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Using Open Access Resources in Data Literacy Instruction: Renewing the IL Curriculum by Aligning It with Changing Needs

Don MacMillen
University of Calgary

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Using open access resources in data literacy instruction: renewing the IL curriculum by aligning it with changing needs

Don MacMillan

Liaison Librarian, Biological Sciences, Physics,
Astronomy & Mathematics

University of Calgary

Calgary, Canada



LIWest 2014-Portland



LIWest 2014-Portland



What we did

Reinvent information literacy (IL) program –
integrate genetics & biochemistry content

Course-integrated library/Lab project
Biology 311 (October) - Biochemistry 393
(February)

Investigate the molecular & structural basis of
inherited diseases using disciplinary data

550 students per class
24 lab sections
10 IL workshops in library classrooms



Inquiry-based exercises

BIOL 311

- *Molecular* basis of inherited diseases
- Student-directed analysis of molecular genetic causes and treatments for a specific inherited disease

Poster

- Students present results of their analysis to peers through a poster presentation at end of term - 6% of final grade

BCEM 393

- *Structural* perspective on molecular basis of inherited diseases
- Student-directed analysis of mutations in proteins leading to a specific inherited disease

Poster

- Students present results of molecular visualization analysis to peers through a poster presentation at end of term - 6% of final grade

Course related LibGuides

<http://tinyurl.com/7jgay9e>

Library

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Biological Sciences

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Biology 311-Principles of Genetics [Print Page](#)

WHAT'S ON THIS PAGE?

[Session Goals](#)

[NCBI](#)

[OMIM](#) (Online Mendelian Inheritance in Man)

[PubMed](#)

[Patents](#)

[Citing Your Sources](#)

SESSION GOALS

At the end of this session you

- Find one **review journal** (Literature) database.
- Locate a **Patent** relationship.
- Use the **OMIM** (Online Mendelian Inheritance in Man) to find gene and protein that are related to a disease.
- Cite your sources using the appropriate citation style.

CONTACT DON MACMILLAN
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Contact Info:
TFDL 460D
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Services Area)

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[Send Email](#)

Links

NATIONAL CENTER FOR BIOTECHNOLOGY INFORMATION (NCBI)

Created in 1988, the **National Centre for Biotechnology Information (NCBI)** is a clearinghouse for molecular biology and genetics information. It includes links to full-text articles and numerous genetics and protein databases including the following:

- **PubMed** - The place to find full-text articles. Includes 22 million articles. ([PubMed Tutorials](#))
- **OMIM** (Online Mendelian Inheritance in Man)

Library

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BCEM 393 - Introduction to Biochemistry [Print Page](#)

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[OMIM](#) (Online Mendelian Inheritance in Man)

[RCSB's Protein Data Bank \(PDB\)](#)

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[Online Survey](#)

SESSION GOALS

At the end of this session you should be able to acquire a structural perspective on the molecular basis of genetically-inherited diseases by using the following tools:

- **PubMed** (Biomedical Literature) and **OMIM** (Online Mendelian Inheritance in Man).
- **Protein Data Bank** or PDB for information about your protein's 3D coordinates.
- **BLAST** to identify homologous or similar proteins and use **ClustlW** to align them.
- **PyMOL** to visualize in 3D, the effects of a mutation on protein structure and function.

Prepare and present an oral presentation on the structural and molecular basis of genetically inherited diseases.

Shortcut to this page: <http://tinyurl.com/7jgay9e>

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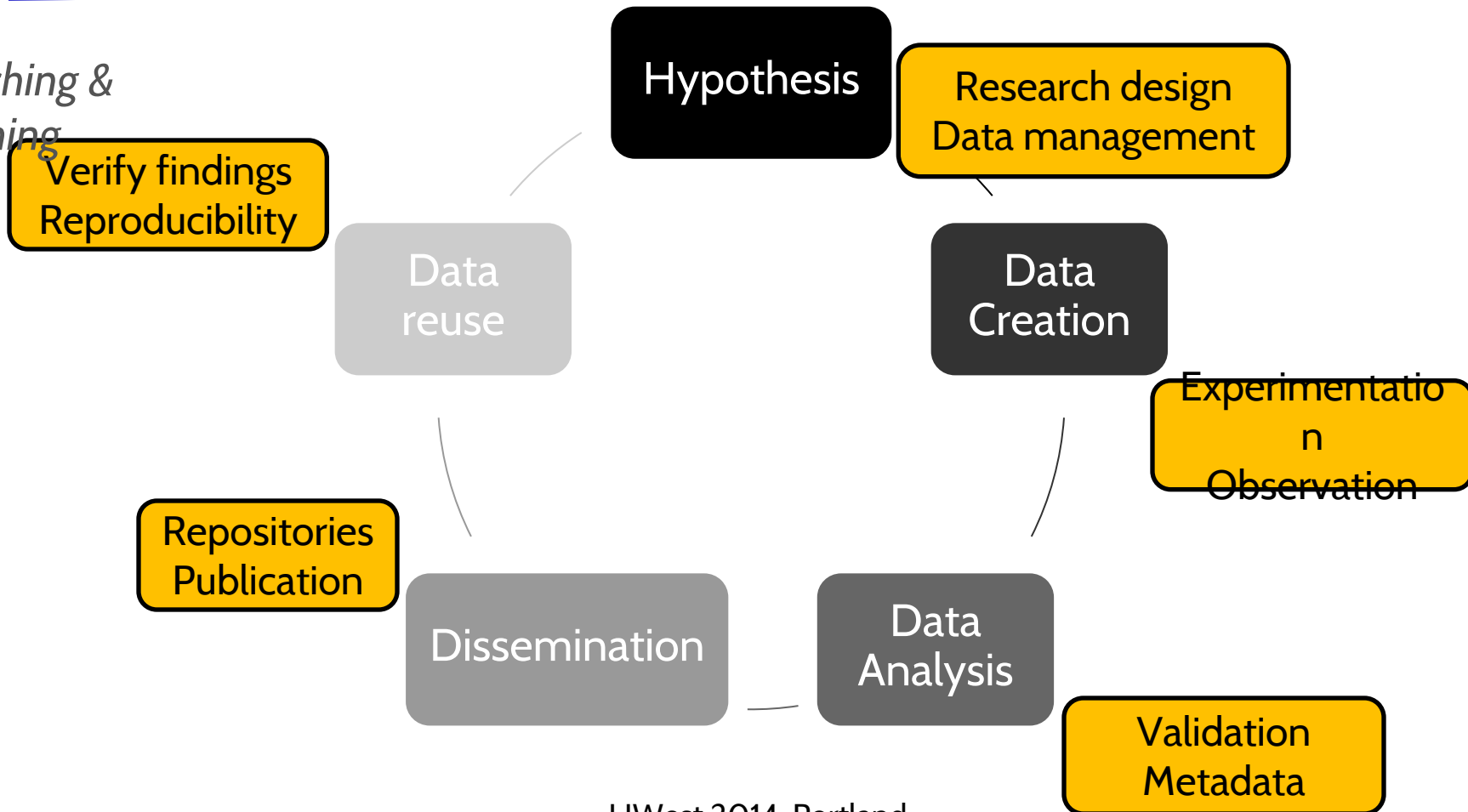
Phone: 403.210.8632
Email: macmilld@ucalgary.ca

NATIONAL CENTER FOR BIOTECHNOLOGY INFORMATION (NCBI)

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Scientific Data Life Cycle

Teaching & learning





Why Data Literacy?

Data-intensive disciplines – robust infrastructure – unique research outcomes

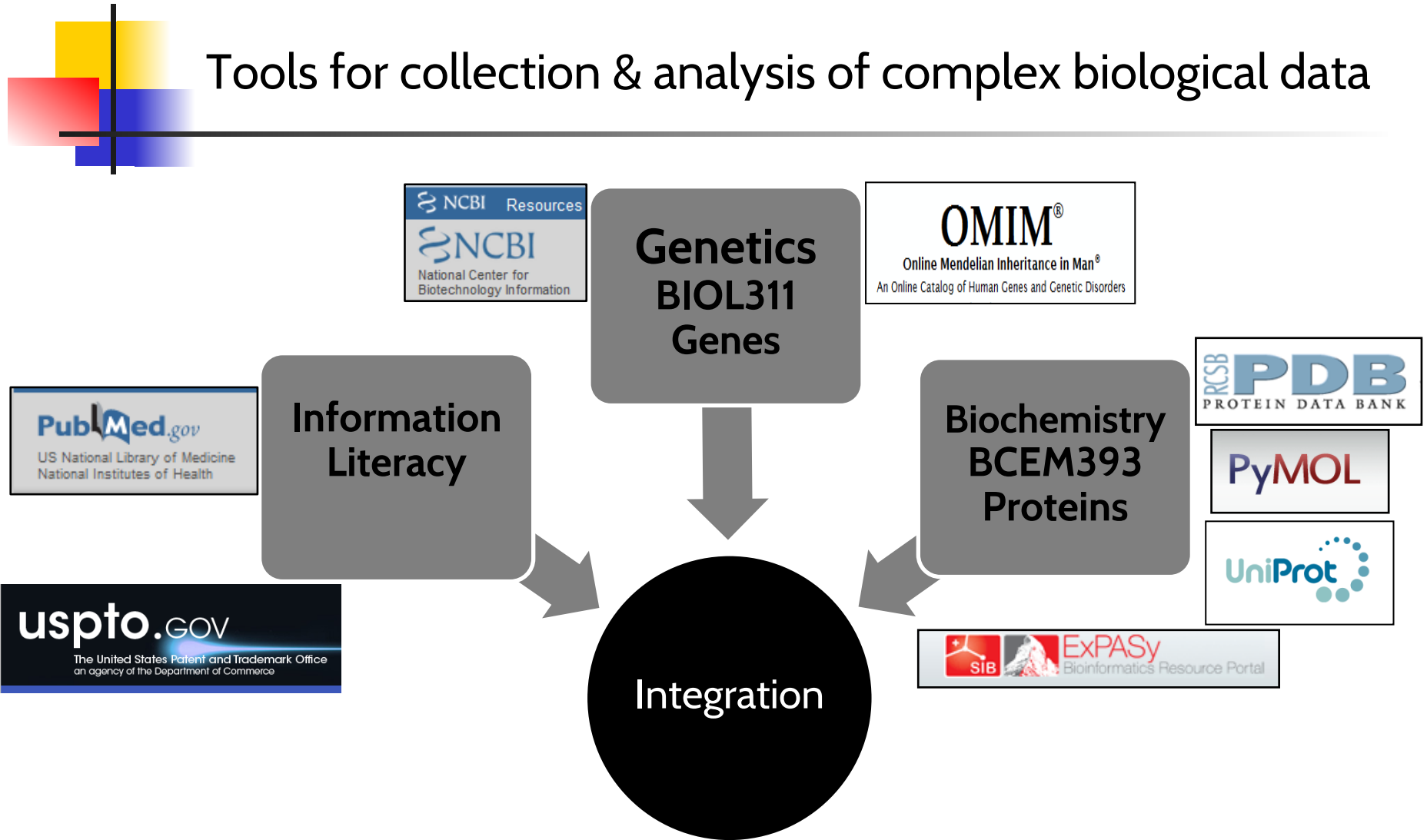
Bioinformatics tools facilitates discovery & analysis of life sciences data

Students conduct research using “real-world” solutions using domain repositories

Librarian re-skilling – enhance our data competencies, domain expertise & relevance

Bioinformatics

Tools for collection & analysis of complex biological data





What is Bioinformatics data?

- Your handout is a sample page from the Protein Data Bank (PDB)
Data repository of 3D protein structural information
- What if we asked students
“What is the important info on this page”

Search
Advanced
Browse

Everything Author Macromolecule Sequence Ligand ?

e.g., PDB ID, molecule name, author

Search History, Previous Results

↓ PDB-101 Hide

Structural View of Biology
Understanding PDB Data
Molecule of the Month
Educational Resources
Author Profiles

↓ MyPDB Hide

Login to your Account
Register a New Account
MyPDB Help Page

↓ Home Hide

News & Publications
Usage/Reference Policies
Deposition Policies
Website FAQ
Deposition FAQ
Contact Us
About Us
Careers
External Links
New Website Features

↓ Deposition Hide

All Deposit Services
Electron Microscopy
X-ray | NMR
Validation Server
BioSync Beamlines/Facilities
Related Tools

↓ Tools Hide

Download Files
Compare Structures
Drug & Drug Target
Mapping
File Formats
RESTful Web Services
Widgets

Summary 3D View Sequence Annotations Seq. Similarity 3D Similarity Literature Biol. & Chem. Methods Geometry Links

FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE FROM HUMAN LIVER TISSUE

DOI:10.2210/pdb1qo5/pdb

1QO5

Display Files
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Primary Citation

The structure of human liver fructose-1,6-bisphosphate aldolase.

Dalby, A.R., Tolan, D.R., Littlechild, J.A.

Journal: (2001) Acta Crystallogr., Sect. D 57: 1526-1533

PubMed: 11679716

Search Related Articles in PubMed

PubMed Abstract:

The X-ray crystallographic structure of the human liver isozyme of fructose-1,6-bisphosphate aldolase has been determined by molecular replacement using a tetramer of the human muscle isozyme as a search model. The liver aldolase (B isozyme) crystallized in space group C2, ... [Read More & Search PubMed Abstracts]

↓ Molecular Description Hide

Classification: Lyase

Structure Weight: 710444.68

Molecule: FRUCTOSE-BISPHOSPHATE ALDOLASE B

Polymer: 1 Type: protein Length: 363

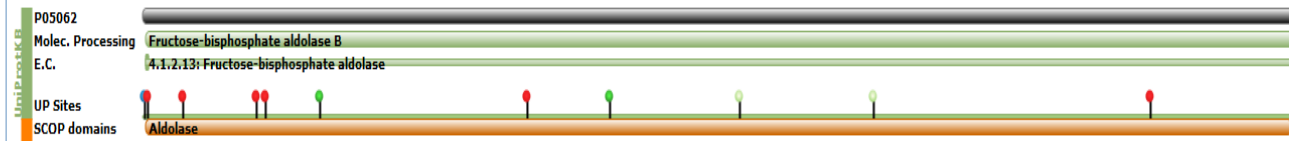
Chains: A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R

EC#: 4.1.2.13

Organism: Homo sapiens

Gene Names: ALDOB ALDB

UniProtKB: Protein Feature View | Search PDB | P05062



Biological Assembly 1 ?



3D View

More Images...

Symmetry: D2 view

Stoichiometry: Homo 4-mer - A4

Biological assembly 1 generated by PQS (software)

Downloadable viewers:

Simple Viewer Protein Workshop
Kiosk Viewer

↓ MyPDB Personal Annotations Hide

To save personal annotations, please



What is Bioinformatics data?

- Now imagine the question(s) is:
 - “What is the *length* of your protein-number of amino acids?”

or

- “What Enzyme Classification or (EC#) does your enzyme belong?”



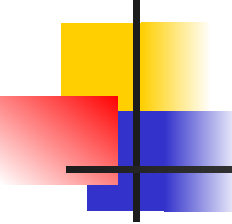
How we did it

Authentic pathway activity that replicates researcher workflow

Scaffolded steps, hands on practice

Emphasize interoperability

Short term lab assignment + longer term major assignment



Bioinformatics - Interoperability

Genetics

PubMed
(Scholarly Literature)

OMIM
(Database of genetic diseases)

Gene (Nucleotide sequences)

Biochemistry

Protein Data Bank
(Protein Structure)

UniProt (Protein Sequence/Function)

BLAST & ClustlW
(Sequence similarity & Alignment)

PyMOL
(3D Visualization)



Sample Questions

- **BIOL 311- Genetics**

- On which chromosome is your gene located?
- What is the inheritance pattern of your disease topic?

- **BCEM 393- Biochemistry**

- Locate your protein's 3D coordinates
- What is the length of your protein (e.g. number of Amino Acids)?

Gene Data Example

NCBI's Gene portal – links to gene & protein data and PubMed

(e.g. Cystic fibrosis = CFTR Gene)

CFTR cystic fibrosis transmembrane conductance regulator (ATP-binding cassette sub-family C, member 7) *Homo sapiens* (Human)

Gene ID: 1080, updated on 8-Jun-2014

Summary

Official Symbol CFTR provided by HGNC

Official Full Name cystic fibrosis transmembrane conductance regulator (ATP-binding cassette sub-family C, member 7) provided by HGNC

Primary source [HGNC:1884](#)

Locus tag tcag7.78

See related [Ensembl:ENSG0000001626](#); [HPRD:03883](#); [MIM:602421](#); [Vega:OTTHUMG00000023076](#)

Gene type protein coding

RefSeq status REVIEWED

Organism [Homo sapiens](#)

Lineage Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorhini; Catarrhini; Hominidae; Homo

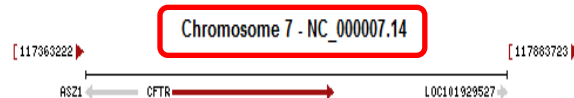
Also known as CF; MRP7; ABC35; ABCC7; CFTR/MRP; TNR-CFTR; dJ760C5.1

Summary This gene encodes a member of the ATP-binding cassette (ABC) transporter superfamily. ABC proteins transport various molecules across extra- and intra-cellular membranes. There are seven distinct subfamilies (ABC1, MDR/TAP, MRP, ALD, OABP, GCN20, White). This protein is a member of the MRP subfamily that is involved in multi-drug resistance. It functions as a chloride channel and controls the regulation of other transport pathways. Mutations in this gene are associated with the autosomal recessive disorders cystic fibrosis and congenital bilateral nasolacrimal duct obstruction. Alternatively spliced transcript variants have been described, many of which result from mutations in this gene. [provided by RefSeq, Jul 2008]

Genomic context

Location: 7q31.2

Annotation release	Status	Assembly	Chr	Location
106	current	GRCh38 (GCF_000001405.26)	7	NC_000007.14 (1174707)
105	previous assembly	GRCh37.p13 (GCF_000001405.25)	7	NC_000007.13 (1171200)



Full text in PMC_nucleotide

GAP

Gene neighbors

Genome

GEO Profiles

GTR

HomoloGene

Map Viewer

MedGen

Nucleotide

OMIM

Probe

Protein

PubChem Compound

PubChem Substance

PubMed

PubMed (GeneRIF)

PubMed (OMIM)

PubMed(nucleotide/PMC)

RefSeq Proteins

RefSeq RNAs

RefSeqGene

Summary

Genomic context

Genomic regions, transcripts, and products

Bibliography

Phenotypes

Variation

Interactions

Pathways

General gene information

Markers, Related pseudogene(s), History

General protein information

Reference sequences

Related sequences

Additional links

Locus-specific Databases

Related information

Order cDNA clone

3D structures

BioAssay

BioAssay by Target (List)

BioAssay by Target (Summary)

BioAssay, by Gene target

BioAssay, RNAi Target, Active

BioProjects

BioSystems

Books

CCDS

Protein Data Example

Protein Data Bank (PDB) – Repository of 3D protein structural data – portal to PubMed and related data sources

RCSB PDB
PROTEIN DATA BANK

Search
Advanced
Browse

Everything
e.g., PDB ID, m

Search History, Previous Results

↓ PDB-101 Hide
Structural View of Biology
Understanding PDB Data
Molecule of the Month
Educational Resources
Author Profiles

↓ MyPDB Hide
Login to your Account
Register a New Account
MyPDB Help Page

↓ Home Hide
News & Publications
Usage/Reference Policies
Deposition Policies
Website FAQ
Deposition FAQ
Contact Us
About Us
Careers
External Links
New Website Features

↓ Deposition Hide
All Deposit Services
Electron Microscopy
X-ray | NMR
Validation Server
BioSync Beamlines/Facilities
Related Tools

↓ Tools Hide
Download Files
Compare Structures
Drug & Drug Target
Mapping
File Formats
RESTful Web Services
Widgets

Summary 3D View Sequence Annotations Seq. Similarity 3D Similarity Literature Biol. & Chem. Methods Geometry Links

FRUCTOSE 1,6-BISPHOSPHATE

DOI:10.2210/pdb1qo5/pdb

Primary Citation

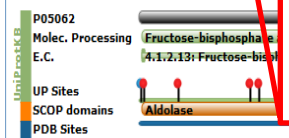
The structure of human liver fructose-1,6-bisphosphate aldolase (B isozyme) crystallized in space group C2, with parameters a = 291.1, b = 489.8, c = 103.4 Å, alpha = 90, beta = 103.6, gamma = 90 degrees. These large unit-cell parameters result in the presence of 18 subunits in the asymmetric unit: four catalytic tetramers and a dimer from a fifth tetramer positioned on the twofold crystallographic axis. This structure provides further insight into the factors affecting isozyme specificity. It reveals small differences in secondary structure in regions previously determined to be isozyme specific. Two of these regions are at the solvent-exposed enzyme surface away from the active site. The most significant changes are in the flexible C-terminal region of the enzyme, where there is an insertion of an extra alpha-helix. Point mutations of the human liver aldolase are responsible for the disease hereditary fructose intolerance. Sequence information is provided for the new crystal structure in order to indicate how these mutations bring about reduced enzyme activity and affect structural stability.

PubMed: 11679716

PubMed Abstract:
The X-ray crystallographic structure of the human liver isozyme of fructose-1,6-bisphosphate aldolase (B isozyme) crystallized in space group C2, with parameters a = 291.1, b = 489.8, c = 103.4 Å, alpha = 90, beta = 103.6, gamma = 90 degrees. These large unit-cell parameters result in the presence of 18 subunits in the asymmetric unit: four catalytic tetramers and a dimer from a fifth tetramer positioned on the twofold crystallographic axis. This structure provides further insight into the factors affecting isozyme specificity. It reveals small differences in secondary structure in regions previously determined to be isozyme specific. Two of these regions are at the solvent-exposed enzyme surface away from the active site. The most significant changes are in the flexible C-terminal region of the enzyme, where there is an insertion of an extra alpha-helix. Point mutations of the human liver aldolase are responsible for the disease hereditary fructose intolerance. Sequence information is provided for the new crystal structure in order to indicate how these mutations bring about reduced enzyme activity and affect structural stability.

Molecular Description

Classification: Lyase
Structure Weight: 710444.68
Molecule: FRUCTOSE-BISPHOSPHATE ALDOLASE
Polymer: 1
Chains: A, B, C, D, E, F, G, H, I, J, K, L
EC#: 4.1.2.13
Organism: Homo sapiens
Gene Names: ALDOB ALDB
UniProtKB: | Protein Feature View |



NCBI Resources How To

PubMed.gov
US National Library of Medicine
National Institutes of Health

PubMed
Advanced

Display Settings: Abstract

Acta Crystallogr D Biol Crystallogr. 2001 Nov;57(Pt 11):1526-33. Epub 2001 Oct 25.

The structure of human liver fructose-1,6-bisphosphate aldolase.

Dalby AR¹, Tolan DR, Littlechild JA.

Author information

Abstract

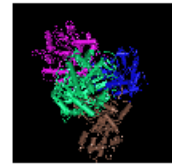
The X-ray crystallographic structure of the human liver isozyme of fructose-1,6-bisphosphate aldolase has been determined by molecular replacement using a tetramer of the human muscle isozyme as a search model. The liver aldolase (B isozyme) crystallized in space group C2, with parameters a = 291.1, b = 489.8, c = 103.4 Å, alpha = 90, beta = 103.6, gamma = 90 degrees. These large unit-cell parameters result in the presence of 18 subunits in the asymmetric unit: four catalytic tetramers and a dimer from a fifth tetramer positioned on the twofold crystallographic axis. This structure provides further insight into the factors affecting isozyme specificity. It reveals small differences in secondary structure in regions previously determined to be isozyme specific. Two of these regions are at the solvent-exposed enzyme surface away from the active site. The most significant changes are in the flexible C-terminal region of the enzyme, where there is an insertion of an extra alpha-helix. Point mutations of the human liver aldolase are responsible for the disease hereditary fructose intolerance. Sequence information is provided for the new crystal structure in order to indicate how these mutations bring about reduced enzyme activity and affect structural stability.

PMID: 11679716 [PubMed - indexed for MEDLINE]

Publication Types, MeSH Terms, Substances, Secondary Source ID

LinkOut - more resources

Structures reported by this article



Fructose 1,6-Bisphosphate Aldolase From Human Liver Tissue
PDB: 1QO5
 Source: Homo sapiens
 Method: X-Ray Diffraction
 Resolution: 2.5 Å

Related information

- Related Citations
- Gene
- Gene (GeneRIF)
- HomoloGene
- MedGen
- Nucleotide (RefSeq)
- Nucleotide (Weighted)
- OMIM (calculated)
- Protein (RefSeq)
- Protein (Weighted)
- Substance (MeSH Keyword)
- Taxonomy via GenBank
- UniGene
- Domains
- Protein
- Structure
- GEO Profiles
- Cited in PMC

PyMOL
Three-dimensional (3D) molecular visualization system
 Students introduce mutations to study impact on protein structure, function & related diseases (e.g. KRAS mutation causes certain types of cancer)

The PyMOL Molecular Graphics System

File Edit Build Movie Display Setting

Please visit <http://www.pymol.org> or contact sales@pymol.org when you

This Executable Build integrates Adjusting settings to improve performance
 Executive: Loading version 1.30
 You clicked /3GFTa//A/GLY*60/CA
 Selector: selection "sele" defined
 ExecutiveRMS: RMS = 0.003 (3)
 Mutagenesis: 27 rotamers loaded.

PyMOL>

PyMOL Viewer

```

/3GFTa//A/1          6          11          16
MET THR GLU TYR LYS LEU VAL VAL VAL GLY ALA GLY GLY VAL GLY LYS
/ras_prot//A/3      6          11          16
  
```

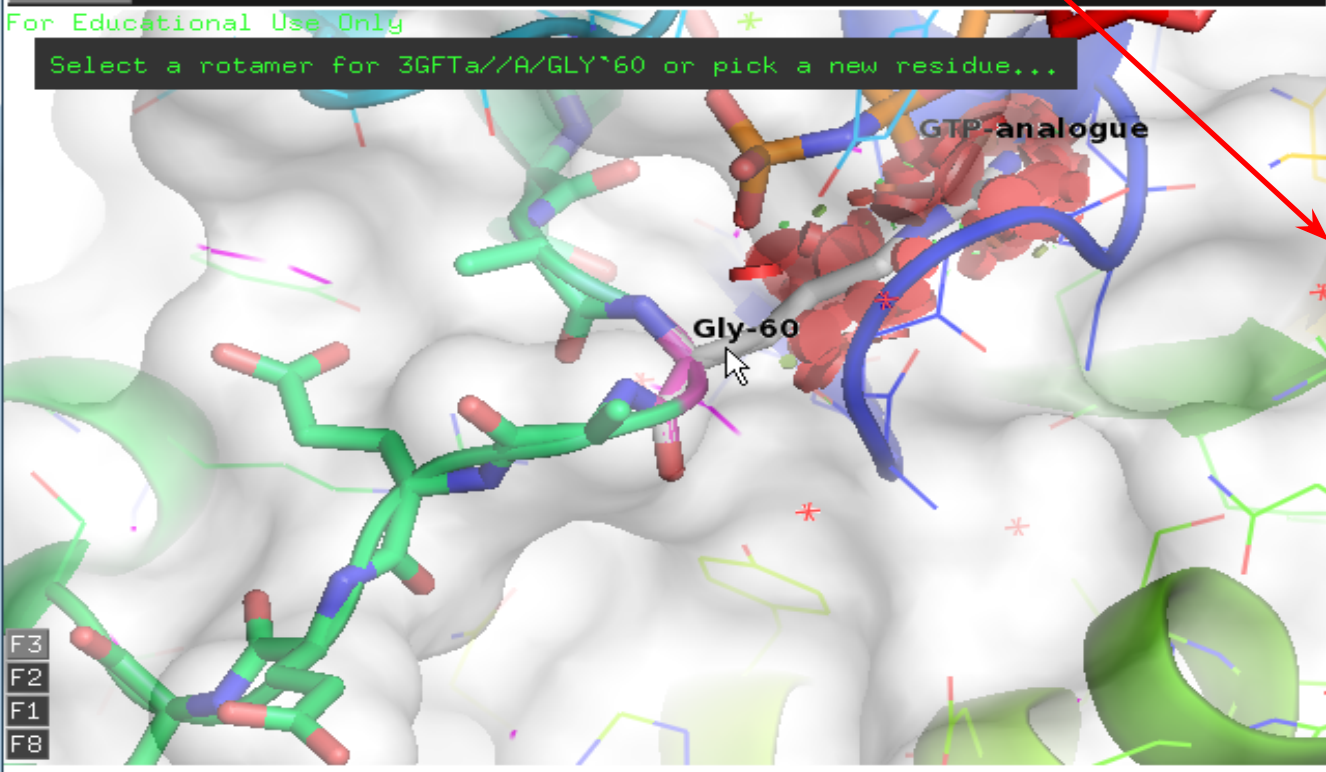
For Educational Use Only

Select a rotamer for 3GFTa//A/GLY*60 or pick a new residue...

GTP-analogue

Gly-60

F3
F2
F1
F8



Help

Orient Draw Ray

Rock Get View

Builder

Rebuild Abort

all	A	S	H	L	C
3GFTa	A	S	H	L	C
(GNP)	A	S	H	L	C
(60s_loop)	A	S	H	L	C
ras_prot	A	S	H	L	C
(G60)	A	S	H	L	C
3GFTa_e_chg	A	S	H	L	C
3GFTa_e_map	A	S	H	L	C
3GFTa_e_pot	A	S	H	L	C

Mutagenesis

Mutate to ARG

N-Cap: Open

C-Cap: Open

Hydrogens: Current

Show Lines

Backbone Depen. Rotamers

Apply

Clear

Done

Mouse Mode 3-Button Viewing

Buttons	L	M	R	Wheel
& Keys	Rota	Move	MovZ	Slab
Shft	+Box	-Box	Clip	MovS
Ctrl	+/-	PkAt	Pk1	MvSZ
CtSh	Sele	Orig	Clip	MovZ
SnglClk	+/-	Cent	Menu	
DblClk	Menu	-	PkAt	

Selecting Residues

State 1/ 27

Navigation buttons: back, forward, search, etc.



Implications for Libraries

Data competencies inform domain expertise
and...vice versa

Align library activities with faculty needs,
data life cycle, (Jaguszewski & Williams 2013)

Librarian's need to offer more
expertise...value (Kenney (Ithaka), 2014)

Collaboration & “soft skills” critical to
leveraging expertise and expanding services

Results in a more rigorous & sustainable IL
program



Impact on student learning

Innovative learning experience for students -
data integrates & informs content

Students will be able to manage and analyze
their data more efficiently

Students able to find “real world” solutions
to research questions

Peer-reviewed presentations demonstrate
deeper understanding of subjects



Best Practices

Must be course-integrated – worth %

Scaffolded, sequential steps – simple to complex – data & bibliographic resources

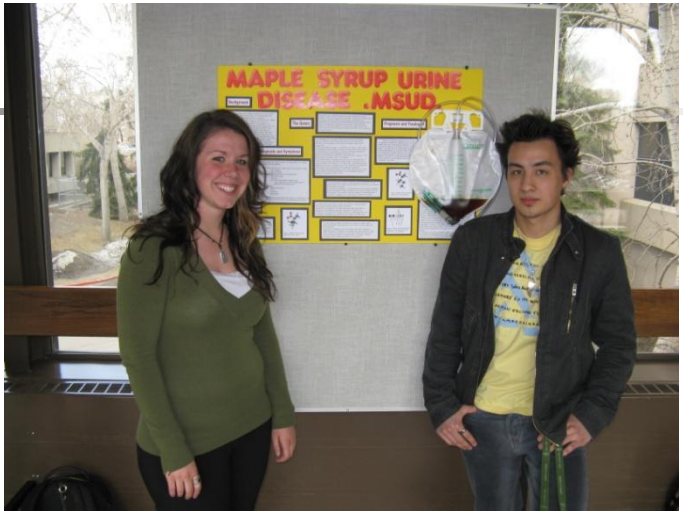
Students learn best by doing – allow hands-on interactivity & flexibility

Tailor relevant data sources to specific questions

Consistent instruction across all lab sections – TA's not always experts

A few of our students ...

Participation in the third annual Biological Student's Conference





Student feedback

- “It was good that we were able to use things that we learned in BIOL 311 to understand things in BCEM 393. I think that I learned more because I could see how labs and topics in the two courses related to each other”
- “I liked how the library and computer labs were hands-on. The TAs and library people were there to help us and not just tell us what to do. I think it was more fun and we got more out of it by doing things on our own instead of following a step-by-step recipe in the lab manual”
- “The presentations gave me the chance to learn many valuable skills. I liked picking the disease to study and doing the project with a partner. I also liked hearing about how other groups went about doing their projects in different ways”



Assessment

- Students prepare poster & presentation (mark and peers)
- Peer-Review “Marking Rubric”
- TooFast
<https://www.toofast.ca/>
- Impact on academic productivity - effective?

Peer-Review Marking

Rubric

Laboratory exercise 2 – Genetics and protein structure

APPENDIX C: PEER-REVIEW MARKING RUBRIC FOR PRESENTATIONS

Names: _____

Topic: _____

	4 – Excellent	3 – Good	2 – Fair	1 – Area of growth	Grade (out of 4)
Delivery	<ul style="list-style-type: none"> Hold attention of entire audience with the use of eye contact, seldom looking at notes Speak with fluctuation in volume and inflection to maintain audience interest and emphasize key points 	<ul style="list-style-type: none"> Consistent use of direct eye contact with audience, but still returns to notes Speak with satisfactory variation of volume and inflection 	<ul style="list-style-type: none"> Display minimal eye contact with audience, while reading mostly from the notes Speak in uneven volume with little or no inflection 	<ul style="list-style-type: none"> Hold no eye contact with audience, as entire report is read from notes Speak in low volume and/or monotonous tone, which causes audience to disengage 	____ / 4
Content/ organization	<ul style="list-style-type: none"> Demonstrate full knowledge by answering all class questions with explanations and elaboration Provide clear explanation of effects of mutation on protein structure and how this affects the inheritance pattern of the disease 	<ul style="list-style-type: none"> Are at ease with expected answers to all questions, without elaboration Provide somewhat clear explanation of effects of mutation on protein structure and how this affects the inheritance pattern of the disease 	<ul style="list-style-type: none"> Are uncomfortable with information and are able to answer only rudimentary questions Attempt to explain the effects of the mutation on protein structure, but do not adequately show why the disease is dominant or recessive 	<ul style="list-style-type: none"> Do not have grasp of information and cannot answer questions about subject Do not clearly explain the effects of the mutation on protein structure nor how these effects cause the disease's inheritance pattern 	____ / 4
Enthusiasm/ audience awareness	<ul style="list-style-type: none"> Demonstrate strong enthusiasm about topic during entire presentation Significantly increase audience understanding and knowledge of topic; convince an audience to recognize the validity and importance of the subject 	<ul style="list-style-type: none"> Show some enthusiastic feelings about topic Raise audience understanding and awareness of most points 	<ul style="list-style-type: none"> Show little or mixed feeling about the topic being presented Raise audience understanding and knowledge of some points 	<ul style="list-style-type: none"> Fail to increase audience understanding of knowledge of topic Show no interest in topic presented 	____ / 4

TOTAL: ____ / 12

APPENDIX B: G.T.A. MARKING RUBRIC FOR PRESENTATIONS

Name: _____

Topic: _____

Content (6 marks):

Give 2 marks if that aspect is well done, 0.5 marks for evidence of effort, and 0 for no effort.

- _____ appropriate amount of background information is presented, with protein and mutation clearly identified and described
- _____ the effects of the mutation on protein structure are clearly explained through a detailed description of the disruption of any non-covalent interactions and the introduction of any steric clashes
- _____ the effects of the mutation on protein function are clearly explained, providing a model that can be used to explain the links between the inheritance pattern and the effects of the mutation on protein structure and function (*i.e.*, why is the disease recessive or dominant based on the mutation's effect on protein structure and function?)

Presentation (6 marks):

Give 1 mark if that aspect is well done, 0.5 marks for evidence of effort, and 0 for no effort.

- _____ demonstrates good speaking skills (tone, volume, pace, avoiding “ums”, “you know”, etc.)
- _____ logical and confident delivery of material
- _____ presenter makes eye contact, engages the audience and is enthusiastic
- _____ presentation is clear and visually appealing
- _____ equal participation of group members
- _____ references are properly cited and presented in the presentation

Answering questions (2 marks):

- 2 marks will be given if all questions are answered thoroughly
- 1 mark will be given if the questions are only partially answered
- 0 marks will be given if the questions are not answered satisfactorily

Asking questions to others (2 marks):



Bibliography

- Jaguszewski, J.M., Williams, K. (2013). *New Roles for New Times: Transforming Liaison Roles in Research Libraries*. Association of Research Libraries. Retrieved from <http://www.arl.org/storage/documents/publications/NRNT-Liaison-Roles-final.pdf>
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Thank You!

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Resources

- NCBI
<http://www.ncbi.nlm.nih.gov/>
- OMIM
<http://www.ncbi.nlm.nih.gov/omim>
- Protein Data Bank
<http://www.rcsb.org/pdb/home/home.do>
- UniProt
<http://www.uniprot.org/>
- PyMOL
<http://www.pymol.org/>
- Course related Libguides
<http://libguides.ucalgary.ca/content.php?pid=55723&sid=413079>