



Université Dr Taher Moulay Saïda
جامعة د. الطاهر مولاي سعيدة

Bioinformatics

for

Biochemistry Master's Program

Dr. Abdelkrim Rachedi

Course program

1. General introduction to bioinformatics.

2. Databases in biology:

- > 2.1. Introduction to databases in general.
- > 2.2. Databases for the primary structure of Proteins and Nucleic Acids, access and usage.
- > 2.3. Sequence Alignment concepts, methods and applications.
- > 2.4. Databases for the structural data of Proteins and Nucleic Acids, access and usage.
- > 2.5. Structural Alignment concepts, methods and applications.

3. Algorithm in biology:

- > 3.1. Introduction to Algorithms in general.
- > 3.2. Sequence Alignment algorithms and weighing matrices.
- > 3.3. Structural Alignment algorithms and weighing matrices.
- > 3.4. 3D-Structure prediction algorithms and applications.

Course program

4. Macromolecules 3D-structure determination methods; strengths and weaknesses:

- > 4.1. Concepts of X-ray Crystallography Method.
- > 4.2 Concepts of Synchrotron X-Ray Diffraction Method.
- > 4.3. Concepts of Nuclear Magnetic Resonance Method.
- > 4.4. Concepts of Cryo-Electron Microscope Method.
- > 4.5. Concepts of SAXS Method.

5. Analyse de la structure 3-Dimensionnel des Macromolecules (protéines et acides nucléiques):

- > 5.1. Methods of macromolecular structure analysis.
- > 5.2. Evaluation of macromolecular structure.
- > 5.3. Impact of macromolecular structure quality on understanding the biological function.

Course program

6. Molecular modeling of 3D-structure and function of proteins:

- > 6.1 Concepts.
- > 6.2 Algorithms.
- > 6.3 Methods.
- > 6.4 Applications.
- > 6.5 Reliability of the generated models and conclusions.

7. Ligands Binding and Drug Design:

- > 7.1 Introduction about Ligands and Drugs.
- > 7.2 Calculation of Ligands Binding Environment and Active Site.
- > 7.3 Macromolecular binding motifs and Ligands.
- > 7.4 Drug Design concepts and applications.
- > 7.5 Modeling new drugs and Technics of Molecular Docking.

Course Web Page

Course material is found at:

<http://www.bioinformaticstools.org/Masters/>



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Department of Biology, Faculty of Sciences
Year 2013-2014

Bioinformatics teaching programmes
for: 1st year Masters

- [Masters in Biodiversity](#)
- [Masters in Biotechnology](#)
- [Masters in Biochemistry](#)



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Course Material – examples



Department of Biology, Faculty of Sciences
Year 2013-2014

Bioinformatics 1st year Masters in Biochemistry

- [Find course material](#)
- [Submit Assignments](#)

[Submit Assignments in PDF or DOC] ([Students only](#))

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Course Material – examples



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Course Material – examples

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Login App. V.1.0	
UserName:	<input type="text"/> (*)
Password:	<input type="password"/> (*)
Press to	<input type="button" value="Login Appl"/>
(*) mandatory fields	
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Course Material – examples

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- [0-blsample.fa](#)
- [0-broad.fasta](#)
- [0-ebi-wubl-prot.fas](#)
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Course Material – examples

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Teaching Tools



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[Visual Biochemistry.exe](#)

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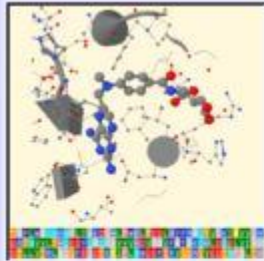
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Online Services:

- [STAD: Structural Targets Annotation Database](#)
 - [All Targets Status Page](#)
 - [Targets Stats Board](#)
 - [Targets Structural Gallery](#)
 - [Targets News](#)
 - [Download Targets](#)
- [NALD: Nucleic Acids and Ligands Database, Ligand Binding Motifs, Classes & Disease Links](#)
- [NEURO: A system for integrating data on the Nervous System](#)
- [SSFS: Sequence, Structure and Function Server \(under development\)](#)
- [NCTPR: Nucleic Acid Codes Translation to Proteins and Reverse](#)
- [Rapid Building of Protein/DNA Motifs in Standard 3D-Conformations](#)

SSFS <http://www.bioinformaticstools.org/ssfs>



Sequence, Structure and Function Server

Keywords:
(type in a PDB id, enzyme id, keyword, protein name, ligand name/id or author)

Sequence:

to be activated soon ...

(Paste in AA sequence in FASTA format)



Sequence, Structure and Function Server v.β-2010,
Wits Bioinformatics, University of The
Witwatersrand, South Africa.

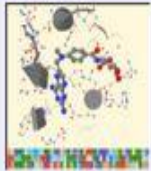
Currently developed at and maintained by University
Dr. Tahar Moulay, Saida, Algeria

E-mail: rachedi@bioinformers.co.uk





SSFS <http://www.bioinformaticstools.org/ssfs>



Sequence, Structure and Function Server

Do another search: [Go](#)
(type in a PDB id, enzyme id, keyword, protein name, ligand name/id or author)

[Main](#)
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PDB entries (13144 hits) related to your query "hydrolase" are:

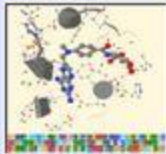


ID	Title	Ligands	Method	Resolution
1021	HOW AMINO-ACID INSERTIONS ARE ALLOWED IN AN ALPHA-HELIX OF T4 LYSOZYME	CL BME	X-RAY	1.74
1031	HOW AMINO-ACID INSERTIONS ARE ALLOWED IN AN ALPHA-HELIX OF T4 LYSOZYME	CL BME	X-RAY	1.90
1041	HOW AMINO-ACID INSERTIONS ARE ALLOWED IN AN ALPHA-HELIX OF T4 LYSOZYME	None	X-RAY	2.80
1071	STRUCTURAL BASIS OF ALPHA-HELIX PROPENSITY AT TWO SITES IN T4 LYSOZYME	CL BME	X-RAY	1.80
1081	STRUCTURAL BASIS OF ALPHA-HELIX PROPENSITY AT TWO SITES IN T4 LYSOZYME	CL BME	X-RAY	1.80
1091	STRUCTURAL BASIS OF ALPHA-HELIX PROPENSITY AT TWO SITES IN T4 LYSOZYME	CL BME	X-RAY	1.85
1101	STRUCTURAL BASIS OF ALPHA-HELIX PROPENSITY AT TWO SITES IN T4 LYSOZYME	CL BME	X-RAY	1.70
1111	STRUCTURAL BASIS OF ALPHA-HELIX PROPENSITY AT TWO SITES IN T4 LYSOZYME	CL	X-RAY	1.80



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SSFS <http://www.bioinformaticstools.org/ssfs>



Sequence, Structure and Function Server

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Entry Summary

Entry	1021 (3D-view the whole entry)
Header	HYDROLASE(O-GLYCOSYL)
Title	HOW AMINO-ACID INSERTIONS ARE ALLOWED IN AN ALPHA-HELIX OF T4 LYSOZYME
Authors	D. W. HEINZ, W. A. BAASE, F. W. DAHLQUIST, B. W. MATTHEWS
Primary Title	HOW AMINO-ACID INSERTIONS ARE ALLOWED IN AN ALPHA-HELIX OF T4 LYSOZYME.
Reference	NATURE . Vol.361561. 1993
Experiment	<u>Method</u> : X-RAY DIFFRACTION <u>Parameters</u> : Resolution: 1.74 Angs, Ref-Value: 17.4, Space Group: P 32 2 1
Chains	A
Enzyme	
Source	ENTEROBACTERIA PHAGE T4
Taxonomy	10665
UniProt	Chain A: P00720 .



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Sequence, Structure and Function Server Main Page

[Summary](#) | [Sequence](#) | [Secondary Structure](#) | [Structural Domains](#) | [Ligand Binding](#) | [Geometry](#)

Chain: A

CE 175A
 BME 901:A

Scene Rendering:

Cartoons Spacefill Backbone
 Ribbons Trace Strands
 Wireframe Meshribbon Rockets

H Bonds (only on Trace mode)

Reset scene

Scene Colour:
chain




Background:
Black

spin

Mouse Controls & Measurements

```
MNIFEMLRIDGLRLKIYKDTEGYTIGIGHLLKSPSLNAAAKSELDKAI GRNT  
NGVITKDEFEKLFNQDVDAAVRGILRNAKLPVYDSLDAVRRARLINVFOGGEI  
GVAGFINSLRMLQQKRWDEAAVNLAKSRWYNQIPNRKRVITTFRTIGIWDAYK
```

NACP: <http://www.bioinformaticstools.org/n2p>



Nucleic Acid Codes to Proteins .. v.1.0

Enter nucleic acid sequence: (DNA or RNA) [NACP How2](#)

Frames:

Genetic Codes:

[Show Genetic Code](#) (select Genetic Code from above list to show)

Nucleic Acid Codes to Proteins (NACP) is a tool for translating nucleic acid sequences (DNA or RNA) following any of the known genetic codes (e.g. Standard, Mitochondrial, bacteria .. etc) into the six reading frames of protein product.

Input of Nucliec Acids Sequence:


- A nucleic acids sequence, DNA or RNA, can typed or pasted into the text window. Sequence can be in **Free text** or **Fasta** format.

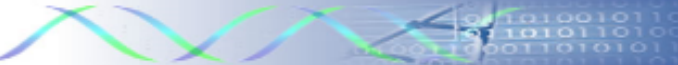
Genetic Codes:


- Translations can be done based on Standard genetic code which is a default selection.
- Other known non-standard genetic codes are also available from **Genetic Codes** list.
- The Genetic Codes used in the translation can be shown by clicking the button [Show Genetic Code](#)



NACP: <http://www.bioinformaticstools.org/n2p>







Nucleic Acid

Enter nucleic acid sequence: (DNA or RNA) NACP How2

>eg. nucleic acid sequences
AGCATTACGATGAAAGCATTACGATGAAAGTGTGCATAGTAGTAGATGATCCCATACAT
CAGATGACAGTCAGGGAAAAAATCAGTGAGAGCATTACGATGAAAGTGTTCAGTGAGTGT
GCATAGTAGTAGATGATCCCATACATCAGATGACAGTCAGGGAAATCAGTGAGAGCATTTA
CGATGAAAGTGTGCATAGTAGTAGATGATCCCATACATCAGATGACAGTCAGGGAAATCAG
TGCATTTAAATCAGTGAGAGCATTACGATGAAAGTGTACGAGCATTACGATGAAAGTGT
GCATAGTAGTAGATGATCCAGCATTACGATGAAAGTGTGCATAGTAGTAGATGATCCCAT
ACATCAGATGACAGTCAGGGAAATCAGTGACATACATCAGATGACAGTCAGGGAAATCAGTG
ATGAAAGTGTGCATAGTAGTAGATGATCCCATACATCAGATGACAGTCAGGGAAATCAGTG

Frames: All 5'-3'

Genetic Codes: Standard Code

Show Genetic Code (select Gene)

Submit
Reset


>Frame_1 EG. NUCLEIC ACID SEQUENCES
SIYDESIYDESVHSSR*SHTSDDSQGNQ*EHLR*KCSVSVHSSR*SHTSDDSQGNQ*EHLR*KCA***M
IPYIR*QSGKSVHLNQ*EHLR*KCTSIYDESVHSSR*SSIYDESVHSSR*SHTSDDSQGNQCIHQMTVRE
ISDESVHSSR*SHTSDDSQGNQ


>Frame_2 EG. NUCLEIC ACID SEQUENCES
AFTMKAFTMKVCIVVDDPIHQMTVREKISESIYDESQ*VCIVVDDPIHQMTVREISESIYDESVHSSR*
SHTSDDSQGNQCI*ISESIYDESVRFTMKVCIVVDDPAFTMKVCIVVDDPIHQMTVREISAYIR*QSGK
SVMKVCIVVDDPIHQMTVREIS


>Frame_3 EG. NUCLEIC ACID SEQUENCES
HLR*KHLR*KCA***MIPYIR*QSGKSVRAFTMKVFSECA***MIPYIR*QSGKSVRAFTMKVCIVVDD
PIHQMTVREISAFKSVRAFTMKVYEHLR*KCA***MIQHLR*KCA***MIPYIR*QSGKSVHTSDDSQGN
Q**KCA***MIPYIR*QSGKSV



NACP: <http://www.bioinformaticstools.org/n2p>







Nucleic Acid Codes

Enter nucleic acid sequence: (DNA or RNA) NACP How2

Frames: F1

Genetic Codes:
Trematode Mitochondrial

Show Genetic Code (select Genetic Code from above list)

Submit
Reset

Genetic code: Trematode Mitochondrial

Codon	AA	Codon	AA	Codon	AA	Codon	AA
TTT	F	CTT	L	ATT	I	GTT	V
TTC	F	CTC	L	ATC	I	GTC	V
TTA	L	CTA	L	ATA	M	GTA	V
TTG	L	CTG	L	ATG	M	GIG	V
TCT	S	CCT	P	ACT	T	GCT	A
TCC	S	CCC	P	ACC	T	GCC	A
TCA	S	CCA	P	ACA	T	GCA	A
TCG	S	CCG	P	ACG	T	GCG	A
TAT	Y	CAT	H	AAT	N	GAT	D
TAC	Y	CAC	H	AAC	N	GAC	D
TAA	*	CAA	Q	AAA	N	GAA	E
TAG	*	CAG	Q	AAG	K	GAG	E
TGT	C	CGT	R	AGT	S	GGT	G
TGC	C	CGC	R	AGC	S	GGC	G