

Title: *Structure based functional identification of an uncharacterized protein from Coxiella burnetii involved in adipogenesis*

Author Names: Tajul Islam Mamun, Mohammed Bourhia, Taufiq Neoaj, Shopnil Akash, Md. A. K. Azad, Md. Sarowar Hossain, Md. Masudur Rahman, Yousef A. Bin Jordan, Samir Ibenmoussa & Baye Sitotaw

Abstract: *Coxiella burnetii*, the causative agent of Q fever, is an intracellular pathogen posing a significant global public health threat. There is a pressing need for dependable and effective treatments, alongside an urgency for further research into the molecular characterization of its genome. Within the genomic landscape of *Coxiella burnetii*, numerous hypothetical proteins remain unidentified, underscoring the necessity for in-depth study. In this study, we conducted comprehensive in silico analyses to identify and prioritize potential hypothetical protein of *Coxiella burnetii*, aiming to elucidate the structure and function of uncharacterized protein. Furthermore, we delved into the physicochemical properties, localization, and molecular dynamics and simulations, and assessed the primary, secondary, and tertiary structures employing a variety of bioinformatics tools. The in-silico analysis revealed that the uncharacterized protein contains a conserved Mth938-like domain, suggesting a role in preadipocyte differentiation and adipogenesis. Subcellular localization predictions indicated its presence in the cytoplasm, implicating a significant role in cellular processes. Virtual screening identified ligands with high binding affinities, suggesting the protein's potential as a drug target against Q fever. Molecular dynamics simulations confirmed the stability of these complexes, indicating their therapeutic relevance. The findings provide a structural and functional overview of an uncharacterized protein from *C. burnetii*, implicating it in adipogenesis. This study underscores the power of in-silico approaches in uncovering the biological roles of uncharacterized proteins and facilitating the discovery of new therapeutic strategies. The findings provide valuable preliminary data for further investigation into the protein's role in adipogenesis.

Keywords: *Coxiella burnetii* Q fever Hypothetical proteins In silico analysis Genome characterization Mth938-like domain Protein structure prediction Physicochemical properties

<https://www.nature.com/articles/s41598-024-66072-3#:~:text=The%20findings%20provide%20a%20structural,discovery%20of%20new%20therapeutic%20strategies.>