

Structural model for Gas1p family members by combined threading and secondary structure prediction methods - (session: Other)

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The Gas1p is a *S.Cerevisiae* membrane glycoprotein that plays a key role in cell wall assembly [1], and belongs to the Gas1p family 72 of β -1,3 glucanases. Several others family members were isolated from *S.Cerevisiae* and from *Candida* species, *S.Pombe* and other fungal organisms.

In particular, five gas genes were present in *S.Cerevisiae* coding for different Gas enzymes, each characterized by a different modular organization of domains.

The catalytic domain (C-domain) is the most conserved among all members of the family and its structural features are particularly relevant to investigate structure-function relationships in this class of enzymes.

Aim of this work was the prediction of the 3D structure of this domain and the comparison of C-domains of different members of the Gas1p family. Due to the unavailability of a 3D structure template suited for homology model construction, we combined threading methods [2] and secondary structure predictions to derive 3D models of some Gas1p family members.

Base on this analysis we propose that the C-domain assumes a TIM-barrel fold and that the portion of the active site residues in our models are compatible with the catalytic characteristic proposed for GHA clan members [3] and we conduct a detailed analysis and comparison of the structural features of C-domains of some of the different members of Gas1p family. SOLO POSTER

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2. Jones D. , Thornton J., Protein fold recognition, *J. Comput. Aided. Mol.Des.*, 1993, 4: 439-456.
3. Henrissat B., Callebaut I., Fabrega S., Lehn P., Mornon J.P., Davies G., Conserved catalytic machinery and the prediction of a common fold for several families of glycosyl hydrolases, *PNAS*, 1996, 93(11):5674