

## **Molecular modeling and structural analysis of the Myelin basic protein-Q65ZS4**

**José Gilberto Jardine<sup>1</sup>, Goran Neshich<sup>1</sup>, Ivan Mazoni<sup>1</sup>, Daniel Martins<sup>2</sup>, Sérgio Marangoni<sup>2</sup>, José Camillo Novello<sup>2</sup>, Wagner F. Gattaz<sup>3</sup>, Emmanuel Dias-Neto<sup>3</sup>**

<sup>1</sup>Embrapa Information Technology, Av. André Tosello 209, Campinas, SP, Brazil.

<sup>2</sup>Laboratório de Proteômica, Depto de Bioquímica - IB - UNICAMP, Campinas, SP, Brasil.

<sup>3</sup>Laboratório de Neurociências - LIM-27 Inst. de Psiquiatria - Faculdade de Medicina da USP

Corresponding author: J. G. Jardine

E-mail: [jardine@cnptia.embrapa.br](mailto:jardine@cnptia.embrapa.br)

### **Abstract**

Schizophrenia (SCZ) is a chronic, debilitating psychotic mental disorder that affects about 1 percent of the population in different countries. SCZ is characterized by a series of negative and positive symptoms including psychomotor retardation, attentional impairment, decreased emotional expression, psychomotor agitation, and auditory hallucinations. A quantitative proteomic analysis of the Anterior Temporal Lobe (ATL) of SCZ and control samples reveal some differentially expressed proteins as Myelin Basic Protein (MBP). MBP is the major constituent of the myelin sheath of oligodendrocytes and Schwann cells in the CNS. MBP has a neuroprotective role in vivo which is controlled by neurotrophic factors. Our study is based on the model of this protein. Homology modeling was done by using the crystallographic structure of a Immunodominant Epitopes homologous protein (PDB code: 1FV1/C) as a template. Analysis of the model structure using BlueStar Sting software indicates that some amino acids present energy of contacts higher than those on the average. Those residues can have an important role in the stability of this protein when cross referenced with the residues showing order of cross presence and cross link higher than the usual measures.

Key words: **Schizophrenia, Myelin basic protein, Molecular modeling, Structural Analysis of protein, bioinformatics.**