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Data Article

From hundreds to thousands: Widening the normal human Urinome

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ABSTRACT

The limits on protein detection in urine are unknown. Improving the analytical approach to detection would increase the number of identified proteins and potentially strengthen their predictive potential in diseases.

Here, we present the data that resulted from a combination of analytical procedures for maximizing sensitivity and reproducibility of normal human urinary proteome analysis. These procedures are ultracentrifugation, vesicle separation, combinatorial peptide ligand libraries (CPLL) and solvent removal of pigments. Proteins were identified by an Orbitrap Velos Mass Spectrometry. 3429 proteins are characterized, 1724 of which are novel discoveries.

The data are related to Santucci et al. (in press) [1] and available both here and at *ChorusProject.org* under project name "From hundreds to thousands: widening the normal human Urinome". The material supplied to Chorus Progect.org includes technical MS spectra data only.

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Specifications table

Subject area	Biology
More specific subject area	Characterization of urine proteome in normal conditions. It was developed a new strategy of analysis which allowed the extension of the number of identified proteins to 3429 (1724 were of new description here). The list of identified proteins is reported in Supplementary Table 1.
Type of data	Excel tables
How data was acquired	*Ultracentrifuge*: Beckman Optima^{TM} l-90K (Ti 90 rotor). *Mass spectroscopy*: for analysis of all urinary sub-fractions was used a linear Trap Quadropole (LTQ) Orbitrap Velos Pro Mass Spectrometry.
Data format	Raw MS files as processed with the Thermo Scientific Proteome Discoverer software: peak were searched by the MASCOT and SEQUEST against Uniprot human database, filtered for a maximum 1% FDR using Percolator; the Peptide Mass Deviation was set to 10 ppm and a minimum of six 6 amino acids per identified peptide were required [2,3]. The Database search parameters were mass tolerance precursor 20 ppm [4], mass tolerance fragment CID 0.8 Da with dynamic modification of deamidation (N, Q), oxidation (M) and static modification of alkylation with IAM (C). Label free experiments and statistical analysis were performed with Perseus software.
Experimental factors	*Sample Collection and Urine Preparation*: Second morning urine (approximately 160 mL) from healthy volunteers were collected, centrifuged at 4 °C for 10 min at 1000*g*. Urine were frozen and maintained at −80 until further processing [5–14]. Second step was centrifugation at 17,000*g* for 30 min at 16 °C. The sample, after Bradford protein assay [15], was stored at −80 °C until use.
Experimental features	Procedure used for analysis of the urinary proteome: Vesicle Isolation, butanol precipitation, Combinatorial Solid-Phase Ligand Library chromatography, Mass spectrometry and Bioinformatic analysis.
Consent	Informed consent was obtained from all the participants in the study.
Data source location	Genova, Italy.
Data accessibility	The data are available at *ChorusProject.org* under project name "From hundreds to thousands: widening the normal human Urinome". Row data relative to MS spectra are available at *ChorusProject.org* under project name "From hundreds to thousands: widening the normal human Urinome". Data are also directly available with this article

Value of the data

- Sub-fractionating normal urine by successive steps allowed to identify 3429 proteins, a net +50% increment compared to traditional methods of analysis.
- Vesicles separation, CPLL and solvent treatments are the basic steps.
- 1724 of the urine proteins identified here are of newly identified and described. Improved characterization of the normal urinary proteome opens doors for the analysis of urine biomarkers in human diseases.

1. Data, experimental design, materials and methods

3429 Non-redundant proteins discovered in our urine proteomic analysis are characterized and are noted in Supplementary Table 1 [1]. 1615 of these proteins were contained in vesicles while the remaining 1794 were equally distributed among CPLL (1488) and butanol insoluble fractions (322). Several proteins were detected exclusively in one of the phases of the procedure, suggesting that each step is crucial in the fractionation strategy. Many (1724) proteins are here described whose presence in urine have never been reported and represent a potential source of information considering that urine is the unique site of excretion of products of interaction of metabolic processes.

1.1. Urinary vesicles isolation

The 17,000*g* urinary supernatant (80 mL) was ultracentrifuged at 48,000 rpm for 75 min at 18 °C. The ultracentrifugation step was repeated by adding the same volume used before until vesicles [16] were isolated. The pellets, washed in DTT (200 mg/mL) and Tris–HCl 65 mM pH 8.8, was centrifuged a 14,000 rpm for 10 min at 4 °C and stored at −80 °C until mass spectrometry analysis.