Computational analysis and functional prediction of ubiquitin hypothetical protein: A possible target in parkinson disease

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Parkinson´s disease (PD) is a high prevalent progressive neurodegenerative disorder characterized by degeneration of dopaminergic neurons and intracytoplasmatic aggregation of ?-synuclein called Lewy Bodies. Anomalies in the proteasomal and endosomal ubiquitin related degradation of ?-synuclein have been related with PD. Among the different proteins described in ubiquitin pathway, the hypothetical protein CAB55973.1 was identified previously. Here we modeled this hypothetical protein in order to contribute to the understanding of PD pathogenesis that should be served as an input in the future as drug targets. This study predicted a three-dimensional model of the complete sequence of hypothetical protein CAB55973.1 with a high value of identity and a good homology quality. Subcellular localization was found in the cytoplasm, mainly in the endosomal membrane. 36 protein-protein interactions related to PD were found. 11 residues were predicted to interact with target proteins for ubiquitination. Binding site prediction showed that one domain (residues 163 to 238) might be involved in ubiquitination of target proteins. In this ubiquitin domain, residues were distributed similarly to those of the binding site of the ubiquitin interacting with the UIM of Hrs protein (PDB 2D3G). The hypothetical protein was constructed based on the complete sequence alignment, which allowed predicting the structure with a high accuracy. The functional prediction showed that only one domain of the hypothetical protein might be involved in the ?- synuclein ubiquitination of the endosomal pathway of the PD. © 2016 Bentham Science Publishers.

Homology mathematical modeling

Hypothetical protein

In-silico

Parkinson disease

Ubiquitin

ubiquitin

alpha synuclein

antiparkinson agent

ubiquitin

Article

gene mutation

human

mathematical model

Parkinson disease

peptide mapping

protein analysis

protein binding

protein expression

protein localization

protein protein interaction

protein secondary structure

protein structure

proteomics

quality control

reliability

sequence alignment

signal transduction

amino acid sequence

binding site

biology

cell fractionation

chemical structure

chemistry

drug effects

genetics

molecular genetics

Parkinson disease

theoretical model

ubiquitination

alpha-Synuclein

Amino Acid Sequence

Antiparkinson Agents

Binding Sites

Computational Biology

Humans

Models, Molecular

Models, Theoretical

Molecular Sequence Data

Parkinson Disease

Protein Structure, Secondary

Subcellular Fractions

Ubiquitination

Ubiquitins