



Bioinformatique –Biologie- -Blida

04 au 06 Avril 2017

# PROGRAMME

Mardi 4 Avril 2017

**8h30** - Réception et inscription (Accueil)

**9h00** - Cérémonie d'ouverture

*Laboratoire de neuro-immunologie, département d'immunologie, Institut Pasteur d'Algérie*

**CO<sub>3</sub>/12h20-STRUCTURAL/FUNCTIONAL MOTIFS IN THE ENZYMES OF THE KREBS CYCLE**

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**Abstract** →



People's Democratic Republic of Algeria  
The Ministry of Higher Education and scientific research



UNIVERSITY DR. MOULAY TAHER. . SAÏDA  
FACULTY OF SCIENCES  
Departement : Biology

## Structural/Functional Motifs in the Enzymes of the Krebs cycle

– A new set of Functional Motifs –

Database URL: <http://bioinformaticstools.org/prjs/cacfms/>

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## Introduction

### Literature Review

Motifs and  
biological  
function

Krebs cycle  
Enzymes

Protein Data  
Bank

Material and  
Methods

Interpretations  
of result

CacFmS  
Database

Metabolism is important for cell survival which is undertaken by specific enzymes. Healthy cells usually have normal metabolism pathways while sick cells show abnormal pathways. Understanding the function of enzymes responsible for metabolism pathways is one way to better treat metabolic related illnesses.

As it has accumulated by a vast number of research studies, 3-dimensional (3D) structure of enzymes dictates the function they do, in other words, the function of enzymes necessitate a certain 3D structure where active/binding site residues are exposed in favorable spatial environment and electro-chemical conditions that allow the carrying out of the reactions needed for their biological function.

In this work, enzymes involved in the Citric Acid Cycle (CAC) metabolism pathway have been selected for a structural-bioinformatics study to try and discover some of the underlying basis behind their biological function.

It was necessary to use spatial structures of proteins from the international database known as the Protein Data Bank or PDB which stores proteins and enzymes in complex forms with substrates or Ligands.

The study resulted in the detection, identification and description of a new group of structural elements that are spatially (3D) arranged and are deemed important in the function of the CAC enzymes. These structural elements are called here Structural/Functional Motifs (or SFMs) which can shed light on the biological function of proteins and be used in a number of applications including the molecular modelling techniques and De Novo Drug Design of new drugs targeting metabolism related diseases.

SFMs data and the Binding Environment details have been annotated into the online database “Citric Acid Cycle Binding Structural & Functional Motifs” or CacSFMs database which is accessed at the URL address: <http://bioinformaticstools.org/prjs/cacfms/>

**Keywords:** Enzymes, Structure, Function, Structural/Functional Motifs, Molecular Modelling, *De Novo Drug Design*, Databases.