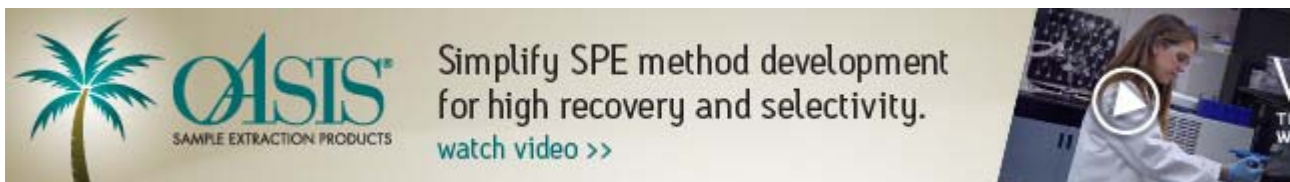


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Journal of Chromatography B

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Regular papers

2 **Characterization and identification of alanine to serine sequence variants in an IgG4 monoclonal antibody produced in mammalian cell lines** Original Research Article
 Pages 1-8
 Jinmei Fu, Jacob Bongers, Li Tao, Dan Huang, Richard Ludwig, Yunping Huang, Yueming Qian, Jonathan Basch, Joel Goldstein, Ramji Krishnan, Li You, Zheng Jian Li, Reb J. Russell
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Highlights

- ▶ Alanine to serine sequence variants were identified in an antibody by LC/MS/MS.
- ▶ The sequence variants were confirmed by

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-  [Volume 825 \(2005\)](#)
-  [Volume 824 \(2005\)](#)
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► DNA sequencing of the mater cell bank revealed one vari-
mutation at the DNA level.

- 3   [Short-incubation mass spectrometry assay for lysosomal storage disorders in newborn and high-risk population screening](#) Original Research Article
Pages 9-17

Thomas P. Mechtler, Thomas F. Metz, Hannes G. Müller, Katharina Ostermann, Rene Ratschmann, Victor R. De Jesus, Bori Shushan, Joseph M. Di Bussolo, Joseph L. Herman, Kurt R. Herkner, David C. Kasper


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Highlights

► We report a short-incubation mass spectrometry-based pr
enzymes. ► Optimized sample handling and online clean-up
► Up to 5 lysosomal enzyme activities are analyzed simulta
spots. ► Method validation was performed under routine clir
environment.



- 4   [Trace determination of \$\beta\$ -blockers and \$\beta_2\$ -agonists in distilled and waste-waters using liquid chromatography–tandem mass spectrometry and solid-phase extraction](#) Original Research Article
Pages 27-38

Alaa A. Salem, Ibrahim A. Wasfi, Salama S. Al-Nassibi


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Highlights

► We developed a sensitive method for determining β -block
LC–MS. ► The method was tested for trace determinations
 β -agonists. ► Recovery of 77.20–97.30% and detection limi
were obtained. ► Drugs at concentrations of 3.44–234.28 p
and Abu Dhabi WWTPs. ► Results suggest that treatment p
to degrade these compounds.

- 5   [Pharmacokinetics of protocatechuic acid in mouse and its quantification in human plasma using LC–tandem mass spectrometry](#) Original Research Article
Pages 39-44

Wei Chen, Dian Wang, Li-shu Wang, Di Bei, Jiang Wang, William A. See, Susan R. Mallery, Gary D. Stoner, Zhongfa Liu

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Highlights

► We developed and validated an LC–MS/MS method for th
plasma. ► This method was used to characterize the pharm
mouse. ► This method detected PCA in the plasma of patier

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of BRB. ► This method provides a translational tool for prec of PCA.

6  

[Dynamic affinity chromatography in the separation of sulfated lignins binding to thrombin](#)

Original Research Article

Pages 45-51

Aiye Liang, Jay N. Thakkar, Michael Hindle, Umesh R. Desai

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Highlights

► Sulfated LMWL fractions were isolated by dynamic thromb chromatography. ► The fractions differ significantly in their biochemical properties. ► One fraction of the three studied exhibited antagonism of clotting. ► This fraction selectively attenuated pathway. ► Identified the 1st LMWL structure that exhibits a pathway.

7  

[Simultaneous determination of morinidazole, its *N*-oxide, sulfate, and diastereoisomeric *N*⁺-glucuronides in human plasma by liquid chromatography–tandem mass spectrometry](#)

Original Research Article

Pages 52-58

Ruina Gao, Dafang Zhong, Ke Liu, Yu Xia, Rongwei Shi, Hua Li, Xiaoyan Chen

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Highlights

► Simultaneously determine morinidazole and its four metabolites. ► Gradient elution was used to obtain the resolution of two metabolites. ► The potential interference from the in-source dissociation avoided. ► The method was applied to clinical pharmacokinetic morinidazole injection.

8  

[Chromatographic behaviour of peptides following dimethylation with H₂/D₂-formaldehyde: Implications for comparative proteomics](#)

Original Research Article

Pages 59-66

Joseph M. Boutilier, Hunter Warden, Alan A. Doucette, Peter D. Wentzell

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

Highlights

► The isotope effect (D₀ vs D₄) in dimethyl labelling of peptides. ► Four replicates of 71 peptide pairs are used to assess retention differences. ► Retention differences are statistically significant, but small and consistent. ► Computational results are consistent with observations for other peptides. ► Dimethyl labelling is a viable alternative for relative peptide quantification.

- 9   **Determination of non-steroidal anti-inflammatory drugs in urine by hollow-fiber liquid membrane-protected solid-phase microextraction based on sol-gel fiber coating** Original Research Article
Pages 67-75
 Ali Sarafraz-Yazdi, Amirhassan Amiri, Gholamhossein Rounaghi, Hossein Eshtiagh-Hosseini
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Highlights

► HFLM-SPME was proposed for the determination of NSAIDs. ► PEG-g-MWCNTs was used as extraction phase to prepare the fiber. ► The HFLM-SPME method, integrating the advantages of HFLM and HF-LPME. ► This method has a considerably low LOD and a wide linear range.

- 10   **Bioanalytical method validation of rapamycin in ocular matrix by QTRAP LC-MS/MS: Application to rabbit anterior tissue distribution by topical administration of rapamycin nanomicellar formulation** Original Research Article
Pages 76-86
 Ravinder Earla, Kishore Cholkar, Sriram Gunda, Rajya Lakshmi Earla, Ashim K. Mitra
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Highlights

► An LC-MS/MS method was validated in ocular matrix. ► This method was successfully applied to estimate the rapamycin concentration in ocular matrix. ► This system demonstrates that 0.2% rapamycin nanomicellar formulation successfully delivers therapeutic drug levels in the eye.

- 11   **Determination of piperphentonamine and metabolites M1 and M6 in human plasma and urine by LC/MS/MS and its application in a pharmacokinetics study in Chinese healthy volunteers** Original Research Article
Pages 87-93
 Aixin Shi, Xin Hu, Kexin Li, Jian Li, Liping Han, Huayin Wan, Rubing Li
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Highlights

► Piperphentonamine hydrochloride for injection is an origin drug in China, which belongs to calcium sensitizers. ► A LC/MS/MS method for the determination of piperphentonamine and metabolites M1 and M6 in human plasma and urine was established in this paper. ► This method can perform quantitative analysis of piperphentonamine and metabolites M1 and M6 in human plasma and urine of healthy Chinese subjects. ► The pharmacokinetic parameters of piperphentonamine and metabolites M1 and M6 after intravenous bolus of piperphentonamine and metabolites in healthy Chinese subjects were evaluated.

- 12   **Microfractionation bioactivity-based ultra performance liquid chromatography/quadrupole time-of-flight mass spectrometry for the identification of nuclear factor- κ B inhibitors and β_2 adrenergic receptor agonists in an alkaloidal extract of the folk herb *Alstonia scholaris*** Original Research Article
Pages 98-104
Yuanyuan Hou, Xuelin Cao, Liqiang Wang, Binfeng Cheng, Linyi Dong, Xiaodong Luo, Gang Bai, Wenyan Gao
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Highlights

- A microfractionation bioactivity-based fingerprint of *A. scholaris* was established.
- This method was coupled with two dual-luciferase reporter assays.
- Inhibitors and β_2 AR agonists can be screened simultaneously.
- Three dual-functional indole alkaloids with dual-target were identified.
- This method is suitable for identifying dual-target compounds in complex systems.

- 13   **Insulin related compounds and their identification** Original Research Article
Pages 105-112
Cheol-Ki Min, Jin-Won Lee, Chang-Kyu Kim, Seong Hwan Kim, Sang Yeol Lee, Sang-Myung Lee, Young-Jin Son
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Highlights


- We report six human insulin-related compounds from two strains.
- Insulin-related compounds were purified and identified by HPLC-MS/MS.
- An analytical HPLC method was introduced to detect human insulin, which is a major impurity during human insulin production.
- The formation mechanisms of insulin-related compounds were studied.
- The identities of the related compounds were confirmed.
- Taken together, our results provide new insights into insulin-related compounds and effective analytical methods for their detection.

- 14   **Determination of five di-(2-ethylhexyl)phthalate metabolites in urine by UPLC-MS/MS, markers of blood transfusion misuse in sports** Original Research Article
Pages 113-121
Núria Monfort, Rosa Ventura, Georgina Balcells, Jordi Segura
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Highlights

- Di-(2-ethylhexyl)phthalate (DEHP) is the most commonly used plasticizer in medical devices.
- DEHP metabolites have been proposed as markers of the transfusion.
- A method to quantify five DEHP metabolites in urine was validated.
- Cutoff concentrations were proposed to determine the presence of DEHP metabolites in urine.

possible transfusion. ► The method is proposed as screening detection in doping control.

- 15  **The principle of pooled calibrations and outlier retention elucidates optimum performance of ion chromatography** Original Research Article
Pages 122-127
 Jens E.T. Andersen, Maria Mikolajczak, Katarzyna Olga Wojtachnio-Zawada, Henrik Vigan Nicolajsen
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Highlights

► Outliers of IC should be retained in order to secure correct Pooled calibrations provide excellent correspondence between method for the determination of the full-calibration range in IC contents determined by IC do not correlate with the sensitivity correspond well to the uncertainty predicted by Horwitz.

- 16  **Analytical method for the sensitive determination of major di-(2-propylheptyl)-phthalate metabolites in human urine** Original Research Article
Pages 128-136
 Wolfgang Gries, Dietmar Ellrich, Katja Küpper, Birgit Ladermann, Gabriele Leng
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Highlights

► DPHP-metabolites OH-MPHP, oxo-MPHP and cx-MPHxP urine. ► GC–HRMS, GC–MS/MS, HPLC–MS/MS methods are Detection limits range between 0.05 and 0.2 µg/L urine for each Sensitive determination of DPHP metabolites in environment

- 17  **Rapid and selective screening of melamine in bovine milk using molecularly imprinted matrix solid-phase dispersion coupled with liquid chromatography-ultraviolet detection** Original Research Article
Pages 137-142
 Hongyuan Yan, Xiaoling Cheng, Ning Sun, Tianyu Cai, Ruijun Wu, Kun Han
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Highlights

► A simple and rapid MI-MSPD method for determination of Water-compatible MIP was obtained by cyromazine as dumm water solution. ► Rapid screening of melamine in milk, while matrix were eliminated. ► Extraction efficiency was markedly equilibrium time. ► This method improved the selectivity and template leakage on quantitative analysis.

- 18   **Purification of baicalin and wogonoside from *Scutellaria baicalensis* extracts by macroporous resin adsorption chromatography** Original Research Article
Pages 143-149
Zhanquan Du, Kun Wang, Yuan Tao, Lixia Chen, Feng Qiu
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Highlights



► Simultaneous separation and purification of baicalin and wogonoside on macroporous resin. ► Process parameters were optimized for the separation procedure. ► HPD-100 resin was successfully applied to separate baicalin and wogonoside with high contents. ► The developed method is suitable for laboratory preparative-scale separation.

Short Communications

- 19   **Sensitive determination of the peptide AP301 – A motif of TNF- α – From human plasma using HPLC–MS/MS**
Pages 18-22
Daniel Mascher, Werner Tscherwenka, Hermann Mascher, Bernhard Fischer
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Highlights



► A new method is described for the determination of AP301. ► A LLOQ of 1 ng/mL using HPLC–MS/MS is reached. ► This information of penetration of it from lung into circulation. ► The concentration of this compound in a biological matrix has not been published yet.

- 20   **Analysis of coenzyme Q₁₀ in lymphocytes by HPLC–MS/MS**
Pages 23-26
A. Arias, J. García-Villoria, A. Rojo, N. Buján, P. Briones, A. Ribes
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Highlights

► The reference range of CoQ₁₀ was narrower when normalized to grams of protein than when normalized to grams of dry weight. ► Isolated lymphocytes are a reliable matrix for the diagnosis and follow-up of patients with CoQ₁₀ deficiency. ► HPLC–MS/MS is a good procedure to measure CoQ₁₀.

- 21   **Capillary electrophoresis to quantitate gossypol enantiomers in cotton flower petals and seed**
Pages 94-97
Sergey Vshivkov, Egor Pshenichnov, Zamira Golubenko, Alik Akhunov, Shadman Namazov, Robert D. Stipanovic

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Highlights

► Gossypol occurs as a mixture of enantiomers in cottonseed oil. ► Gossypol is more toxic to non-ruminant animals. ► Plant breeders are developing a low percent of (-)-gossypol. ► A capillary electrophoresis method was used to quantitate the enantiomers. ► Breeders can use this method to select for a low (-)-gossypol seed trait.

22   [Preparative separation of glycoalkaloids \$\alpha\$ -solanine and \$\alpha\$ -chaconine by centrifugal partition chromatography](#)



Pages 150-154

Jacques Attoumbré, David Lesur, Philippe Giordanengo, Sylvie Baltora-Rosset

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Highlights

► α -Solanine and α -chaconine were extracted from *Solanum tuberosum* Pompadour. ► CPC was used to develop an efficient preparative procedure. ► The efficiency of the separation depended on the solvent system. ► Highest purity and yield were achieved for α -chaconine.

23   [A rapid quantitative method of carisoprodol and meprobamate by liquid chromatography–tandem mass spectrometry](#)

Pages 155-160

Shannon Essler, Kerry Bruns, Michael Frontz, J. Rod McCutcheon



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Highlights

► Carisoprodol and meprobamate are commonly encountered in forensic toxicology. ► In this method, sample preparation can be performed with minimal materials and effort. ► Using LC/MS/MS provides less need for sample cleanup, adds speed and specificity to the analysis. ► The method uses internal standards for both analytes.

Erratum

Corrigendum

24   [Corrigendum to: "Determination of the gamma secretase activity in human plasma by online extraction and electrospray tandem mass spectrometry" \[J. Chromatogr. B 878 \(2010\) 2348–2354\]](#)
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Clinton F. Stewart

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