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Structure-based Identification of a Novel NTPase from Methanococcus jannaschii

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Almost half of the entire set of predicted genomic products from $Methanococcus\ jannaschii$ are classified as functionally unknown hypothetical proteins. We present a structure-based identification of the biochemical function of a protein with hitherto-unknown function from a M. jannaschii gene, Mj0226. The crystal structure of Mj0226 protein determined at 2.2Å resolution reveals that the protein is a homodimer and each monomer folds into an elongated α/β structure. Comparisons of Mj0226 protein with protein structures in the database indicated that a part of protein is homologous to some of the nucleotide-binding proteins. Biochemical analysis shows that Mj0226 protein is a novel nucleotide triphosphatase that can efficiently hydrolyze nonstandard nucleotides such as XTP to XMP or ITP to IMP, but not the standard nucleotides, in the presence of Mg^{2+} or Mn^{2+} ions.