

METABOLOMICS-ASSISTED DRAFT METABOLIC NETWORK RECONSTRUCTION OF *PRIESTIA ENDOPHYTICA* UCM B-5715

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Priestia endophytica UCM B-5715 synthesizes a variety of biologically active compounds, such as pigments, substances with anticancer activity, and plant hormone precursors, which makes it a promising industrial strain. However, biotechnologically relevant metabolic pathways and biochemical reaction cascades of this bacterium remain undiscovered.

The information regarding its primary and secondary metabolism, gene regulation, and protein-protein interactions is scattered. This study aimed to gain an insight into the metabolic network interconnections of *P. endophytica* UCM B-5715 and construct a knowledgebase merging genomic, proteomic, and metabolomic data on this microorganism. To conduct metabolomic profiling, the strain *P. endophytica* UCM B-5715 was grown on beef-extract agar for 24 hours. Exo- and endometabolites were extracted following standard protocol and separated by gas chromatography-mass spectrometry. The results were imported into MetaboAnalyst5.0 for evaluation. The strain's whole genome annotated assembly was obtained from the GenBank database (GCA_900115845.1) and manually reannotated via ebi-blastp search against the uniprotkb_bacteria database. Merlin software was used for metabolic network reconstruction. Gene-Protein-Reaction associations and gap-fill analysis were introduced manually into the model based on genome annotation, experimental data, and literature evaluation. We obtained 101 metabolites that were categorized into 7 categories. The majority of metabolites were clustered into the organic acids, carbohydrates, and fatty acyls RefMet super-classes, which comprised 28%, 25%, and 25% of the total number of compounds, respectively. Over Representation Analysis indicated that 25 pathways were significantly associated with the metabolic profile obtained, Protein biosynthesis, Aspartate metabolism, and Glutathione metabolism showing the largest enrichment ratio. Manual genome reannotation showed that 2016 genes out of 5144 had an enzyme-coding function. According to gene content analysis, 40% of genes in the network code for amino acid metabolism enzymes. Both nucleotide metabolism genes and genes involved in cofactor biosynthesis represent 18% of the enzyme-encoding genome. The pathways of terpenoids and polyketides biosynthesis, indole alkaloid biosynthesis, cyanoamino acid biosynthesis, and xenobiotic degradation are reported in the strain *P. endophytica* UCM B-5715 for the first time. The model contains 73 KEGG pathways featuring 1559 reactions. There are 5750 reactants and 7023 products in *P. endophytica* UCM B-5715 metabolic network in total. Thus, with the help of metabolomic profiling and genome reannotation, we developed a draft metabolic network reconstruction of *P. endophytica* UCM B-5715, which deepens the current knowledge of its metabolism and sheds light on the previously unexplored biotechnologically important traits.

