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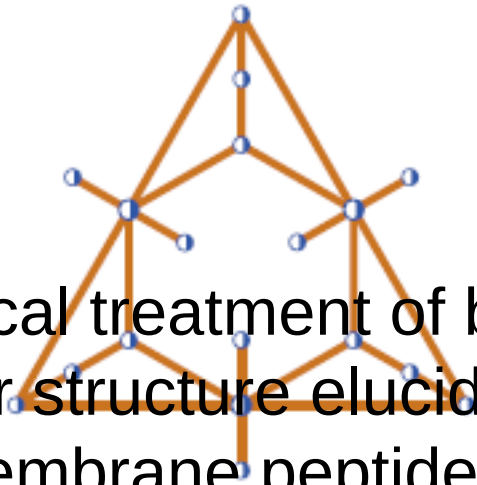

Mathematical treatment of biochemical data for structure elucidation of transmembrane peptide regions

Content :

We present an approach towards structure elucidation of bilitranslocase (BTL) transmembrane regions. BTL is a membrane protein which transports bilirubin from blood to liver cells. The sequence and secondary structure information of transmembrane segments of proteins with known 3D structure is exploited to predict the transmembrane domains of structurally unresolved target protein. With the help of known structures the trans-membrane domains are encoded in such a way that it is possible to group and classify them with respect to their specific sub-structural characteristics and to build a model for prediction of transmembrane segments. In order to explore the bilitranslocase transport mechanism, we tested a set of non-congeneric compounds for their competitive inhibition constants in the investigated protein-substrate system. The information about chemical structure of small molecules that inhibit bilitranslocase helps us to build a hypothesis about the transport mechanism of the studied biological system.

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