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Data Article

Mass spectrometry data from a quantitative analysis of protein expression in gills of immuno-challenged blue mussels (*Mytilus edulis*)

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ABSTRACT

Here, we provide the dataset associated with our research article on the potential effects of ocean acidification on antimicrobial peptide (AMP) activity in the gills of *Mytilus edulis*, "Impact of ocean acidification on antimicrobial activity in gills of the blue mussel (*Mytilus edulis*)" [1]. Blue mussels were stimulated with lipopolysaccharides and samples were collected at different time points post injection. Protein extracts were prepared from the gills, digested using trypsin and a full in-depth proteome investigation was performed using liquid chromatography coupled to tandem mass spectrometry (LC–MS/MS). Protein identification and quantification was performed using the MaxQuant 1.5.1.2 software, "MaxQuant enables high peptide identification rates, individualized p.p.b.-range mass accuracies and proteome-wide protein quantification" [2].

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Specifications Table

Subject area	*Biology*
More specific subject area	*Protein expression in Mytilus edulis*
Type of data	*Table,.xlsx file*
How data was acquired	*Data dependent LC-MS/MS acquired on a Q Exactive instrument (Thermo Fisher Scientific) coupled to a ultra nanoflow high-performance liquid chromatography (HPLC) system (EASY-nLC™ 1000, Thermo Fisher Scientific)*
Data format	*Processed, analyzed*
Experimental factors	a) *Lipopolysaccharide stimulation of blue mussels and protein extraction from gills* a) *LC-MS/MS analysis for protein identification and quantification*
Experimental features	*Blue mussels were stimulated with lipopolysaccharides and samples were collected at different time points post injection. Protein extracts were prepared from the gills, digested using trypsin and a full in-depth proteome investigation was performed using LC-Orbitrap MS/MS technique. The spectra (.RAW) were acquired using Xcalibur software 3.0.63 and further database searches were performed using MaxQuant* 1.5.1.2. *The search results were stored as.xls-files.*
Data source location	*Uppsala, Sweden*
Data accessibility	*Data are within this article* (Supplementary Table 1)

Value of the data

- The data further validate the protein expression changes presented in Hernroth et al. [1].
- The data can be used to validate protein identification in *Mytilus edulis* from other studies.
- The in depth proteomic data enables comparison with RNA expression data.

1. Data

This dataset comprise the output file (Supplementary Table 1, available online) from the database search of LC–MS/MS raw files obtained from bottom-up MS analysis of gills from *Mytilus edulis* immune-challenged by lipopolysaccharide injection. Samples were collected at five time points post injection of lipopolysaccharide (Table 1). One control group of mussels injected with only *Mytilus* physiological saline (PS)-buffer was included. Each group included five individual mussels.

2. Experimental design, materials and methods

2.1. Experimental set up

Thirty mussels were kept in the running seawater system of SLC-Kristineberg ($\sim$32 PSU, 14 °C) and divided into six 15 L basins with five individuals in each. Bacterial contamination was avoided by pre-challenging with lipopolysaccharide (LPS; #L7261, Sigma Aldrich) dissolved in PS-buffer [3]. One control group of mussels was injected with only PS-buffer and the other five groups were injected with 0.2 μg LPS g^{-1} mussel (wet weight), into the adductor muscle. The gills of mussels from the control group were dissected at time 0 followed by dissection of one group at a time after 0.5, 1.5, 3, 5 and 8 h post injection. The dissected gill tissues were immediately put on dry ice before being stored at −80 °C until further prepared.