of monoclonal antibodies using direct coupled pH gradient cation exchange chromatography to high-resolution native mass spectrometry	F, Füssl, K Cook, K Scheffler, A Farrell, S Mittermayr, J Bones	Analytical Chemistry	2018
Monoclonal antibodies sequence assessment using a hybrid quadrupole-Orbitrap mass spectrometer	A Farrell, S Carillo, K Scheffler, K Cook, J Bones	Analytical Methods	2018
Charge variant native mass spectrometry benefits mass precision and dynamic range of monoclonal antibodies intact mass analysis	AO Bailey, G Han, W Phung, P Gazis, J Sutton, JL Josephs, W Sandoval	MAbs	2018
A case study to identify the drug conjugation site of a site-specific antibody-drug-conjugate using middle-down mass spectrometry	O Hernandez-Alba, S Houel, S Hessman, S Erb, D Rabuka, R Huguet, J Josephs, A Beck, PM Drake, S Cianferani	Journal of the American Society for Mass Spectrometry	2019
Detection of the myostatin-neutralizing antibody Domagrozumab in serum by means of Western blotting and LC-HRMS	K Walpurgis, A Thomas, M Thevis	Drug Testing and Analysis	2019
Comprehensive characterisation of the heterogeneity of adalimumab via charge variant analysis hyphenated on-line to native high resolution Orbitrap mass spectrometry	F Füssl, A Trappe, K Cook, K Scheffler, O Fitzgerald, J Bones	Mabs	2019
SEC-ICP-MS and on-line isotope dilution analysis for characterisation and quantification of immunochemical assays	D Clases, RG de Vega, D Bishop, P Doble	Analytical and Bioanalytical Chemistry	2019
Characterization of native reversible self-association of a monoclonal antibody mediated by Fab-Fab interaction	L Gentiluomo, D Roessner, W Streicher, S Mahapatra, P Harris, W Strieß	Journal of Pharmaceutical Sciences	2020
Stable isotope dilution LC-HRMS assay to determine free SN-38, total SN-38, and SN-38G in a tumor xenograft model after intravenous administration of antibody–drug conjugate (Sacituzumab Govitecan)	R Pandey, A Gruslova, J Chiou, AJ Brenner, S Tiziani	Analytical Chemistry	2020
Impact of dextran on thermal properties, product quality attributes, and monoclonal antibody stability in freeze-dried formulations	C Haeuser, P Goldbach, J Huwyler, W Friess, A Allmendinger	European Journal of Pharmaceutics and Biopharmaceutics	2020



Antibodies

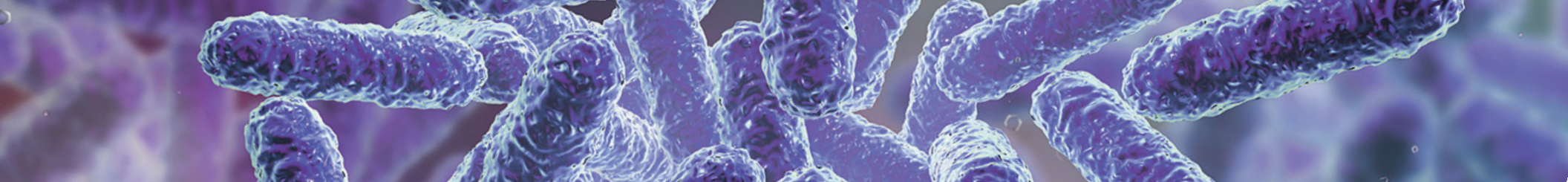
Title	Authors	Journal	Date
Analysis of cetuximab N-Glycosylation using multiple fractionation methods and capillary electrophoresis mass spectrometry	C Váradi, C Jakes, J Bones	Journal of Pharmaceutical and Biomedical Analysis	2020
Fluorescent detection of O-GlcNAc via tandem glycan labeling	ZL Wu, A Luo, A Grill, T Lao, Y Zou, Y Chen	Bioconjugate Chemistry	2020
An evaluation of instrument types for mass spectrometry-based multi-attribute analysis of biotherapeutics	Z Zhang, PK Chan, J Richardson, B Shah	mAbs	2020
Mass Spectrometry characterization of higher order structural changes associated with the Fc-glycan structure of the NISTmAb reference material, RM 8761	K Groves, A Cryar, AE Ashcroft, M Quaglia	Journal of the American Society for Mass Spectrometry	2020
Development of a 3D-LC/MS workflow for fast, automated, and effective characterization of glycosylation patterns of biotherapeutic products	J Camperi, L Dai, D Guillaume, C Stella	Analytical Chemistry	2020
Comparative elucidation of Cetuximab heterogeneity on the intact protein level by cation exchange chromatography and capillary electrophoresis coupled to mass spectrometry	F Füssli, A Trappe, S Carillo, C Jakes, J Bones	Analytical Chemistry	2020
Comparing different domains of analysis for the characterisation of N-glycans on monoclonal antibodies	S Carillo, R Pérez-Robles, C Jakes, MR da Silva, SM Martín, A Farrell, N Navas, J Bones	Journal of Pharmaceutical Analysis	2020
Rapid Intact mass based multi-attribute method in support of mAb upstream process development	C Lanter, M Lev, L Cao, V Loladze	Journal of Biotechnology	2020

Environmental

Title	Authors	Journal	Date
Identification of novel phosphorus-based flame retardants in curtains purchased in Japan using Orbitrap mass spectrometry	Y Miyake, M Tokumura, Q Wang, T Amagai, Y Takegawa, Y Yamagishi, S Ogo, K Kume, T Kobayashi, S Takasu, K Ogawa, K Kannan	Environmental Science and Technology Letters	2018
Efficacy of endothall dimethylalkylamine salt applied to static irrigation channels during winter to control aquatic weeds in temperate Australia	D Clements, KL Butler, TD Hunt, Z Liu, TM Dugdale	Journal of Aquatic Plant Management	2018
Sediment facilitates microbial degradation of the herbicides endothall monoamine salt and endothall dipotassium salt in an aquatic environment	MS Islam, TD Hunt, Z Liu, KL Butler, TM Dugdale	Environmental Research and Public Health	2018
Rapid removal of poly- and perfluorinated compounds from investigation-derived waste (IDW) in a pilot-scale plasma reactor	RK Singh, N Multari, C Nau-Hix, RH Anderson, SD Richardson, TM Holsen, SM Thagard	Environmental Science and Technology	2019
Analysis of university workplace building surfaces reveals usage-specific chemical signatures	LI McCall, VM Anderson, RS Fogle III, JJ Haffner, E Hossain, R Liu, AH Ly, H Ma, M Nadeem, S Yao	Building and Environment	2019
Aliphatic amines at the Cape Verde atmospheric observatory: Abundance, origins and sea-air fluxes	M van Pinxteren, KW Fomba, D van Pinxteren, N Triesch, EH Hoffmann, CHL Cree, MF Fitzsimons, W von Tümpling, H Herrmann	Atmospheric Environment	2019
Heteroxanthin as a pigment biomarker for <i>Gonyostomum</i> semen (Raphidophyceae)	CHC Hagman, T Rohrlack, S Uhlig, V Hostyeva	PLOS One	2019
Low maize pollen collection and low pesticide risk to honey bees in heterogeneous agricultural landscapes	C Urbanowicz, N Baert, SE Bluher, K Böröczky, M Ramos, SH McArt	Apidologie	2019
Deposition and source identification of nitrogen heterocyclic polycyclic aromatic compounds in snow, sediment, and air samples from the Athabasca Oil Sands Region	L Chibwe, CA Manzano, D Muir, B Atkinson, JL Kirk, CH Marvin, X Wang, C Teixeira, D Shang, T Harner, AO De Silva	Environmental Science and Technology Letters	2019
Investigations on the decomposition of AdBlue urea in the liquid phase at low temperatures by an electrochemically induced pH shift	P Braun, B Durner, HP Rabl, FM Matysik	Monatshefte für Chemie - Chemical Monthly	2019
Hydrodynamic exposure and time since application influence endothall amine potency against submersed aquatic plants	TM Dugdale, S Islam, TD Hunt, Z Liu, KL Butler, D Clements, MD Netherland	Aquatic Botany	2019
Separation and quantification of imidazoles in atmospheric particles using LC-Orbitrap-MS	M Teich, M Schmidpott, D van Pinxteren, J Chen, H Herrmann	Journal of Separation Science	2019
Removal of tetracycline from an aqueous solution using manganese dioxide modified biochar derived from Chinese herbal medicine residues	Q Shen, Z Wang, Q Yu, Y Cheng, Z Lui, T Zhang, S Zhou	Environmental Research	2020
Toxin analysis of freshwater cyanobacterial and marine harmful algal blooms on the west coast of Florida and implications for estuarine environments	JS Metcalf, SA Banack, RA Wessel, M Lester, JG Pim, JR Cassani, PA Cox	Neurotoxicity Research	2020

Environmental

Title	Authors	Journal	Date
Quantification of brominated polycyclic aromatic hydrocarbons in environmental samples by liquid chromatography tandem mass spectrometry with atmospheric pressure photoionization and post-column infusion of dopant	M Masuda, Q Wang, M Takumura, Y Miyake, T Amagai	Analytical Sciences	2020
Elevated levels of per- and polyfluoroalkyl substances in Cape Fear River striped bass (<i>Morone saxatilis</i>) are associated with biomarkers of altered immune and liver function	TC Guillette, J McCord, M Guillette, ME Polera, KT Rachels, C Morgeson, N Kotlarz, DRU Knappe, BJ Reading, M Strynar, SM Belcher	Environmental International	2020
Mechanisms of pH-dependent uptake of ionizable organic chemicals by fish from oil sands process-affected water (OSPW)	M Brinkmann, H Alharbi, U Fuchylo, S Wiseman, G Morandi, H Peng, JP Giesy, PD Jones, M Hecker	Environmental Science and Technology	2020
A unique approach to monitor stress in coral exposed to emerging pollutants	D Stien, M Suzuki, AMS Rodrigues, M Yvin, F Clergeaud, E Thorel, P Lebaron	Scientific Reports	2020
Ecotoxicity assessment and bioconcentration of a highly brominated organophosphate ester flame retardant in two amphibian species	SA Robinson, SD Young, C Brinovcar, A McFee, AO De Silva	Chemosphere	2020



Toxicology

Title	Authors	Journal	Date
Role of P-glycoprotein in deoxynivalenol-mediated in vitro toxicity	L Ivanova, CK Fæste, A Solhaug	Toxicology Letters	2018
Delphinidin protects colon carcinoma cells against the genotoxic effects of the mycotoxin altertoxin II	G Aichinger, H Puntcher, J Beisl, ML Kütt, B Warth, D Marko	Toxicology Letters	2018
Dietary administration of black raspberries modulates arsenic biotransformation and reduces urinary 8-oxo-2'-deoxyguanosine in mice	P Tu, J Xue, X Bian, L Chi, B Gao, J Leng, H Ru, TJ Knobloch, CM Weghorst, K Lu	Toxicology and Applied Pharmacology	2019
Improved accuracy of saxitoxin measurement using an optimized enzyme-linked immunosorbent assay	JR McCall, WC Holland, DM Keeler, DR Hardison, RW Litaker	Toxins	2019
Behavioural and metabolomic changes from chronic dietary exposure to low-level deoxynivalenol reveal impact on mouse well-being	CK Faeste, F Pierre, L Ivanova, A Sayyari, D Massotte	Archives of Toxicology	2019
Two novel azaspiracids from <i>Azadinium poporum</i> , and a comprehensive compilation of azaspiracids produced by Amphidomataceae, (Dinophyceae)	B Krock, U Tillmann, J Tebben, N Trefault, H Gu	Harmful Algae	2019
Dermal exposure to plasticizers in nail polishes: An alternative major exposure pathway of phosphorus-based compounds	M Tokumura, M Seo, Q Wang, Y Miyake, T Amagai, M Makino	Chemosphere	2019
Unique structural/stereo-isomer and isobar analysis of novel fentanyl analogues in postmortem and DUID whole blood by UHPLC-MS-MS	S Sofalvi, ES Lavins, IT Brooker, CK Kaspar, J Kucmanic, CD Mazzola, CL Mitchell-Mata, CL Clyde, RN Rico, LG Apollonio, C Goggin, B Marshall, D Moore, TP Gilson	Journal of Analytical Toxicology	2019
LC-HRMS and chemical derivatization strategies for the structure elucidation of Caribbean Ciguatoxins: Identification of C-CTX-3 and -4	F Kryuchkov, A Robertson, CO Miles, EM Mudge, S Uhlig	Marine Drugs	2020
Second laboratory validation of β -N-methylamino-L-alanine, N-(2-aminoethyl) glycine, and 2,4-diaminobutyric acid by ultra-performance liquid chromatography and tandem mass spectrometry	SA Banack	Neurotoxicity Research	2020
Isolation of the <i>Tephrosia vogelii</i> extract and rotenoids and their toxicity in the RTgill-W1 trout cell line and in zebrafish embryos	AH Said, A Solhaug, M Sandvik, FE Msuya, MS Kyewalyanga, AJ Mmochi, JL Lyche, S Hurem	Toxicol	2020
Thioprolin formation as a driver of formaldehyde toxicity in <i>Escherichia coli</i>	JA Patterson, H He, JS Folz, Q Li, MA Wilson, O Fiehn, ST Bruner, A Barr-Even, AD Hanson	Biochemical Journal	2020
A chemical biology approach to probing the folding pathways of the inhibitory cystine knot (ICK) peptide ProTx-II	S McCarthy, J Robinson, K Thalassinou, AB Tabor	Frontiers in Chemistry	2020
Triphenyl phosphate permeates the blood brain barrier and induces neurotoxicity in mouse brain	X Liu, X Zhao, Y Wang, J Hong, M Shi, D Pfaff, L Guo, H Tang	Chemosphere	2020
Ergot alkaloid mycotoxins: physiological effects, metabolism and distribution of the residual toxin in mice	P Reddy, J Hemsworth, KM Guthridge, A Vinh, S Vassiliadis, V Ezernieks, GC Spangenberg, SJ Rochfort	Scientific Reports	2020
Fatal intoxication with ivabradine: First case report	A Knapp-Gisclon, M Zerach, C Mayer-Duverneuil, C Rambaud, GL de la Grandmasion, JC Alvarez	Forensic Science International	2020



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Title	Authors	Journal	Date
High-speed isocratic and gradient liquid-chromatography separations at 1500 bar	J De Vos, M De Pra, G Desmet, R Swart, T Edge, F Steiner, S Eeltink	Journal of Chromatography A	2015
Repeatability of gradient ultrahigh pressure liquid chromatography–tandem mass spectrometry methods in instrument-controlled thermal environments	JP Grinias, JMT Wong, RT Kennedy	Journal of Chromatography A	2016
Synthesis and evaluation of sulfobetaine zwitterionic polymer bonded stationary phase	D Yu, Z Guo, A Shen, J Yan, Z Dong, G Jin, Z Long, L Liang, X Liang	Talanta	2016
Ultra-fast high-efficiency enantioseparations by means of a teicoplanin-based chiral stationary phase made on sub-2 μm totally porous silica particles of narrow size distribution	OH Ismail, A Ciogli, C Villani, M De Martino, M Pierini, A Cavazzini, DS Bell, F Gasparrini	Journal of Chromatography A	2016
Total peak shape analysis: detection and quantitation of concurrent fronting, tailing, and their effect on asymmetry measurements	MF Wahab, DC Patel, DW Armstrong	Journal of Chromatography A	2017
A 14 parameter study of UHPLC's for method development transfer and troubleshooting	IAH Ahmad, F Hrovat, A Soliven, A Clarke, P Boswell, T Tarara, A Blasko	Chromatographia	2017
Separations at the speed of sensors	DC Patel, MF Wahab, TC O'Haver, DW Armstrong	Analytical Chemistry	2018
A very simple resolution enhancement technique for analytical signals using the properties of even-derivatives	MF Wahab, TC O'Haver, F Gritti, G Hellinghausen, DW Armstrong	Analyst	2018
Improving visualization of trace components for quantification using a power law based integration approach	G Hellinghausen, MF Wahab, DW Armstrong	Journal of Chromatography A	2018
Power law approach as a convenient protocol for improving peak shapes and recovering areas from partially resolved peaks	MF Wahab, F Gritti, TC O'Haver, G Hellinghausen, DW Armstrong	Chromatographia	2019
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Title	Authors	Journal	Date
In-line Fourier-transform infrared spectroscopy as a versatile process analytical technology for preparative protein chromatography	S Großhans, M Rüdert, A Sanden, N Brestrich, J Morgenstern, S Heissler, J Hubbuch	Journal of Chromatography A	2018
Modification of carbon nanotubes by amphiphilic glycosylated proteins	W Fang, MB Linder, P Laaksonen	Journal of Colloid and Interface Science	2018
Development of a multi-functional concurrent assay using weak cation-exchange solid-phase extraction (WCX-SPE) and reconstitution with a diluted sample aliquot for anti-doping analysis	Y Kim, M Jeon, H Min, J Son, J Lee, OS Kwon, MH Moon, KH Kim	Rapid Communications in Mass Spectrometry	2018
LC-MS/MS quantification of airborne fungal α -amylase at a production facility	AC Vente, RAM van der Hoeven, F Chen, ALL Duchateau	Trends in Chromatography	2018
Development of two complementary LC-HRMS methods for analyzing sotatercept in dried blood spots for doping controls	T Lange, K Walpurgis, A Thomas, H Geyer, M Thevis	Bioanalysis	2019
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Extractable impurities from fluoropolymer-based membrane filters – interference in high-throughput, untargeted analysis	PY Puah, DJH Lee, KH Mak, HJ Ang, HC Chen, PY Moh, ST Fong, YS Ling	RSC Advances	2019
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Adolescent cocaine exposure enhances the GABAergic transmission in the prelimbic cortex of adult mice	P Shi, J Nie, H Liu, Y Li, X Lu, X Shen, F Ge, T Yuan, X Guan	The Journal of the Federation of American Societies for Experimental Biology	2019
Dissociable dopamine dynamics for learning and motivation	A Mohebi, JR Pettibone, AA Hamid, JMT Wong, LT Vinson, T Patriarchi, L Tian, RT Kennedy, JD Berke	Nature	2019
Incentive and dopamine sensitization produced by intermittent but not long access cocaine self-administration	AB Kawa, AC Valenta, RT Kennedy, TE Robinson	European Journal of Neuroscience	2019
Different effects of carbohydrate binding modules on the viscoelasticity of nanocellulose gels	BJM Rooijackers, S Arola, R Velagapudi, MB Linder	Biochemistry and Biophysics Reports	2020
Gamma radiolysis of TODGA and CyMe4BTPhen in the ionic liquid tri-n-octylmethylammonium nitrate	P Zsabka, K Van Hecke, A Wilden, G Modolo, M Hupert, V Jaspers	Solvent Extraction and Ion Chromatography	2020
Volumetric absorptive microsampling and dried blood spot microsampling vs. conventional venous sampling for tacrolimus trough concentration monitoring	H Veenhof, RA Koster, LAT Junier, SP Berger, SJL Bakker, DJ Youw	Clinical Chemistry and Laboratory Medicine	2020

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The <i>Penium margaritaceum</i> genome: Hallmarks of the origins of land plants	C Jiao, I Sørensen, X Sun, H Sun, H Behar, S Alseekh, G Philippe, KP Lopez, L Sun, R Reed, S Jeon, R Kiyonami, S Zhang, AR Fernie, H Brumer, DS Domozych, Z Fei, JKC Rose	Cell	2020
Quantification of endogenous steroid sulfates and glucuronides in human urine after intramuscular administration of testosterone esters	G Forsdahl, K Zanitzer, D Erceg, G Gmeiner	Steroids	2020
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The ethanolamine-sensing transcription factor EutR promotes virulence and transmission during <i>Citrobacter rodentium</i> intestinal infection	CA Rowley, AM Sauder, MM Kendall	Molecular Pathogenesis	2020
Interaction of maternal choline levels and prenatal Marijuana's effects on the offspring	MC Hoffman, SK Hunter, A D'Alessandro, K Noonan, A Wyrwa, R Freedman	Psychological Medicine	2020
Development and validation of a liquid chromatography high-resolution mass spectrometry (LC-HRMS) bioanalytical method for quantifying cannabinoids in whole blood: Application for determining recent cannabis use	MW DeGregorio, SA Audino, E Montoya, A Phong, CJ Kao, GT Wurz	Journal of AOAC International	2020
Tandem detection of organic and inorganic gunshot residues using LC-MS and SEM-EDS	C Bonnar, EC Moule, N Lucas, KE Seyfang, RP Dunsmore, RS Popelka-Filcoff, K Redman, KP Kirkbride	Forensic Science International	2020
Ventromedial hypothalamic nucleus neuronal subset regulates blood glucose independently of insulin	JN Flak, PB Goforth, J Dell-Orco, PV Sabatini, C Li, N Bozadjieva, M Sorensen, A Valenta, A Rupp, AH Affinati, C Cras-Méneur, A Ansari, J Sacksner, N Kodur, DA Sandoval, RT Kennedy, DP Olson, MG Meyers	The Journal of Clinical Investigation	2020
Profiles of human milk oligosaccharides and their relations to the milk microbiota of breastfeeding mothers in Dubai	CA Moubareck, M Lootah, M Tahlak, K Venema	Nutrients	2020
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Fast nevirapine impurity profiling using UHPLC-DAD	H Franz, S Fabel	AN170	2014
Improvement in speed and reproducibility of protein digestion utilizing novel sample preparation technology in a full solution work	J Bardsley, J Jones, V Barattini, P Humphryes, T Liddicoat	PN21209	2015
Rapid discovery of differentially expressed proteins in T2D plasma samples using improved UHPLC chromatography and pSMART data acquisition	S Peterman, M Lopez, D Sarracino, A Prakash, M Vogelsang, B Krastins, G Byram, G Vadali, M Mohiuddin, P Muraca, AB Goldfine, ME Patti	PN64369	2015
Combination of bottom-up and top-down characterization of biologics using a high throughput capable workflow in proteome discoverer software	K Scheffler, T Ueckert, C Paschke, B Delanghe	PN64482	2015
Fast and ultrafast LC-MS/MS methods for robust and reliable analysis of pesticides in food using the Vanquish UHPLC system	G Greco, CPB Martins, K Bousova, R Swart	AN 1138	2015
How scalable are the dispersion processes in real columns packed with solid core material?	T Edge, L Pereira, D Steiner	PN21220	2015
Determination of A-type and B-type procyanidins in apple, cocoa and cinnamon extracts	JA Glinski, D Thomas, A Wong, VB Glinski, I Acworth	PN71285	2016
The Vanquish Platform: Major improvement in throughput and resolution of xanthenes in mangosteen pericarp	Q Zhang, B Bailey, M Plante, I Acworth	AN172	2016
The importance of correct UHPLC instrument setup for protein aggregate analysis by size-exclusion chromatography	A Farrell, J Bones, K Cook	AN 21602	2016
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Characterizing therapeutic monoclonal antibodies	M De Pra, C Pohl	WP21502	2016
Monitoring peptide PEGylation by HPLC with charged aerosol detection	D Thomas, I Acworth, S Meier, B Kaboord, H Yang, C Fisher	PN72093	2016
Ternary gradient for tenofovir disoproxil fumarate impurity profiling	S Fabel, M Martin	AN 1129	2016



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Title	Authors	Journal	Date
Metoprolol and select impurities analysis using a hydrophilic interaction chromatography method with combined UV and charged aerosol detection	B Bailey	AN1126	2016
UHPLC method development for simultaneous determination of antihypertensive combination agents	S Fabel	AN1122	2016
UHPLC method development for analyzing a once-daily tablet formulation for HIV-1 infection treatment	S Fabel	AN1115	2016
Reliable results in peptide mapping using the vanquish flex UHPLC system	C Paul, M De Pra, EJ Sneekes	AN1132	2016
High salt gradient analysis of post-translational modifications - deamidation monitoring	M Menz, C Paul, EJ Sneekes	AN71811	2016
Analysis of subtle changes in biological systems through use of high resolution, high accuracy UHPLC generated libraries with a Q-Exactive HF mass spectrometer	DA Sarracino, M De Pra, K Murphy, J Neil, MF Lopez	PN71310	2016
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Label-free analysis by UHPLC with charged aerosol detection of glycans separated by charge, size, and isomeric structure	D Thomas, I Acworth	AN1127	2016
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Separation of mixed-base oligonucleotides using a high-resolution, reversed-phase chromatography column	J Baek, J Thayer, S Lin, X Liu	AN21476	2016
Increased speed and sample throughput of opioid analysis from human urine using micro-elution solid phase extraction	J Bardsley, J Jones	AN21578	2016
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The role of temperature and column thermostating in liquid chromatography	M Heidorn	WP71499	2016
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A more flexible column thermostating technique in LC method transfer	M Heidorn	WP71500	2016



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Fast and easy optimization of detection wavelengths with Vanquish fluorescence detectors	H Franz, A Manka	TN166	2016
Boosting trace detection performance with the Vanquish diode array detector and high-sensitivity LightPipe flow cell	A Manka, H Franz	TN165	2016
Rapid, sensitive, and easy UHPLC-MS/MS analysis of fungicides in fruit juices with QuEChERS	Lamb, B King	AN21691	2017
Lifetime stability of size exclusion chromatography columns for protein aggregate analysis	A Farrell, C Jakes, A Ley, M De Pra, F Steiner, J Bones	AN 72362	2017
Comprehensive protein glycosylation comparison of an innovator monoclonal antibodies to a candidate biosimilar by HILIC UHPLC analysis	S Millán, A Trappe, A Farrell, J Bones	AN21651	2017
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Full characterization of heterogeneous antibodies samples under denaturing and native conditions on the Q Exactive BioPharmaceuticals mass spectrometer	K Scheffler, E Damoc	AN72348	2017
Fast profiling of the N-glycan population in biotherapeutic antibodies by UHPLC-FLD with MS confirmation	S Milán, S Mettermayr, A Farrell, J Bones	AN21652	2017
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Achieve confident impurity detection with the Thermo Scientific ISQ EC single quadrupole mass spectrometer	S Meding, K Lovejoy, M Ruehl	AN72391	2017
A pre-concentration and online solid phase extraction setup for the LC-MS analysis of therapeutic protein mixtures	M Samonig, S Patzelt, M Rühl, R Swart	TN184	2017
High-precision, automated peptide mapping of proteins	A Farrell, J bones, K Cook, S Patel, A Schwahn, J Bardsley	AN21682	2017
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Immunoaffinity solid-phase extraction with HPLC-FLD detection for the determination of aflatoxins B2, B1, G2, and G1 in ground hazelnut	M De Pra, S Grosse, F Steiner	LCGC	2018



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Title	Authors	Journal	Date
Growth media effects on post-translational modifications investigated through peptide mapping LC-MS/MS analysis of anti-IL8 monoclonal antibodies	G Oliviero, I Zaborowska, C Jakes, S Carillo, J Bones	AN 21879	2018
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Investigating process-related post-translational modifications in NISTmAb RM 8671 using high-throughput peptide mapping analysis	S Millán, C Jakes, N Dorival, S Carillo, J Bones	AN21781	2018
Subunits analysis approach for the determination of fucosylation levels in monoclonal antibodies using LC-HRAM-MS	C Jakes, S Carillo, I Zaborowska, J Bones	AN21805	2018
Separation of IgG2 and IgG4 therapeutics using weak cation exchange chromatography	J Baek, S Bechler, S Lin, S Tremintin	AN21843	2018
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Evaluation and application of salt- and pH-based ion-exchange chromatography gradients for analysis of therapeutic monoclonal antibodies	A Farrell, C Jakes, J Bones	AN21778	2018
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Accurate and precise quantification of mAb-released N-glycans with an amide HILIC column	X Zhang, Z Sun	AN21764	2018
Easy, fast and reproducible analysis of host cell protein (HCP) in monoclonal antibodies preparations	G Oliviero, K Cook, K Scheffler, F Füssl, J Bones	AN21918	2019



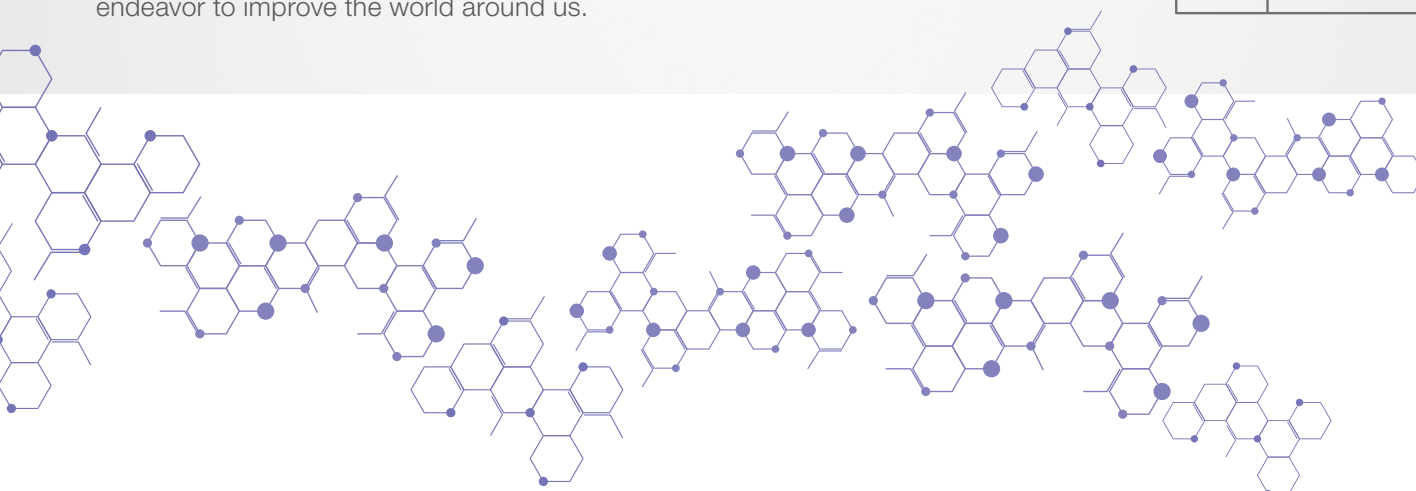
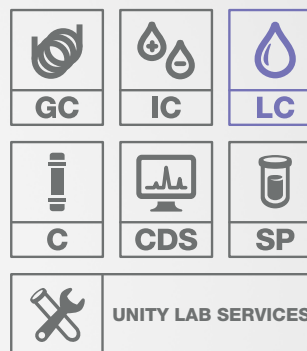
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Performance evaluation of MAbPac RP columns for monoclonal antibodies IdeS subunit analysis	MR da Silva, S Carillo, C Jakes, J Bones	AN21910	2019
Confident monoclonal antibodies sequence verification by complementary LC-MS techniques	A Farrell, S Carillo, J Bones, K Sheffler, K Cook	AN21919	2019
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A global pH-gradient based charge variant analysis directly coupled to HRAM-MS (CVA-MS) for mAb analysis	F Füssl, J Bones, K Cook, K Scheffler	AN21917	2019
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Comparative analysis of innovator and biosimilar monoclonal antibodies using a multi-attribute method	X Zhang, H Liu, R Quintyn, M Du	AN73912	2020
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Sensitive profiling of IgG1 monoclonal antibodies variants under native conditions	S Carillo, J Bones	AB73554	2020

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