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Data article

Supporting data for the MS identification of distinct transferrin glycopeptide glycoforms and citrullinated peptides associated with inflammation or autoimmunity

A. Rosal-Vela [a,1], A. Barroso [b,1], E. Giménez [b], S. García-Rodríguez [b], V. Longobardo [c], J. Postigo [d], M. Iglesias [d], A. Lario [c], J. Merino [d], R. Merino [e], M. Zubiaur [a], V. Sanz-Nebot [b], J. Sancho [a,*]

[a] Instituto de Parasitología y Biomedicina "López-Neyra" (IPBLN), CSIC, Armilla, Granada, Spain
[b] Departament de Química Analítica, Universitat de Barcelona, Spain
[c] Unidad de Proteómica, IPBLN, CSIC, Armilla, Granada, Spain
[d] Facultad de Medicina, Universidad de Cantabria, Santander, Spain
[e] Instituto de Biomedicina y Biotecnología de Cantabria, CSIC, Santander, Spain

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ABSTRACT

This data article presents the results of all the statistical analyses applied to the relative intensities of the detected 2D-DiGE protein spots for each of the 3 performed DiGE experiments. The data reveals specific subsets of protein spots with significant differences between WT and CD38-deficient mice with either Collagen-induced arthritis (CIA), or with chronic inflammation induced by CFA, or under steady-state conditions. This article also shows the MS data analyses that allowed the identification of the protein species which serve to discriminate the different experimental groups used in this study. Moreover, the article presents MS data on the citrullinated peptides linked to specific protein species that were generated in CIA^+ or CFA-treated mice. Lastly, this data article provides MS data on the efficiency of the analyses of the transferrin (Tf) glycopeptide glycosylation pattern in spleen and serum from CIA^+ mice and normal controls. The data supplied in this work is related to the research article entitled "identification of multiple transferrin species in spleen and serum from mice with collagen-induced arthritis which may

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* Correspondence to: Instituto de Parasitología y Biomedicina López-Neyra, CSIC, Avenida del Conocimiento s/n, Parque Tecnológico de la Salud (PTS), 18016 Armilla (Granada), Spain. Tel.: +34 958181664; fax: +34 958181632.
E-mail address: granada@ipb.csic.es (J. Sancho).
[1] A. Rosal-Vela and A. Barroso equally contributed to this work.

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reflect changes in transferrin glycosylation associated with disease activity: the role of CD38" [1]. All mass spectrometry data have been deposited to the ProteomeXchange Consortium via the PRIDE partner repository with identifiers PRIDE: PXD002644, PRIDE: PXD002643, PRIDE: PXD003183 and PRIDE: PXD003163.

Specifications table

Subject area	*Biology*
More specific subject area	*Proteomics and glycoproteomics*
Type of data	*Tables, figures and raw data*
How data was acquired	Scanned 2D-DiGE images were analyzed using the DeCyder7.0 software (GE Healthcare) using the Differential In-gel Analysis (DIA) module to detect and normalize the protein spots. Protein relative abundance across all samples and statistical analyses were performed using the Biological Variation Analysis (BVA) module of the DeCyder software. *MS data for protein identification was acquired using a MALDI TOF/TOF UltrafleXtreme (Bruker), or a* 4800 MALDI-TOF/TOF Analyzer (AB SCIEX). *μLC–TOF–MS data for the analysis of the glycopeptides glycoforms of Tf was acquired with a 1200 series capillary liquid chromatography system (Agilent Technologies) coupled to a 6220 oa-TOF LC/MS mass spectrometer with an orthogonal G1385-44300 interface (Agilent Technologies).*
Data format	*Analyzed (excel files and word tables) and raw data*
Experimental factors	*Mice with Collagen-induced arthritis, or with chronic inflammation, or with no treatment. Protein extraction and/or purification from spleen or serum samples. CyDye labeling. 2-D gel electrophoresis.*
Experimental features	*Protein extracts from mice subjected to different experimental conditions were analyzed by 2D-DiGE, and protein species that differed in abundance were identified by MS/MS. PTMs such as citrullination of the identified proteins, or glycosylation of Tf species were further analyzed by MS.*
Data source location	*UB: Barcelona; UCO: Córdoba; IPBLN: Granada.*
Data accessibility	*Data is within this article. Data also available at the ProteomeXchange Consortium via the PRIDE partner repository, PRIDE: PXD002644, PRIDE: PXD002643, PRIDE: PXD003183 and PRIDE: PXD003163.*

Value of the data

- Application of μLC–TOF–MS for characterization of multiple glycopeptide glycoforms from mouse transferrin.
- Investigation of altered transferrin glycopeptide glycosylation patterns in inflammatory and/or autoimmune diseases.
- Mass spectrometry approach to identify new citrullinated peptides in mice with arthritis (CIA model).
- Properly described approach for 2D-DiGE analysis to identify protein species that differ in abundance due to certain pathologies.
- Basis for the study of altered protein species associated with inflammatory processes or arthritis in humans.