Characterization and identification of alanine to serine sequence variants in an IgG4 monoclonal antibody produced in mammalian cell lines

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

Highlights

► Alanine to serine sequence variants were identified in an IgG4 monoclonal antibody produced in mammalian cell lines by LC/MS/MS. ► The sequence variants were confirmed by
Short-incubation mass spectrometry assay for trace determination of pharmacokinetics of protocatechuic acid in distilled and waste-waters using LC–tandem mass spectrometry and solid-phase extraction

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We report a short-incubation mass spectrometry-based proof-of-concept study for the potential application of this method as a screening tool for lysosomal storage disorders in newborns and high-risk population screening for Niemann–Pick A/B disease in adults.

Highlights

- We developed and validated an LC–MS/MS method for the quantification of protocatechuic acid (PCA) in human plasma using LC–tandem mass spectrometry (LC–MS/MS).
- This method was used to characterize the pharmacokinetics of PCA in a mouse.
- This method detected PCA in the plasma of patients with Niemann–Pick A/B disease.
- DNA sequencing of the maternal cell bank revealed one variant allele associated with the disease.

Trace determination of β-blockers and β2-agonists in distilled and waste-waters using liquid chromatography–tandem mass spectrometry and solid-phase extraction

4

We developed a sensitive method for determining β-blockers and β2-agonists in distilled and waste-waters using LC–MS. The method was tested for trace determinations with low detection limits. Recovery of 77.20–97.30% and detection limits of 0.035–0.15 pg L−1 were obtained. Drugs at concentrations of 3.44–234.28 pg L−1 and Abu Dhabi WWTPs were detected in this study.

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Pharmacokinetics of protocatechuic acid in mouse and its quantification in human plasma using LC–tandem mass spectrometry

5

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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

Highlights

► Sulfated LMWL fractions were isolated by dynamic thrombin chromatography. ► The fractions differ significantly in their biochemical properties. ► One fraction of the three studied α2-antagonism of clotting. ► This fraction selectively attenuates pathway. ► Identified the 1st LMWL structure that exhibits a pathway.

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

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

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

Highlights

► The isotope effect (D0 vs D4) in dimethyl labelling of peptides is manifest. ► Retention differences are statistically significant, but small and non-significant in PCA. ► Computational results are consistent with observations for dimethyl labelling is a viable alternative for relative peptide quantification.

Related articles | Related reference work articles
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

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 HF-LPME and HF-LPME.
► This method has a considerably low LOD.

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

Highlights
► An LC–MS/MS method was validated in ocular matrix.
► It was utilized for quantification of rapamycin, and was stable for 24 hours.
► This method was successfully applied to estimate the rapamycin concentration in various tissues.
► This system demonstrates that 0.2% rapamycin nanomicellar formulation successfully delivers therapeutic drug levels in the eye.

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

Highlights
► Piperphentonamine hydrochloride for injection is an origin human, which belongs to calcium sensitizers.
► A LC/MS/M method was used for the concentrations of piperphentonamine and metabolites M1 and M6 in plasma and urine was established in this paper.
► This method was successfully applied to perform quantitative analysis of piperphentonamine and metabolites M1 and M6 in plasma and urine of healthy Chinese subjects.
► The pharmacokinetic parameters of piperphentonamine in healthy Chinese subjects were evaluated.
Microfractionation bioactivity-based ultra performance liquid chromatography/quadrupole time-of-flight mass spectrometry for the identification of nuclear factor-κB inhibitors and β2 adrenergic receptor agonists in an alkaloidal extract of the folk herb Alstonia scholaris

Page 98-104
Yuanyuan Hou, Xuelin Cao, Liqiang Wang, Binfeng Cheng, Linyi Dong, Xiaodong Luo, Gang Bai, Wenyuan Gao

Highlights

► A microfractionation bioactivity-based fingerprint of A. sch

This method was coupled with two dual-luciferase reporter a inhibitors and β2AR agonists can be screened simultaneousl Three dual-functional indole alkaloids with dual-target were f suitable for identifying dual-target compounds in complex sy

Insulin related compounds and identification

Page 105-112
Cheol-Ki Min, Jin-Won Lee, Chang-Kyu Kim, Seong Hwan Kim, Sang Yeol Lee, Sang-Myung Lee, Young-Jin Son

Highlights

► We report six human insulin-related compounds from two strains. ► Insulin-related compounds were purified and iden methods. ► An analytical HPLC method was introduced to c human insulin, which is a major impurity during human insul formation mechanisms of insulin-related compounds were st identities of the related compounds. ► Taken together, our r insulin-related compounds and effective analytical methods f

Determination of five di-(2-ethylhexyl)phthalate metabolites in urine by UPLC–MS/MS, markers of blood transfusion misuse in sports

Page 113-121
Núria Monfort, Rosa Ventura, Georgina Balcells, Jordi Segura

Highlights

► Di-(2-ethylhexyl)phthalate (DEHP) is the most commonly DEHP metabolites have been proposed as markers of the transfusion. ► A method to quantify five DEHP metabolites f validated. ► Cutoff concentrations were proposed to deter
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

<table>
<thead>
<tr>
<th>Highlights</th>
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<tr>
<td>► 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 contents determined by IC do not correlate with the sensitivities correspond well to the uncertainty predicted by Horwitz.</td>
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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

<table>
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<th>Highlights</th>
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<tr>
<td>► DPHP-metabolites OH-MPHP, oxo-MPHP and cx-MPHxP in urine. ► GC–HRMS, GC–MS/MS, HPLC–MS/MS methods Detection limits range between 0.05 and 0.2 μg/L urine for each Sensitive determination of DPHP metabolites in environment</td>
</tr>
</tbody>
</table>

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

<table>
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<tr>
<td>► A simple and rapid MI-MSPD method for determination of Water-compatible MIP was obtained by cyromazine as dummy water solution. ► Rapid screening of melamine in milk, while matrix were eliminated. ► Extraction efficiency was markedly improved by equilibrium time. ► This method improved the selectivity and template leakage on quantitative analysis.</td>
</tr>
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http://www.sciencedirect.com/science/journal/15700232/908
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

**Highlights**

- Simultaneous separation and purification of baicalin and wogonoside with high contents.
- The developed method 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

**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 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

**Highlights**

- The reference range of CoQ10 was narrower when normalized to grams of protein.
- Isolated lymphocytes are a reliable matrix for the diagnosis and follow-up of patients.
- 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
Gossypol occurs as a mixture of enantiomers in cottonseed, more toxic to non-ruminant animals. Plant breeders are developing seeds low in gossypol. A capillary electrophoresis method can quantitate the enantiomers. Breeders can use this method to develop low gossypol seed trait.

Preparative separation of glycoalkaloids α-solanine and α-chaconine by centrifugal partition chromatography

α-Solanine and α-chaconine were extracted from Solanum Pompadour. CPC was used to develop an efficient preparation procedure. The efficiency of the separation depended on material purity and yields were achieved for α-chaconine.

A rapid quantitative method of carisoprodol and meprobamate by liquid chromatography–tandem mass spectrometry

Carisoprodol and meprobamate are commonly encountered in toxicology. In this method, sample preparation can be per materials and effort. Using LC/MS/MS provides less need for internal standards for both analytes. The method uses internal standards for both analytes.


The corrigendum corrects errors in the original publication.