Interaction network and mass spectrometry data of *Xanthomonas citri* subsp. *citri* surface proteins from differential proteomic analysis of infectious and non-infectious cells

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**A B S T R A C T**

Here we provide the mass-spectrometry and *in silico* interaction network dataset of proteins identified on our research article on surface proteomic analysis from *Xanthomonas citri* subsp. *citri* (XAC) cells grown in vivo (infectious) and in vitro (non-infectious, control) by 2D-DIGE approach. Fluorescence labeling of proteins were performed on intact cells followed by cellular lysis and labeled spots from 2D gel differing in abundance between the two conditions (ANOVA, *p*-value < 0.05) were analyzed by a nano-electrospray tandem mass spectrometry Q-Tof Ultima API mass spectrometer (MicroMass/Waters) (LC-ESI-MS/MS). This article contains raw data of proteins detected in the 79 spots analyzed by LC-ESI-MS/MS approach and also an enrichment analysis on the resulting protein–protein interaction network performed with the Integrated Interactome System (IIS) platform and Cytoscape software. The data are supplementary to our original research article, “*Xanthomonas citri* subsp. *citri* surface proteome by 2D-DIGE: ferric enterobactin receptor and other outer membrane proteins potentially involved in...”
Specifications Table

| Subject area | Biology |
|-------------|---------|
| More specific subject area | Plant–pathogen interaction proteomics |
| Type of data | MS spectra raw files, Figure, Table |
| How data was acquired | Mass Spectrometry Liquid Chromatography: nano-electrospray tandem mass spectrometry Q-Tof Ultima API mass spectrometer system used: MicroMass/Waters |
| Data format | Raw, analyzed |
| Experimental factors | 2D-DIGE proteome analysis of surface-labeled XAC cells (in vivo vs. in vitro) |
| Experimental features | XAC cells were grown in vivo (infectious) and in vitro (non-infectious) conditions and cells were fluorescently labeled previously to cell lysis. Differential spots were isolated, trypsin-digested and peptide samples were analyzed by LC-ESI-MS/MS and proteins identified by Mascot search software. |
| Data source location | Campinas and São Carlos, São Paulo State, Brazil. |
| Data accessibility | All the raw files from mass spectrometry analysis are deposited in Peptide Atlas and can be found through the PASS00850 number or by the link ftp://PASS00850:ZJ7425v@ftp.peptideatlas.org/. |

Value of the data

- Data were generated by a first study on surface proteome of XAC interacting with its citrus host and thus can provide additional information for XAC-host interaction studies in need of proteomic data
- In silico interaction analysis provides an overview of possible protein–protein interactions among XAC cells.

1. Data

Data include raw files of mass spectrometry analysis of tryptic peptides of XAC surface proteins labeled with CyDyes DIGE minimal dyes. Proteins with differential abundance in cells grown in vivo and in vitro were mapped into a protein–protein interaction network (Fig. 1; Supplementary data). Information of overrepresented Gene Ontology (GO) biological processes and KEGG pathways is shown (Table 1).

2. Experimental design, material and methods

XAC genome strain (strain 306) was grown in vivo on detached Citrus aurantifolia leaves (infectious condition) and in vitro in NB medium (non-infectious condition, control), as described by Carnielli et al. [1].
2.1. LC-ESI-MS/MS analysis

Seventy-nine CyeDye labeled spots determined as differential by ANOVA (DeCyder software, GE Healthcare) were excised, digested with trypsin and peptide mixtures from each spot were loaded onto an analytic column C18 1.7 μm BEH 130 (100 μm × 100 mm) RP-UPLC (nanoAcquity UPLC, Waters) coupled to a nano-electrospray tandem mass spectrometry Q-Tof Ultima API mass spectrometer (MicroMass/Waters). A trapping column Symmetry C18 (180 μm × 20 mm) was used for desalting and sample concentration.

Data files generated by the LC-ESI-MS/MS analysis (PeptideAtlas dataset submission PASS00850) were processed using the search engine MASCOT Distiller v.2.3.2.0, 2009 (Matrix Science Ltd.) and the sequences were searched against XAC 306 genome databank (available at NCBI) using Mascot Server v.2.3.01.0 (Matrix Science Ltd.). The following parameters were used for database searches: trypsin with 1 missed cleavage allowed, mass tolerance of 0.1 Da for the precursor ions and a tolerance of...
| ID     | Gene symbol | ENSEMBL | SWISS-PROT                      | Protein structure (PDB) | Conserved domain (CDD) | Gene ontology (GO) | Cellular component | Molecular function       | Biological process                                      |
|--------|-------------|---------|---------------------------------|-------------------------|------------------------|---------------------|--------------------|-----------------------|--------------------------------------------------------|
| Q8PQW5 | glnA        | Not defined | Glutamine synthetase OS=Methylococcus capsulatus (strain ATCC 33,009/NCIMB 11,132/Bath) GN=glnA PE=3 SV=2 | 2gls GLUTAMINE SYNTHETASE | TIGR00653, GlnA, glutamine synthetase, type I | GO:0005737 cytoplasm | GO:0005524 ATP binding | GO:0006542 glutamine-biosynthetic process | GO:0004356 glutamate-ammonia ligase activity GO:0009399 nitrogen fixation |
| Q8PQ7  | XAC0245     | Not defined | No hits found                     | No hits found            | No hits found          | Not defined         | Not defined          | Not defined           | Not defined                                                          |
| Q8PPZ1 | groL        | Not defined | 60 kDa chaperonin OS=Xanthomonas axonopodis pv. citri (strain 306) GN=groL PE=3 SV=1 | 3e76 60 kDa chaperonin   | PRK00013, groEL, chaperonin GroEL | GO:0005737 cytoplasm | GO:0005524 ATP binding | GO:0042026 protein refolding                           |                                                          |
| Q8PN6  | fusA        | Not defined | Elongation factor G OS=Xanthomonas axonopodis pv. citri (strain 306) GN=fusA PE=3 SV=1 | 4kjc elongation factor G | PRK00007, PRK00007, elongation factor G | GO:0005737 cytoplasm | GO:0005525 GTP binding | Not defined                                  |                                                        |
| Q8PN8  | rplP        | Not defined | 50S ribosomal protein L16 OS=Xanthomonas oryzae pv. oryzae (strain KACC10331/ KX085) GN=rplP PE=3 SV=1 | 4kjb 50S ribosomal protein L16 | PRK09203, rplP, 50S ribosomal protein L16 | GO:0005840 ribosome   | GO:0019843 tRNA binding | GO:0006412 translation                                 | GO:0003735 structural constituent of ribosome GO:0000049 tRNA binding |
| ID   | Gene symbol | ENSEMBL | SWISS-PROT | Protein structure (PDB) | Conserved domain (CDD) | Gene ontology (GO) |
|------|-------------|---------|------------|-------------------------|------------------------|-------------------|
|      |             |         |            |                         |                        | Cellular component | Molecular function | Biological process |
|      |             |         |            |                         |                        |                   |                   |                   |
| Q8PN59 | gcvP | Not defined | Glycine dehydrogenase (decarboxylating) OS = *Xanthomonas axonopodis* pv. *citri* (strain 306) GN = gcvP PE = 3 SV = 1 | 4lh4 Glycine dehydrogenase [decarboxylating] | PRK05367, PRK05367, glycine dehydrogenase | Not defined | GO:0004375 glycine dehydrogenase (decarboxylating) activity | GO:0019464 glycine decarboxylation via glycine cleavage system |
| Q8PNG1 | XAC1110 | Not defined | Nucleoid-associated protein XAC1110 OS = *Xanthomonas axonopodis* pv. *citri* (strain 306) GN = XAC1110 PE = 3 SV = 1 | 1pug Hypothetical UPF0133 protein ybaB | PRK00153, PRK00153, hypothetical protein | GO:0043590 bacterial nucleoid | GO:0003677 DNA binding | Not defined |
| Q8PN5 | clpP | Not defined | ATP-dependent Clp protease proteolytic subunit OS = *Xanthomonas oryzae* pv. *oryzae* (strain KACC10331/ KX085) GN = clpP PE = 3 SV = 1 | 2fzs ATP-dependent Clp protease proteolytic subunit | PRK00277, clpP, ATP-dependent Clp protease proteolytic subunit | GO:0005737 cytoplasm | GO:0004252 serine-type endopeptidase activity | Not defined |
| Q8PN2 | mopB | Not defined | Outer membrane porin F OS = *Pseudomonas aeruginosa* (strain ATCC 15,692/PAO1/1C/PRS 101/LMG 12,228) GN = oprF PE = 1 SV = 1 | No hits found | cd07185, OmpA_C-like, Peptidoglycan binding domains similar to the C-terminal domain of outer-membrane protein OmpA | GO:0009279 cell outer membrane | GO:0005509 calcium ion binding | Not defined |
| Q8PN8 | mdh | Not defined | Malate dehydrogenase OS = *Xanthomonas axonopodis* | 1b8v PROTEIN (MALATE DEHYDROGENASE) | PRK05442, PRK05442, malate dehydrogenase | Not defined | GO:00044262 cellular |                   |
| Accession | Gene/Description | Species/Strain | GO Terms |
|-----------|-----------------|----------------|----------|
| Q8PK77    | rpsA            | Not defined    | GO:0030060 L-malate dehydrogenase activity |
|           |                 | 30S ribosomal protein S1 | carbohydrate metabolic process |
|           |                 | Pseudomonas aeruginosa (strain ATCC 15,692/PAO1/1C/PRS 101/LMG 12,228) | GO:0006108 malate metabolic process |
|           |                 | DEM=3 SV=1     | GO:0006099 tricarboxylic acid cycle |
| Q8PMB0    | dnaK            | Not defined    | GO:0005840 ribosome |
|           |                 | Chaperone protein DnaK | GO:0003723 RNA binding |
|           |                 | Xanthomonas axonopodis pv. citri (strain 306) | GO:0006412 translation |
|           |                 | DEM=3 SV=1     | GO:0003735 structural constituent of ribosome |
| Q8PMC2    | XAC1509         | Not defined    | Not defined |
|           |                 | No hits found  | Not defined |
|           |                 | Outer membrane protein assembly factor BamA | Not defined |
|           |                 | Edwardsiella ictaluri (strain 93-146) | Not defined |
|           |                 | DEM=3 SV=1     | Not defined |
| Q8PML3    | oma             | Not defined    | Not defined |
|           |                 | No hits found  | Not defined |
|           |                 | Outer membrane protein assembly factor BamA | Not defined |
|           |                 | DEM=3 SV=1     | Not defined |

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| ID    | Gene symbol | ENSEMBL | SWISS-PROT | Protein structure (PDB) | Conserved domain (CDD) | Gene ontology (GO) |
|-------|-------------|---------|------------|-------------------------|------------------------|--------------------|
| Q8PMV4| mucD        | Not defined | Probable periplasmic serine endoprotease DegP-like OS = *P. aeruginosa* pv. *pseudomonas savastanoi* pv. *phaeolica* (strain 1448A/Race 6) | 3otp Protease do | TIGR02037, degP_htrA DO, periplasmic serine protease, Do/DeqQ family | Not defined |
| Q8PJ70| oar         | Not defined | No hits found | No hits found | pfam13620, Carboxypeptidase regulatory-like domain | GO:0004872 receptor activity |
| Q8PJ69| XAC2673     | Not defined | No hits found | No hits found | No hits found | Not defined |
| Q8PJ68| XAC2674     | Not defined | UPF0056 inner membrane protein YhgN OS = *Shigella flexneri* GN = yhgN PE = 3 SV = 1 | No hits found | COG2095, MarC, Multiple antibiotic transporter [Intracellular trafficking and secretion] | Not defined |
| Q8PI27| iroN        | Not defined | No hits found | No hits found | TIGR01782, TonB-XanthCaul, TonB-dependent receptor | GO:00009279 cell outer membrane |
| Q8PHT1| bfeA        | Not defined | No hits found | No hits found | cd01347, ligand_gated_channel, TonB-dependent/Ligand-Gated channels are created by a monomeric 22 strand (22,24) anti-parallel beta-barrel | GO:00009279 cell outer membrane |

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| Accession | Gene Id | Description | GO:0009279 cell outer membrane | GO:0004872 receptor activity | GO:004473 malate dehydrogenase (oxaloacetate-decarboxylating) (NADP\(^+\)) activity |
|-----------|---------|-------------|-------------------------------|-------------------------------|------------------------------------------------------------------|
| Q8PHT0    | bfeA    | Not defined | No hits found                 | No hits found                 | PRK07232, PRK07232, bifunctional malic enzyme oxidoreductase/ phosphotransacetylase |
| Q8PGZ2    | maeB    | Not defined | NADP-dependent malic enzyme   | No hits found                 | Go:0005829 cytosol                                               |
| Q8PH16    | btuB    | Not defined | No hits found                 | No hits found                 | Go:0004473 malate dehydrogenase (oxaloacetate-decarboxylating) (NADP\(^+\)) activity |
| Q8PH23    | adk     | Not defined | Adenylate kinase              | No hits found                 | Go:0005737 cytoplasm                                            |
| ID     | Gene symbol | ENSEMBL | SWISS-PROT   | Protein structure (PDB)                                                                 | Conserved domain (CDD)                                                                 | Gene ontology (GO)                                                                 |
|--------|-------------|---------|--------------|----------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|
|        |             |         |              |                                                                                        |                                                       |                                                                                 |
| Q8PH89 | fhuE        |         |              | FhuE receptor OS=Escherichia coli (strain K12) GN=fhuE PE=1 SV=2                         | 3efm Ferric alcaligin siderophore receptor                                              | GO:0009279 cell outer membrane                                                        |
|        |             |         |              |                                                                                        | COG:4773, FhuE, Outer membrane receptor for ferric coprogen and ferric-rhodotorulic acid [Inorganic ion transport and metabolism] | GO:0005506 iron ion binding                                                        |
|        |             |         |              |                                                                                        |                                                                                        | GO:0004872 receptor activity                                                      |
|        |             |         |              |                                                                                        |                                                                                        | GO:0015343 siderophore transmembrane transporter activity                          |
| Q8PHB5 | XAC3344     |         |              | Probable fructose-bisphosphate aldolase class 1 OS=Xanthomonas axonopodis pv. citri (strain 306) GN=XAC3344 PE=3 SV=1 | 3mmt Fructose-bisphosphate aldolase                                                   | GO:0004332 fructose-bisphosphate aldolase activity                                   |
|        |             |         |              |                                                                                        | cd00948, FBP_aldolase_I_a, Fructose-1,6-bisphosphate aldolase                         | GO:0005215 transporter activity                                                   |
|        |             |         |              |                                                                                        |                                                                                        | GO:0006096 glycolysis                                                              |
| Q8PFD5 | iroN        |         |              | No hits found                                                                         | No hits found                                                                          |                                                                           |
|        |             |         |              |                                                                                        |                                                                                        |                                                                           |
| Q8PFH2 | argl        |         |              | Arginase OS=Brucella suis biovar 1 (strain 1330) GN=arcB PE=3 SV=1                     | 5cev PROTEIN (ARGINASE)                                                                 | GO:004053 arginase activity                                                        |
|        |             |         |              |                                                                                        | cd009989, Arginase, Arginase family                                                   | GO:0005215 transporter activity                                                   |
|        |             |         |              |                                                                                        |                                                                                        | GO:0006525 arginine metabolic process                                               |
| Q8PG19 | XAC3802     |         |              | No hits found                                                                         | No hits found                                                                          | GO:0046872 metal ion binding                                                        |
|        |             |         |              |                                                                                        |                                                                                        |                                                                                 |

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| Accession | Protein | Description | GO:0005886 (plasma membrane) | GO:0005524 (ATP binding) | GO:0015991 (ATP hydrolysis coupled proton transport) | GO:0045261 (proton-translocating ATP synthase complex, catalytic core F(1)) | GO:0046933 (proton-translocating ATP synthase activity, rotational mechanism) | GO:0046961 (proton-translocating ATPase activity, rotational mechanism) |
|-----------|---------|-------------|-------------------------------|--------------------------|-----------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|
| Q8PGG5 atpA Not defined | ATP synthase subunit alpha | OS = Xanthomonas campestris pv. vesicatoria (strain 85-10) | PRK09281, PRK09281, F0F1 ATP synthase subunit alpha | GO:0005886 (plasma membrane) | GO:0005524 (ATP binding) | GO:0015991 (ATP hydrolysis coupled proton transport) | GO:0045261 (proton-translocating ATP synthase complex, catalytic core F(1)) | GO:0046933 (proton-translocating ATP synthase activity, rotational mechanism) | GO:0046961 (proton-translocating ATPase activity, rotational mechanism) |
| Q8PCN6 xanB Not defined | Xanthan biosynthesis protein | OS = Xanthomonas campestris pv. campestris (strain ATCC 33,913/DSM 3586/NCPPB 528/LMG 568/P 25) | 2x65 MANNOSE-1-PHOSPHATE GUANYLYLTRANSFERASE | TIGR01479, GMP_PMI, mannose-1-phosphate guanylyltransferase/mannose-6-phosphate isomerase | Not defined | GO:0016853 (isomerase activity) | GO:0000271 (polysaccharide biosynthetic process) | GO:0016779 (nucleotidyltransferase activity) | |
| Q8PGY7 XAC3475 Not defined | No hits found | No hits found | pfam13531, SBP_bac_11, Bacterial extracellular solute-binding protein | Not defined | Not defined | Not defined | Not defined | Not defined |
| Q8PER7 XAC4273 Not defined | No hits found | No hits found | No hits found | GO:0016020 (membrane) | GO:0030246 (carbohydrate binding) | GO:0004872 (receptor activity) | GO:0005215 (transporter activity) | GO:0030246 (carbohydrate binding) | GO:0004872 (receptor activity) |
| Q8PER6 XAC4274 Not defined | No hits found | No hits found | No hits found | GO:0016020 (membrane) | GO:0030246 (carbohydrate binding) | GO:0004872 (receptor activity) | Not defined | Not defined |
| ID     | Gene symbol | ENSEMBL | SWISS-PROT | Protein structure (PDB) | Conserved domain (CDD) | Gene ontology (GO) | Cellular component | Molecular function | Biological process |
|--------|-------------|---------|------------|-------------------------|------------------------|---------------------|-------------------|-------------------|-------------------|
| Q8NL22 | tufA        | Not defined |            | Elongation factor Tu, PE = tuf1, V = 1 | PRK00049, elongation factor Tu | GO:0005737 cytoplasm | GO:00005215 transporter activity | GO:0003924 GTP binding| Not defined |
|        |             |          |            | Elongation factor Tu, OS = Xanthomonas campestris pv. vesicatoria (strain 85-10) | GO:0005525 GTP binding |                       |                   |                   |                   |
| P0A0Y2 | rpoA        | Not defined |            | DNA-directed RNA polymerase subunit alpha, PE = rpoA, V = 1 | PRK05182, DNA-directed RNA polymerase subunit alpha | GO:0003677 DNA binding | GO:0003899 DNA-directed RNA polymerase activity | GO:0006351 transcription, DNA-dependent |                   |
|        |             |          |            | DNA-directed RNA polymerase subunit alpha, OS = Xanthomonas oryzae pv. oryzae (strain KACC10331/KX085) | GO:0003746 translation elongation factor activity |                       |                   |                   |                   |
0.1 Da for the fragment ions, carbamidomethyl of cystein as fixed modification, oxidation of methionine (variable), and presence of CyDyes in lysine residues (variable).

2.2. Bioinformatic and network analysis

The identified proteins were submitted to an enrichment analysis by Integrated Interactome System (IIS) platform [2] using the functional annotation database of *Escherichia coli*, since *Xanthomonas* sp. does not have such database annotation. The resulting protein map was visualized on Cytoscape and nodes were assigned in clusters according to the most enriched (lowest enrichment p-value) biological processes or KEGG pathway (Fig. 1). Different colors were used to display proteins from the input (orthologues proteins; in blue) or from the database (in gray). Proteins without a biological process or KEGG pathway annotation are grouped in the center of the network. The annotation table for the input list is shown in Table 1.

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Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.07.054.

Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.07.054.

References

[1] C.M. Carnielli, J. Artier, J.C.F. de Oliveira, M.T.M. Novo-Mansur, *Xanthomonas citri* subsp. *citri* surface proteome by 2D-DIGE: ferric enterobactin receptor and other outer membrane proteins potentially involved in citric host interaction, J. Proteom. (2016), http://dx.doi.org/10.1016/j.jprot.2016.05.007 (in press).

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