In silico prediction of auxiliary activity enzymes secreted by the fungus Chrysoporthe cubensis

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The growing concern over the worldwide shortage of fossil fuels and the increasing emissions of greenhouse gases has provided the development of technologies that use biomass from agricultural residues for the production of biofuels. Our research group has demonstrated that Chrysoporthe cubensis, a plant pathogenic fungus, has produced enzymatic extracts more efficient for plant biomass degradation than commercial preparations. So, it is essential to know in detail the enzymes and proteins secreted by this fungus, especially those involved in the hydrolysis of biomass. In addition to the Glycoside Hydrolyses (GH) enzymes, this fungus can produce Auxiliary Activities (AAs), which are still poorly studied. The presence of this wide range of enzymes may explain the high efficiency of this fungal extract compared to commercial cocktails. It has been proposed a bioinfosecretome study of C.cubensis enzymes with Auxiliary Activities, through in silico predictions of candidate protein secretion using bioinformatics tools. Computational analysis will provide information on the probable secretome of *C.cubensis* and the identification of key enzymes that can be targeted to increase the hydrolytic efficiency, making this extract more interesting for commercial purposes. Protein sequences from eukaryotes belonging to thirteen families of Auxiliary Activities enzymes of Carbohydrate-Active enzymes database (CAZy) were recovered and aligned (tblastn) with the complete genome draft of C.cubensis selecting only the aligned regions with more than 70% of coverage and 40% of identity. The resulting gene coordinates were subjected to a manual curation step for elimination of possible redundancies and then subjected to ab initio gene prediction using the program Augustus. After obtaining the final model of predicted genes, members of AA1 families were selected for comparative studies of sequence variability. Later, the C.cubensis enzymes of interest will be selected and the structural modeling by comparison with structural domains of auxiliary enzymes characterized and belonging to fungi with different lifestyles, in which it will allow to verify unique characteristics of the catalytic sites of *C.cubensis* enzymes that can positively influence the interaction between target and substrate. Thus, through comparative studies of structural diversity among the members of AA1 family, is expected to select enzymes with great potential for commercial application.

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