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Data Article

Physiochemical and protein datasets related to citrus juice sac cells-derived nanovesicles and microvesicles



Gabriella Pocsfalvi^{a,*}, Lilla Turiák^b, Alfredo Ambrosone^c,
Pasquale del Gaudio^c, Gina Puska^d, Immacolata Fiume^a,
Teresa Silvestre^a, Károly Vékey^b

^a Institute of Biosciences and BioResources, National Research Council of Italy, Italy

^b MS Proteomics Research Group, Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Hungary

^c Department of Pharmacy, University of Salerno, Italy

^d Department of Anatomy, Cell and Developmental Biology, Eötvös Loránd University, Budapest, Hungary

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ABSTRACT

Qualitative and quantitative data obtained on micro and nanovesicle enriched fractions isolated from four citrus species, *C. sinensis*, *C. limon*, *C. paradisi* and *C. aurantium* are presented. It includes physiochemical characterization by transmission electron microscopy (TEM) and dynamic laser scattering (DLS); and molecular characterization of the biocargo of citrus vesicles by quantitative label-free proteomics. Vesicular transport related proteins of *C. sinensis* were predicted by (i) finding orthologues based on previously described vesicular transport proteins and (ii) GO term enrichment analysis. Based on the protein content different types of intra and intercellular vesicles were dissected and the distribution of different Enzyme classes (ECs) were determined. This data article is related to “Protein biocargo of citrus fruit-derived vesicles reveals heterogeneous transport and extracellular vesicle populations” (Pocsfalvi et al., 2018).

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* Corresponding author.

E-mail address: gabriella.pocsfalvi@ibbr.cnr.it (G. Pocsfalvi).

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Specifications table

Subject area	Biology, Chemistry, Physics
More specific subject area	Cell-derived nanovesicles and microvesicles
Type of data	Tables and figures (TEM image and DLS graphs)
How data were acquired	TEM, DLS, mass spectrometer (Bruker Maxis II with CaptiveSpray nano-booster ionsource)
Data format	Raw, filtered, analyzed
Experimental factors	Isolation of MV and NV-enriched fractions using ultracentrifugation, for proteomics: lysis of vesicles and in-solution digestion using trypsin
Experimental features	Vesicles were isolated from citrus fruit juice sac cells into two fractions using differential ultracentrifugation. TEM and DLS images were obtained on every fractions. In-solution digestion proteomics using trypsin as digesting enzymes and LC-MS/MS-based protein identification was performed. Bioinformatics and data mining were performed using EggNOG and Blast2Go software.
Data source location	Naples (Italy) and Budapest (Hungary)
Data accessibility	The data are included in the manuscript in an easily accessible format
Related research article	Pocsfalvi G, Turiák L, Ambrosone A, Del Gaudio P, Puska G, Fiume I, Silvestre T, Vékely K: Protein biocargo of citrus fruit-derived vesicles reveals heterogeneous transport and extracellular vesicle populations. <i>J Plant Physiol.</i> 2018, 229: pp. 111–121. https://doi.org/10.1016/j.jplph.2018.07.006 [1].

Value of the data

- The data can be used for the efficient design of nanodelivery vehicles for drugs and natural substances.
- The data can be used as benchmark data for the comparison of nano- and microvesicles isolated from different organisms.
- The data can be used for the establishment of biomarkers for plant-derived vesicles valuable for further biological studies.
- The data can provide insights of enzyme composition of citrus-derived vesicles for nanovector design.
- The data can provide insights to the different types of vesicles expressed in citrus fruit sac cells including transport, secretory and extracellular vesicles.

1. Data

We are sharing physiochemical and protein biocargo data on plant-derived nanovesicles and microvesicles. These include TEM images and graphs showing size-distributions determined by DLS (Supplementary Figure 1, 2 and 3) that confirm the vesicular nature of both micro (MV) and nanovesicle-enriched fractions isolated from three different citrus species *C. sinensis*, *C. limon* and *C. aurantium*. Supplementary Table 1A lists the identified proteins in the MV and Supplementary Table 1B lists the data relative to the NV fractions of four citrus species, *C. sinensis*, *C. limon*, *C. paradisi* and *C. aurantium*. In each samples approximately 600–800 proteins were identified. Supplementary Table 2A reports the relative protein expression levels obtained by label-free protein quantitation. 1700 proteins were quantified in the 8 samples analyzed. Supplementary Table 2B lists the four citrus vesicle protein cargo associated orthogonal genes (OGs) and helps to compare the citrus data with other taxa. Comparison is shown between (i) four citrus and EVpedia present OGs, (ii) the data obtained on *C. limon* and that published by Raimondo et al. (2015), and (iii) the data obtained on *C.*

paradisi and that published by Wang et al. (2014a). EggNOGs OGs were determined by EggNOG mapper version 4.5.1. [8].

Supplementary Table 3 is related to the vesicular transport proteins. Supplementary Table 3A) shows the putative vesicular transport related proteins in the proteome of *C. sinensis* and Supplementary Table 3B lists the potential vesicular transport related cargo proteins identified in citrus fruit juice sac cell derived vesicles. Supplementary Table 4A shows the expression level of various enzymes identified in the citrus vesicles related data while in Supplementary Table 4B the Kegg Pathway are associated to the identified enzymes isolated from citrus vesicles.

2. Experimental design, materials and methods

2.1. Plant material and vesicle isolation

Micro and nanovesicle enriched fractions were isolated from the fruits of four different Citrus species, sweet orange (*C. sinensis*), lemon (*C. limon*), grapefruit (*C. paradisi*) and bitter orange (*C. aurantium*) using differential centrifugation method as described in Pocsfalvi et al., 2018 [1,2].

2.2. Transmission electron microscopy

5 μ L samples at 1 μ g/ μ L protein concentrations in 0.1 M PBS pH 7.6 were deposited onto formvar and carbon coated 300 mesh copper grids for one minute for transmission electron microscopy (TEM) analysis. The droplets were removed, the grids were dried and the samples were negatively stained with 2% (w/v) aqueous uranyl acetate. TEM images were acquired by a Jeol JEM 1011 electron microscope operating at 60 kV and mounted with a Morada CCD camera (Olympus Soft Imaging Solutions).

2.3. Dynamic light scattering

Vesicle size distribution was measured by dynamic light scattering (DLS) using a Zetasizer Ver. 7.01, Malvern Instrument (Malvern, UK) at room temperature. Vesicles were dispersed in water and the intensity of the scattered light was measured with a detector at 90° angle. Mean diameter and size distribution were the mean of three analyses.

2.4. NanoLC-ESI-MS/MS and data analyses

The quality of vesicle samples was controlled using sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE) and in-solution digestion-based shot-gun proteomics as it is reported by Pocsfalvi et al. [1].

NanoLC-ESI-MS/MS analysis was carried out on 1 μ g of tryptic digest using a Dionex Ultimate 3000 nanoRSLC (Dionex, Sunnyvale, Ca, USA) coupled to a Bruker Maxis II mass spectrometer (Bruker Daltonics GmbH, Bremen, Germany) via CaptiveSpray nanobooster ionsource. Peptides were desalted on an Acclaim PepMap100 C-18 trap column (100 μ m \times 20 mm, Thermo Scientific, Sunnyvale, CA, USA) using 0.1% TFA for 8 min at a flow rate of 5 μ L/min and separated on the ACQUITY UPLC M-Class Peptide BEH C18 column (130 Å , 1.7 μ m, 75 μ m \times 250 mm, Waters, Milford, MA, USA) at 300 nl/min flow rate, 48 °C column temperature. Solvent A was 0.1% formic acid, solvent B was acetonitrile, 0.1% formic acid and a linear gradient from 4% B to 50% B in 90 min was used. Mass spectrometer was operated in the data dependent mode using a fix cycle time of 2.5 s. MS spectra were acquired at 3 Hz, while MS/MS spectra at 4 or 16 Hz depending on the intensity of the precursor ion. Singly charged species were excluded from the analysis.

Protein identification, quantitation [1,3-7], statistical analysis and bioinformatics has been performed as it is described in Ref. [1,9,10].

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Transparency document. Supporting information

Transparency document associated with this article can be found in the online version at <https://doi.org/10.1016/j.dib.2018.12.036>.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at <https://doi.org/10.1016/j.dib.2018.12.036>.

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