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Sequence to structure and immunological analysis of MOMP from *Chlamydiae*

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The Major Outer Membrane Protein (MOMP) is the most abundant (60 % by weight) protein in the cell membrane of the *Chlamydiae* family. Its cellular localization makes it important for survival, host cell adhesion, invasion and other pathological schemes of *Chlamydiae*. MOMP has been reported to possess antibody neutralizing properties as well as provoking a unique inflammatory immune response. This protein, conserved in all species of *Chlamydiae* is a vaccine target against human and livestock diseases. This report focuses on bioinformatics and wet laboratory approaches utilized for the analysis of this 40kDa, 389 aa protein. Bioinformatics analysis revealed that MOMP is a β-barrel protein with surface exposed peptide epitopes. Further bioinformatics using the Sybyl-X flexible docking protocol shows that the peptides formed stable complexes with MHC class II and surface exposed aliphatic side chains that may be accessible to T-cell receptors. In fact, other research groups have shown that these peptides have an anti-inflammatory effect in an animal model of atherosclerosis. MOMP was effectively cloned, expressed and purified for structural studies. Analysis of MOMP by circular dichroism revealed that MOMP is a β-sheet rich protein which proved to be more thermostable in the presence of fatty acids and intermediates of the citric acid cycle. Finally, a low-resolution structure 4Å for MOMP has been obtained by molecular replacement based on FadL of *E. coli*. The findings from this work open a new frontier for the development of drugs and vaccines that target MOMP.

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