A Computational Study of the Mechanism for F1-ATPase Inhibition by the Epsilon Subunit

A Computational Study of the Mechanism for F1-ATPase Inhibition by the Epsilon Subunit

Thomson, Karen J.

Name: thesis_kjt_proque ...
Size: 1.206Mb
Format: PDF
Description: ETD thesis
View/Open

Name: 3oaa-1bsn_a-h_sel ...
Size: 27.26Mb
Format: GIF image
Description: Animated GIF of TMD ...
View/Open

Name: 3oaa_gh.gif
Size: 24.18Mb
Format: GIF image
Description: Animated GIF of TMD ...
View/Open

Name: 1bsn_h_movie.gif
Size: 16.25Mb
Format: GIF image
Description: Animated GIF of TMD ...
View/Open

Permanent Link:	http://hdl.handle.net/1805/5024
Date:	2013
Committee Chair:	Pu, Jingzhi
Committee Members:	Ge, Haibo Sardar, Rajesh Long, Eric C. (Eric Charles)
Degree:	M.S.
Degree Year:	2013
Department:	Chemistry & Chemical Biology
Grantor:	Purdue University
Keywords:	ATP synthase ; molecular dynamics ; computer simulation ; CHARMM
LC Subjects:	Molecular dynamics -- Research -- Analysis -- Evaluation ; Adenosine triphosphatase -- Regulation ; Adenosine triphosphatase -- Computer simulation ; Computational biology ; Escherichia coli -- Research ; Proteins -- Structure ; Molecular biology -- Mathematical models ; Chemistry -- Data processing ; Proteins -- Conformation ; Crystallography -- Technique ; Molecular dynamics ; Bioenergetics ; Computer simulation

Abstract:

The multi-protein complex of F0F1 ATP synthase has been of great interest in the fields of microbiology and biochemistry, due to the ubiquitous use of ATP as a biological energy source. Efforts to better understand this complex have been made through structural determination of segments based on NMR and crystallographic data. Some experiments have provided useful data, while others have brought up more questions, especially when structures and functions are compared between bacteria and species with chloroplasts or mitochondria. The epsilon subunit is thought to play a signi cant role in the regulation of ATP synthesis and hydrolysis, yet the exact pathway is unknown due to the experimental difficulty in obtaining data along the transition pathway. Given starting and end point protein crystal structures, the transition pathway of the epsilon subunit was examined through computer simulation.The purpose of this investigation is to determine the likelihood of one such proposed mechanism for the involvement of the epsilon subunit in ATP regulation in bacterial species such as E. coli.

Description:

Indiana University-Purdue University Indianapolis (IUPUI)

This item appears in the following Collection(s)

- Chemistry & Chemical Biology Department Theses and Dissertations (/handle/1805/2052)

Show Statistical Information (#)

My Account

- Login
- Register

Statistics

- Most Popular Items
- Statistics by Country
- Most Popular Authors

FULFILLING *the* PROMISE