
TARDIS

THE AUSTRALIAN REPOSITORIES FOR DIFFRACTION IMAGES
(Androulakis et al (2008) Acta Cryst. D) [PubMed]

Size of data indexed by TARDIS
Compressed: 20.60 GB Uncompressed: ~80 GB Average Dataset Size (Compressed): 1.48 GB

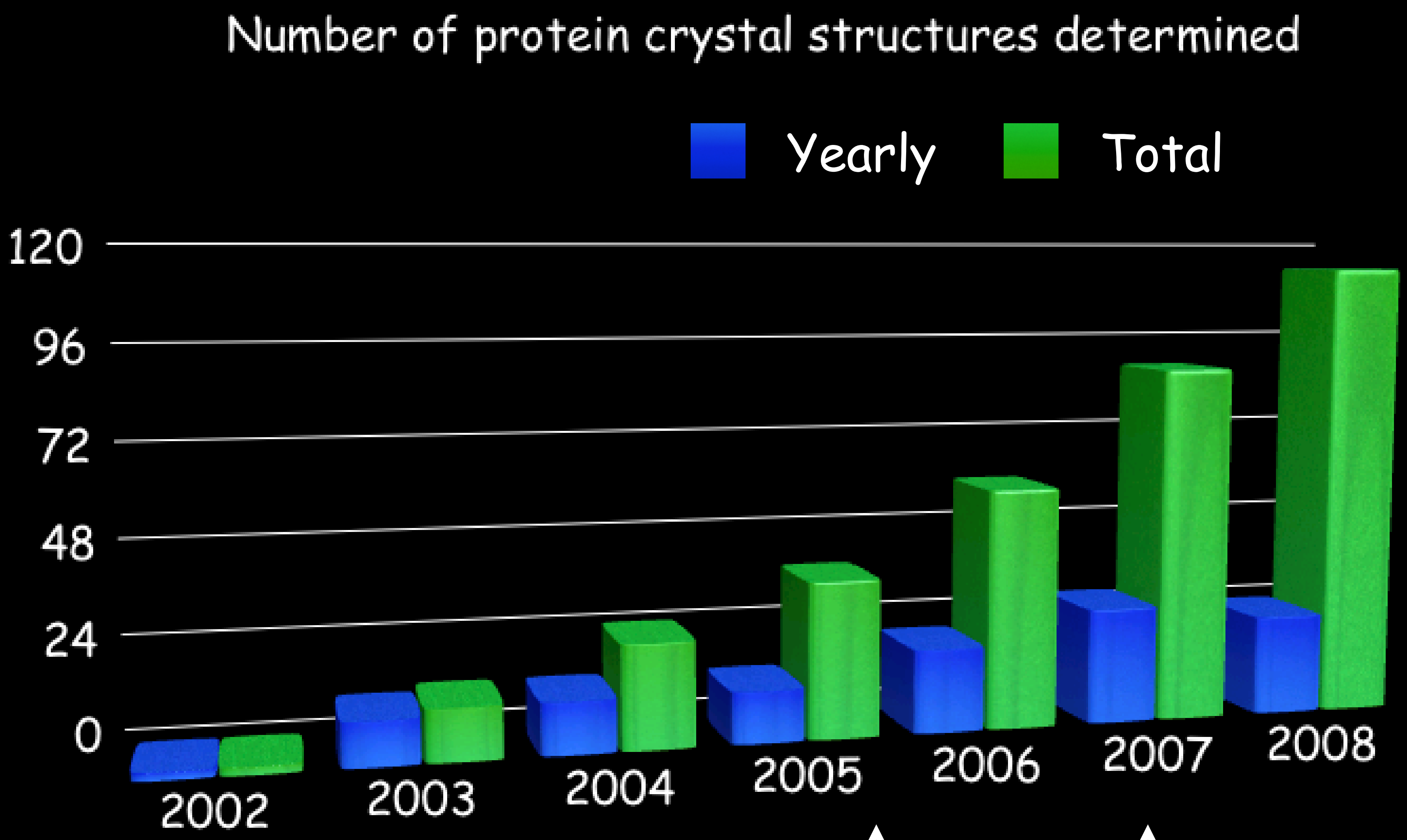
Federated Repositories of X-ray Diffraction Images

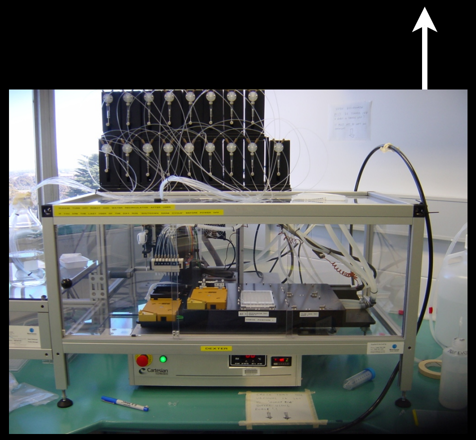
Ashley Buckle

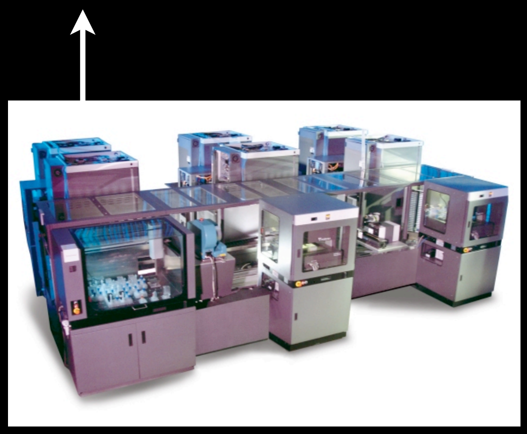
Dept of Biochemistry & Molecular Biology
Monash University, Melbourne, Australia

IUCR, Osaka, August 30th

Protein Crystallography at Monash





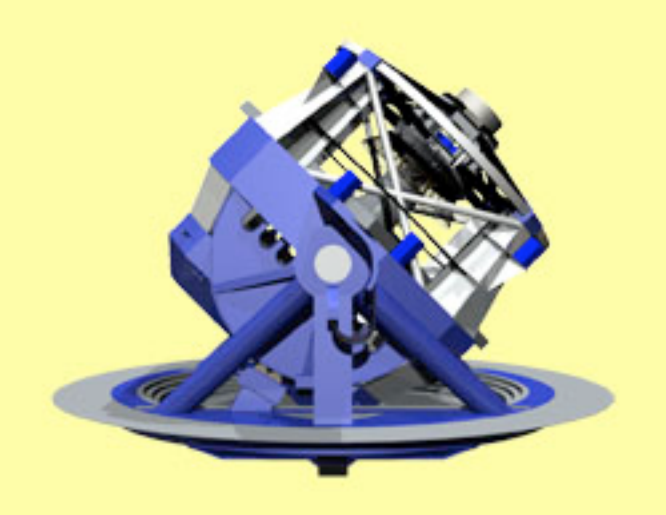


Too much raw data?

Astronomers dont think so...

“....Using these solutions as first steps, the ultimate goal is to meet the needs of the Large Synoptic Survey Telescope (LSST); when LSST begins operation in 2013 it will generate an estimated 15TB of raw data and more than 100TB of processed data every night, 365 days a year. “

source: http://www.gridtoday.com/grid/803617.html



Who stores the raw data?

Laboratory

Pros:

- simple
- cheap

Cons:

- media failure
- staff turnover
- lost disks
- lack of persistence

Institutional libraries

Pros:

- already storing research data
- new role of library
- federated
- economical and scalable
- persistence

Cons:

- data formats - standards?
- data discovery

wwPDB

Pros:

- centralised
- global solution
- standardisation

Cons:

- large data size
- cost

Fedora Commons provides sustainable technologies to **create, manage, publish, share and preserve digital content** as a basis for intellectual, organizational, scientific and cultural heritage by bringing two communities together.

Communities of practice that include scholars, artists, educators, Web innovators, publishers, scientists, librarians, archivists, records managers, and museum curators who present, access, or preserve digital content.

Software developers who work on the cutting edge of open source Web, semantic and enterprise content technologies to ensure that collaboratively created knowledge is available now and in the future.

Open Source Technology

Storage Repository technologies to

{ Download Fedora 3.0
Download Fedora 2.2.3 }

View the Fedora Commons Video First in a Series

Top Ten Reasons to Choose Fedora

Click on any item to learn more.

1. Store whatever you want
2. Easy access
3. Express relationships
4. Free open source software
5. Enables permanence

HatCheck Newsletter

[html] [pdf]

News

New Fedora Commons Wiki
28 August 2008, 2:24 pm

RepoCamp at the Library of Congress
20 August 2008, 3:58 pm

http://fedora-commons.org

Why Fedora?

- Used as a library repository worldwide
  - 148 known as of August 2008
- Examples:
  - eSciDoc Project (key repository for the Max Planck Society)
  - National Science Digital Library (US National Science Federation)
- standards compliant
- open source

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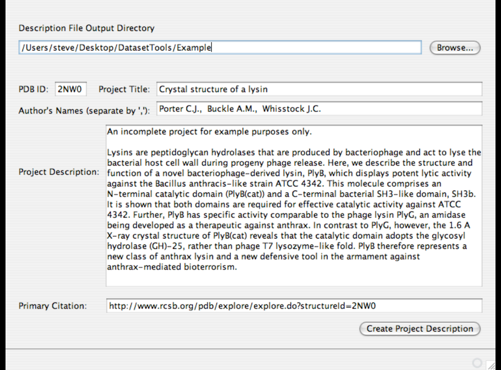
HOME NEWS ABOUT DATA TOOLS PARTNERS SEARCH

Tools for data deposition



Description File Output Directory
/Users/steve/Desktop/DatasetTools/Example

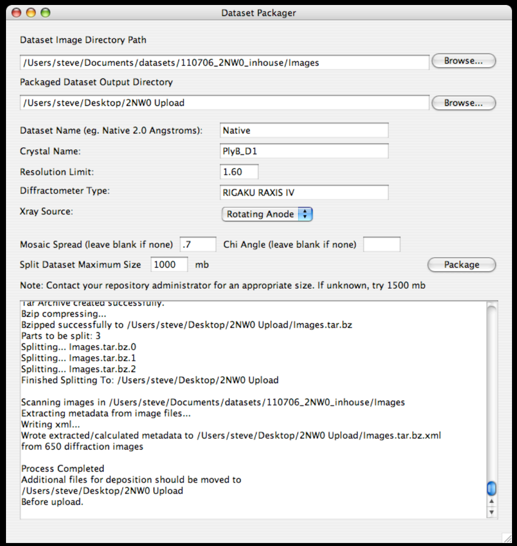
PDB ID: 2NW0 Project Title: Crystal structure of a lysin
Author's Names (separate by ','): Porter C.J., Buckle A.M., Whisstock J.C.

Project Description: An incomplete project for example purposes only.

Lysins are peptidoglycan hydrolases that are produced by bacteriophage and act to lyse the bacterial host cell wall during progeny phage release. Here, we describe the structure and function of a novel bacteriophage-derived lysin, PlyB, which displays potent lytic activity against the Bacillus anthracis-like strain ATCC 4342. This molecule comprises an N-terminal catalytic domain (PlyB(cat)) and a C-terminal bacterial SH3-like domain, SH3b. It is shown that both domains are required for effective catalytic activity against ATCC 4342. Further, PlyB has specific activity comparable to the phage lysin PlyG, an amidase being developed as a therapeutic against anthrax. In contrast to PlyG, however, the 1.6 A X-ray crystal structure of PlyB(cat) reveals that the catalytic domain adopts the glycosyl hydrolase (GH)-25, rather than phage T7 lysozyme-like fold. PlyB therefore represents a new class of anthrax lysin and a new defensive tool in the armament against anthrax-mediated bioterrorism.

Primary Citation: http://www.rcsb.org/pdb/explore/explore.do?structureId=2NW0

Project Descriptor



Dataset Image Directory Path
/Users/steve/Documents/datasets/110706_2NW0_inhouse/Images
Packaged Dataset Output Directory
/Users/steve/Desktop/2NW0 Upload

Dataset Name (eg. Native 2.0 Angstroms): Native
Crystal Name: PlyB_D1
Resolution Limit: 1.60
Diffractometer Type: RIGAKU RAXIS IV
Xray Source: Rotating Anode

Mosaic Spread (leave blank if none) .7 Chi Angle (leave blank if none)
Split Dataset Maximum Size 1000 mb

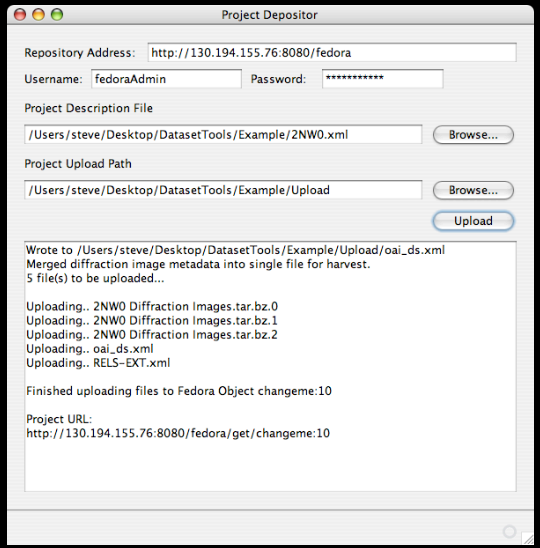
Note: Contact your repository administrator for an appropriate size. If unknown, try 1500 mb

```
Tar Archive created successfully.
Bzip compressing...
Bzipped successfully to /Users/steve/Desktop/2NW0 Upload/Images.tar.bz
Parts to be split: 3
Splitting... Images.tar.bz.0
Splitting... Images.tar.bz.1
Splitting... Images.tar.bz.2
Finished Splitting To: /Users/steve/Desktop/2NW0 Upload

Scanning images in /Users/steve/Documents/datasets/110706_2NW0_inhouse/Images
Extracting metadata from image files...
Writing xml...
Wrote extracted/calculated metadata to /Users/steve/Desktop/2NW0 Upload/Images.tar.bz.xml
from 650 diffraction images

Process Completed
Additional files for deposition should be moved to
/Users/steve/Desktop/2NW0 Upload
Before upload.
```

Dataset Packager



Repository Address: http://130.194.155.76:8080/fedora
Username: fedoraAdmin Password: ***********

Project Description File
/Users/steve/Desktop/DatasetTools/Example/2NW0.xml

Project Upload Path
/Users/steve/Desktop/DatasetTools/Example/Upload

```
Wrote to /Users/steve/Desktop/DatasetTools/Example/Upload/oai_ds.xml
Merged diffraction image metadata into single file for harvest.
5 file(s) to be uploaded...

Uploading.. 2NW0 Diffraction Images.tar.bz.0
Uploading.. 2NW0 Diffraction Images.tar.bz.1
Uploading.. 2NW0 Diffraction Images.tar.bz.2
Uploading.. oai_ds.xml
Uploading.. RELS-EXT.xml

Finished uploading files to Fedora Object changeme:10

Project URL:
http://130.194.155.76:8080/fedora/get/changeme:10
```

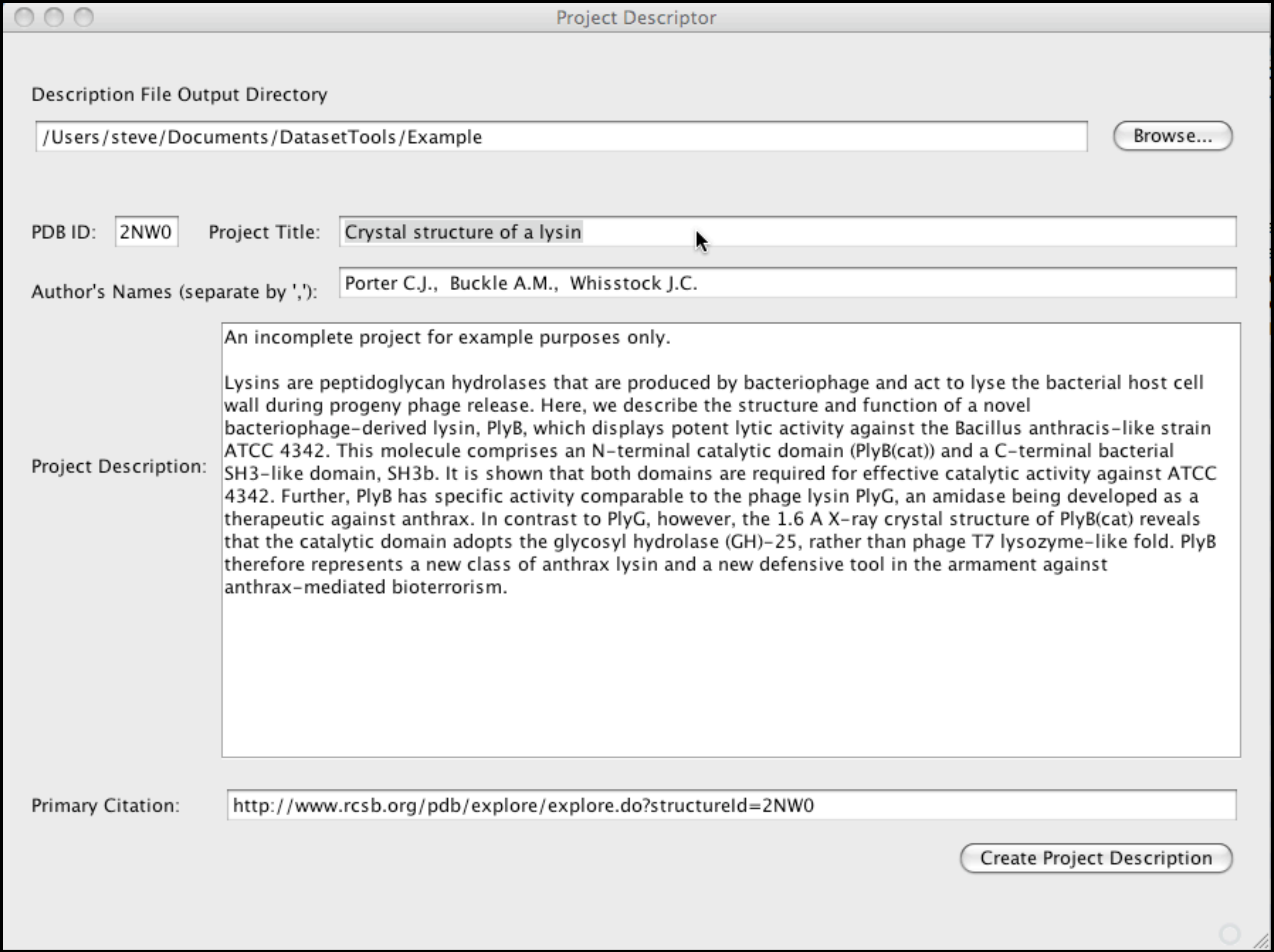
Project Depositor

Package Each Dataset and Annotate Datasets with Metadata

Institutional Repository

Project ingested into repository with packaged, annotated datasets, ready to be discovered by TARDIS

Create Project



Description File Output Directory

/Users/steve/Documents/DatasetTools/Example

PDB ID: 2NW0

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Author's Names (separate by ','): Porter C.J., Buckle A.M., Whisstock J.C.

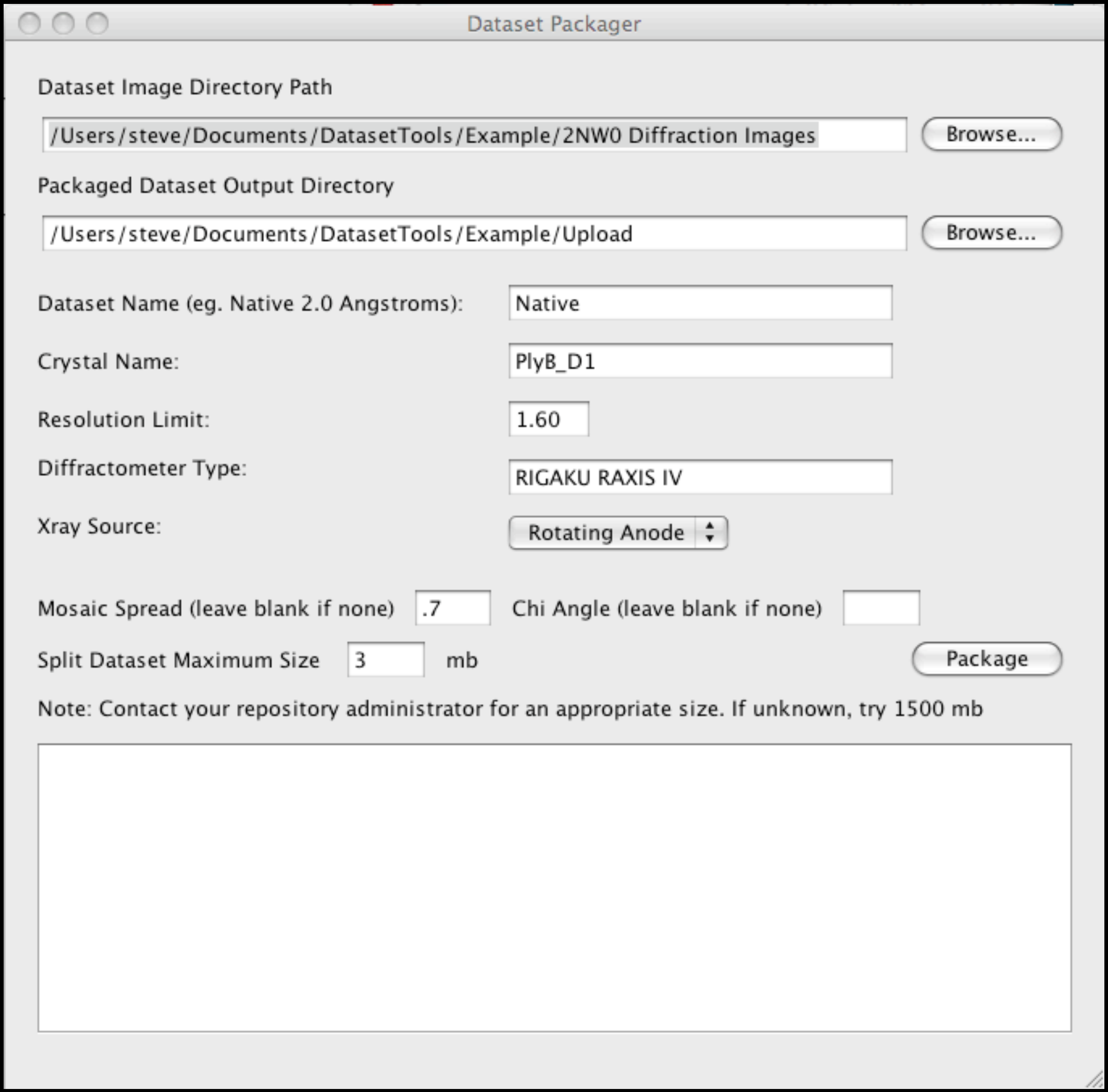
Project Description:

An incomplete project for example purposes only.

Lysins are peptidoglycan hydrolases that are produced by bacteriophage and act to lyse the bacterial host cell wall during progeny phage release. Here, we describe the structure and function of a novel bacteriophage-derived lysin, PlyB, which displays potent lytic activity against the Bacillus anthracis-like strain ATCC 4342. This molecule comprises an N-terminal catalytic domain (PlyB(cat)) and a C-terminal bacterial SH3-like domain, SH3b. It is shown that both domains are required for effective catalytic activity against ATCC 4342. Further, PlyB has specific activity comparable to the phage lysin PlyG, an amidase being developed as a therapeutic against anthrax. In contrast to PlyG, however, the 1.6 A X-ray crystal structure of PlyB(cat) reveals that the catalytic domain adopts the glycosyl hydrolase (GH)-25, rather than phage T7 lysozyme-like fold. PlyB therefore represents a new class of anthrax lysin and a new defensive tool in the armament against anthrax-mediated bioterrorism.

Primary Citation: http://www.rcsb.org/pdb/explore/explore.do?structureId=2NW0

Package Data



Dataset Image Directory Path

/Users/steve/Documents/DatasetTools/Example/2NW0 Diffraction Images

Packaged Dataset Output Directory

/Users/steve/Documents/DatasetTools/Example/Upload

Dataset Name (eg. Native 2.0 Angstroms): Native

Crystal Name: PlyB_D1

Resolution Limit: 1.60

Diffractometer Type: RIGAKU RAXIS IV

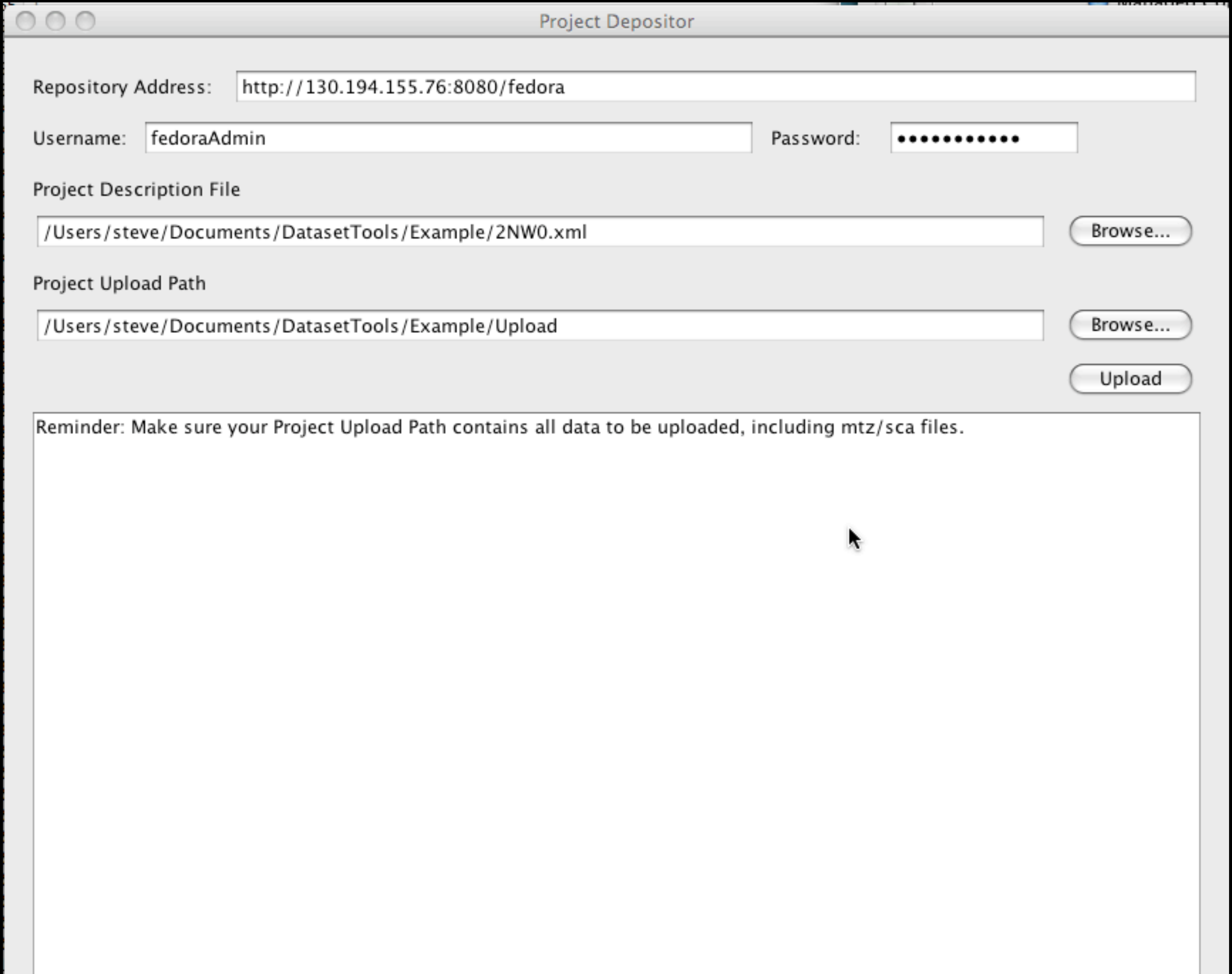
Xray Source: Rotating Anode

Mosaic Spread (leave blank if none) .7 Chi Angle (leave blank if none)

Split Dataset Maximum Size 3 mb

Note: Contact your repository administrator for an appropriate size. If unknown, try 1500 mb

Upload Data



Repository Address: http://130.194.155.76:8080/fedora

Username: fedoraAdmin

Password: ••••••••••••

Project Description File

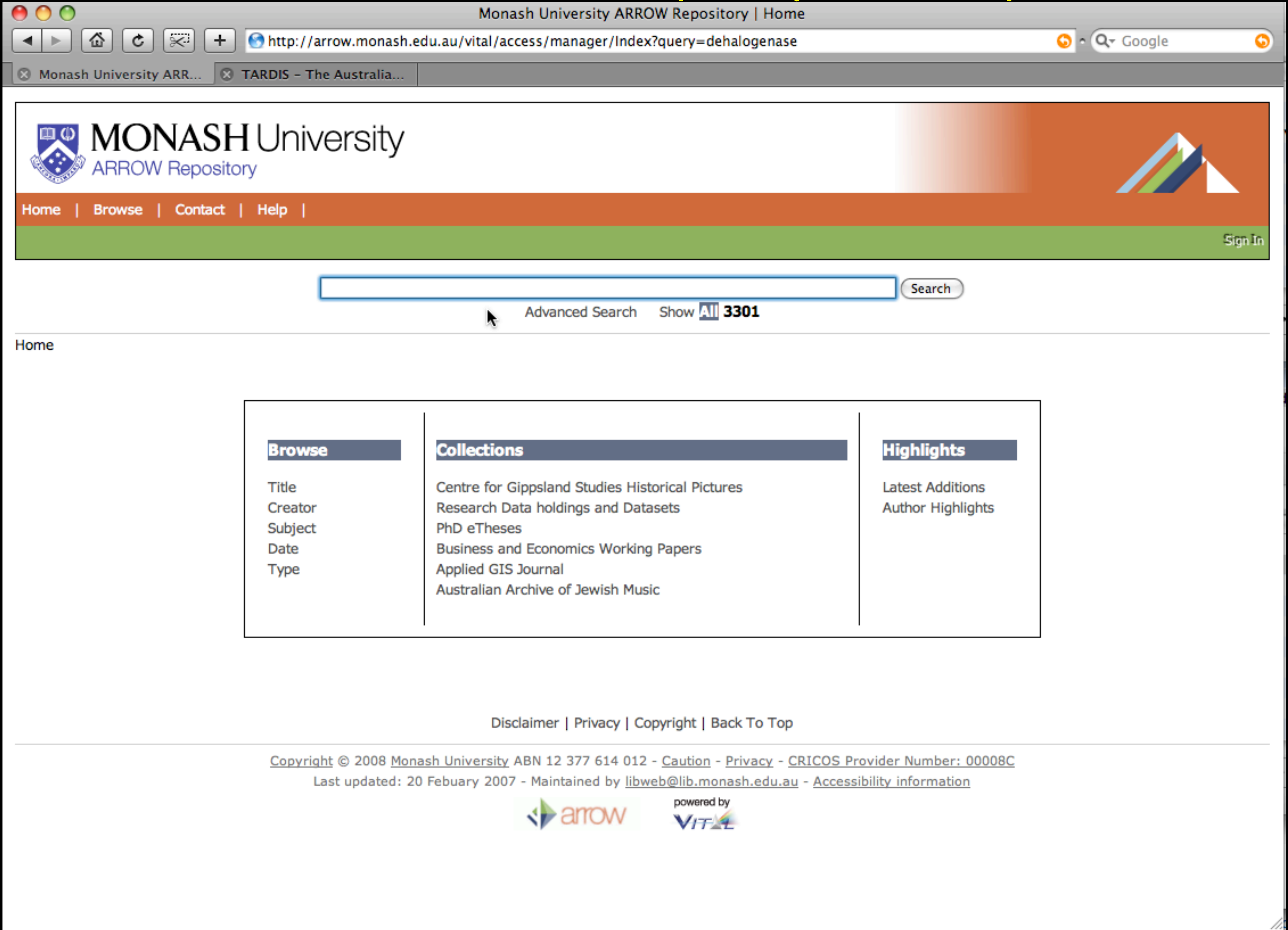
/Users/steve/Documents/DatasetTools/Example/2NW0.xml

Project Upload Path

/Users/steve/Documents/DatasetTools/Example/Upload

Reminder: Make sure your Project Upload Path contains all data to be uploaded, including mtz/sca files.

Data in Library repository



Browse	Collections	Highlights
Title	Centre for Gippsland Studies Historical Pictures	Latest Additions
Creator	Research Data holdings and Datasets	Author Highlights
Subject	PhD eTheses	
Date	Business and Economics Working Papers	
Type	Applied GIS Journal	
	Australian Archive of Jewish Music	

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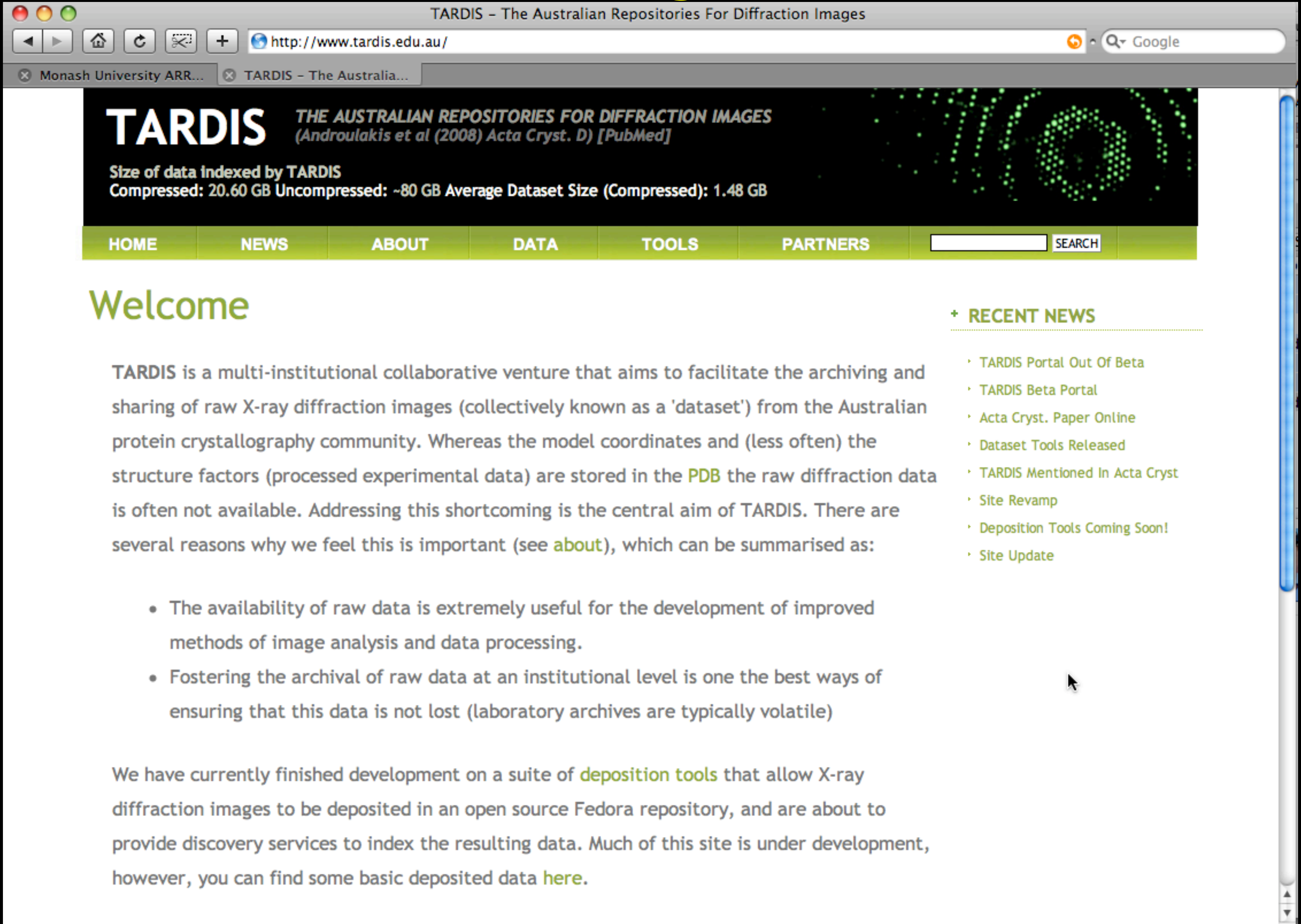
Last updated: 20 Febuary 2007 - Maintained by libweb@lib.monash.edu.au - Accessibility information

Search using TARDIS



TARDIS *THE AUSTRALIAN REPOSITORIES FOR DIFFRACTION IMAGES*
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Size of data indexed by TARDIS
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Welcome

TARDIS is a multi-institutional collaborative venture that aims to facilitate the archiving and sharing of raw X-ray diffraction images (collectively known as a 'dataset') from the Australian protein crystallography community. Whereas the model coordinates and (less often) the structure factors (processed experimental data) are stored in the PDB the raw diffraction data is often not available. Addressing this shortcoming is the central aim of TARDIS. There are several reasons why we feel this is important (see about), which can be summarised as:

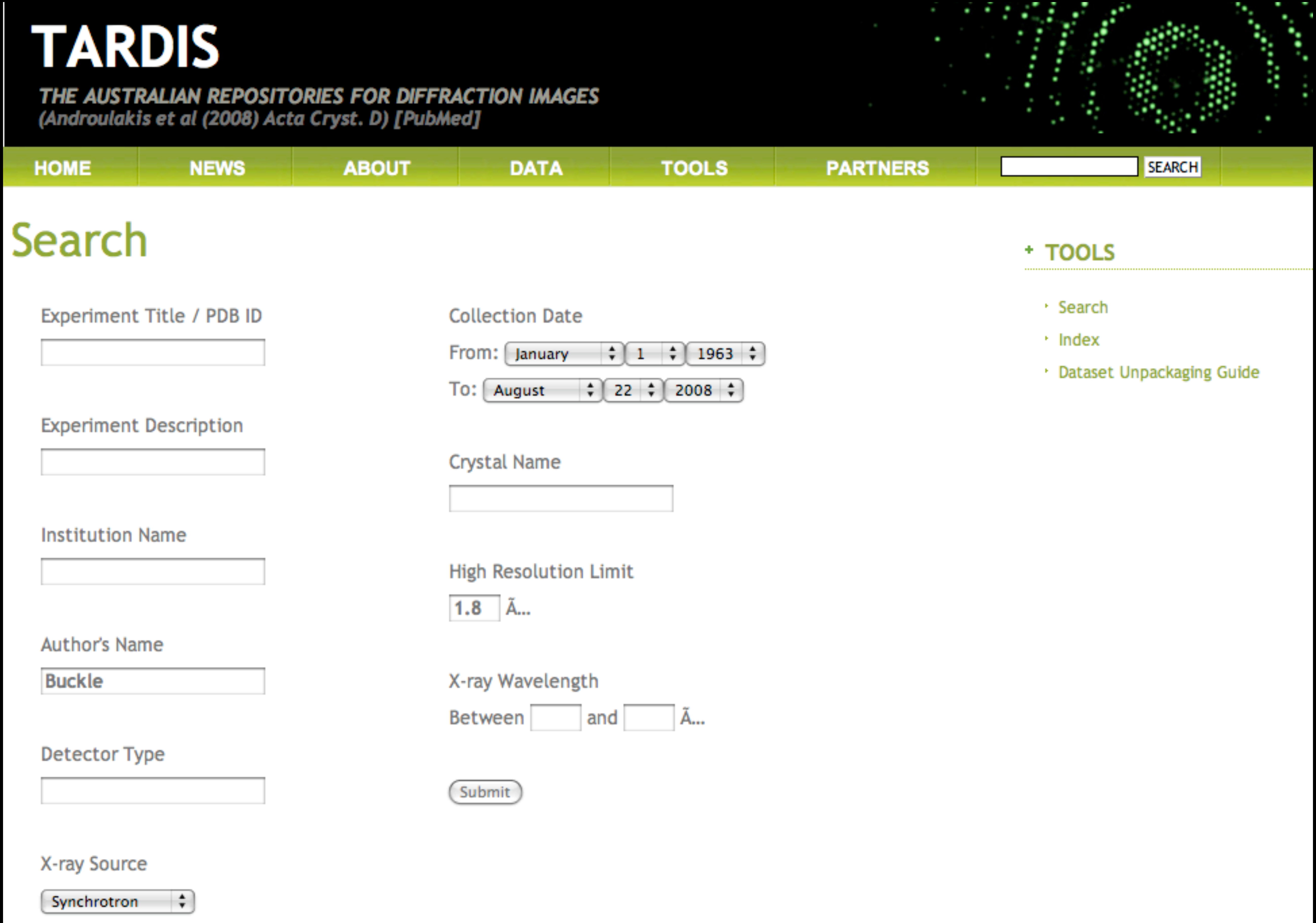
- The availability of raw data is extremely useful for the development of improved methods of image analysis and data processing.
- Fostering the archival of raw data at an institutional level is one the best ways of ensuring that this data is not lost (laboratory archives are typically volatile)

We have currently finished development on a suite of deposition tools that allow X-ray diffraction images to be deposited in an open source Fedora repository, and are about to provide discovery services to index the resulting data. Much of this site is under development, however, you can find some basic deposited data here.

RECENT NEWS

- TARDIS Portal Out Of Beta
- TARDIS Beta Portal
- Acta Cryst. Paper Online
- Dataset Tools Released
- TARDIS Mentioned In Acta Cryst
- Site Revamp
- Deposition Tools Coming Soon!
- Site Update

Advanced Search



TARDIS

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(Androulakis et al (2008) Acta Cryst. D) [PubMed]

Search

Experiment Title / PDB ID:

Experiment Description:

Institution Name:

Author's Name: Buckle

Detector Type:

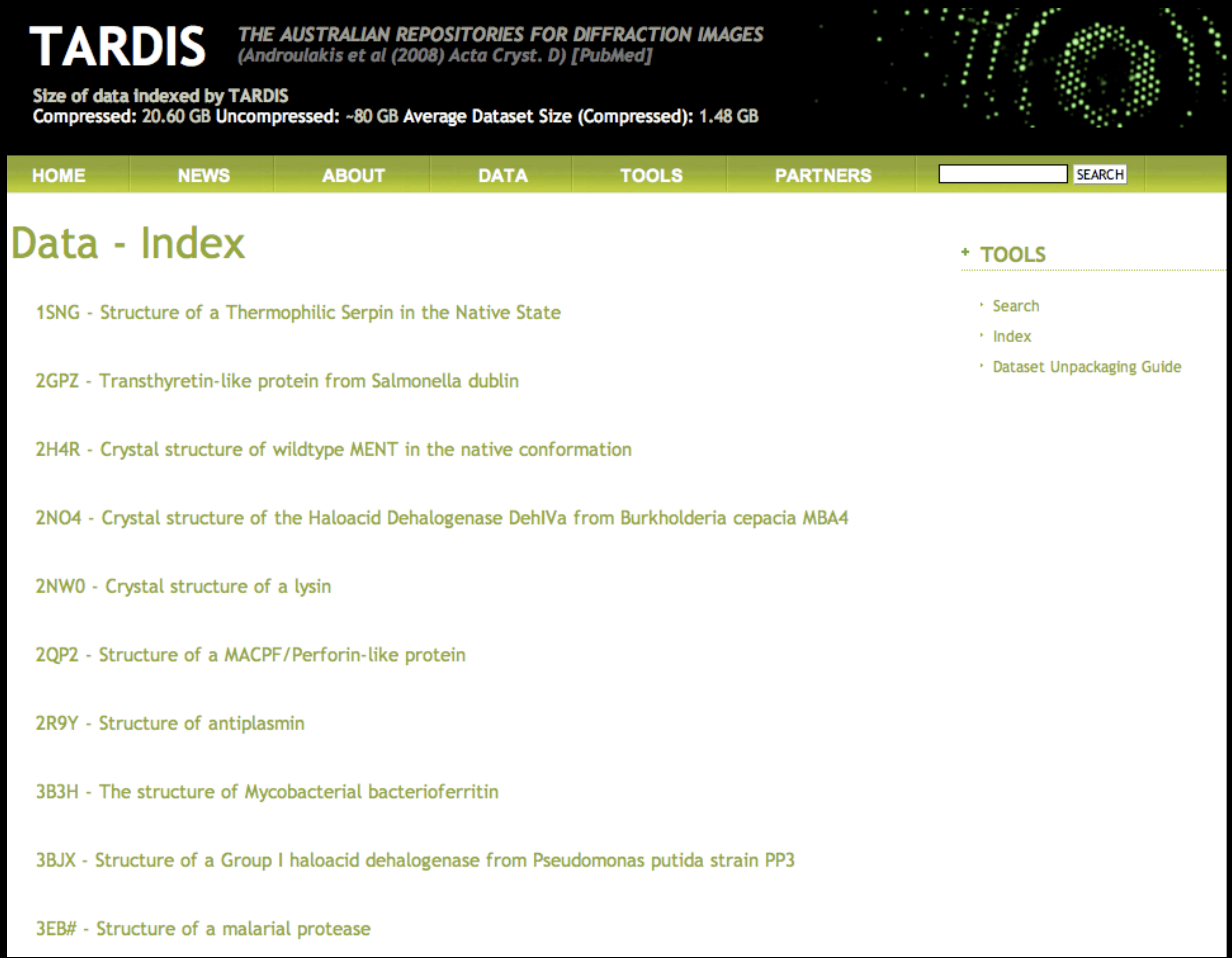
X-ray Source: Synchrotron

Collection Date
From: January 1 1963
To: August 22 2008

Crystal Name:

High Resolution Limit: 1.8 Ã…

X-ray Wavelength
Between and Ã…



TARDIS *THE AUSTRALIAN REPOSITORIES FOR DIFFRACTION IMAGES*
(Androulakis et al (2008) Acta Cryst. D) [PubMed]

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Data - Index

1SNG - Structure of a Thermophilic Serpin in the Native State

2GPZ - Transthyretin-like protein from Salmonella dublin

2H4R - Crystal structure of wildtype MENT in the native conformation

2NO4 - Crystal structure of the Haloacid Dehalogenase DehIVa from Burkholderia cepacia MBA4

2NW0 - Crystal structure of a lysin

2QP2 - Structure of a MACPF/Perforin-like protein

2R9Y - Structure of antiplasmin

3B3H - The structure of Mycobacterial bacterioferritin

3BJX - Structure of a Group I haloacid dehalogenase from Pseudomonas putida strain PP3

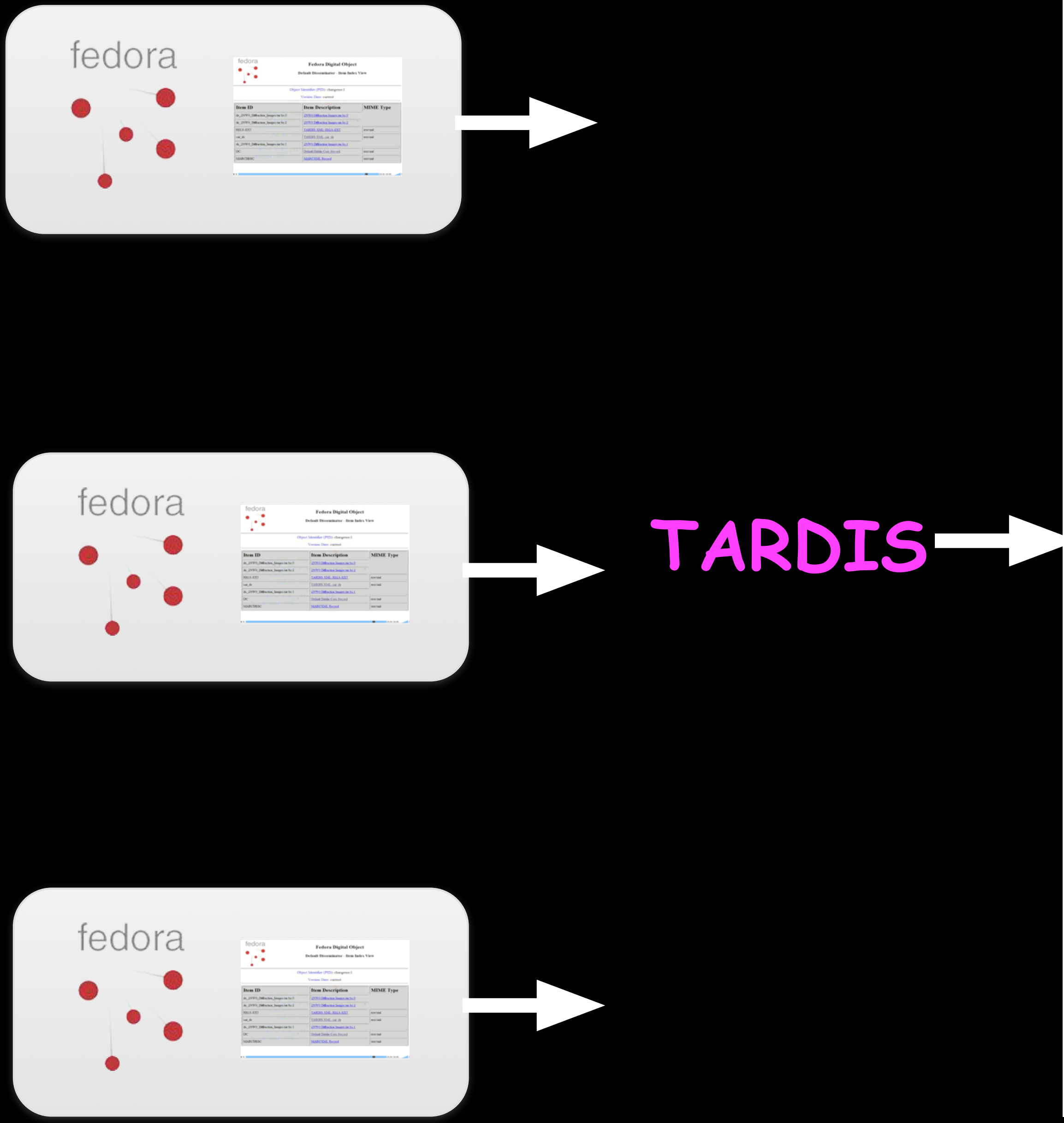
3EB# - Structure of a malarial protease

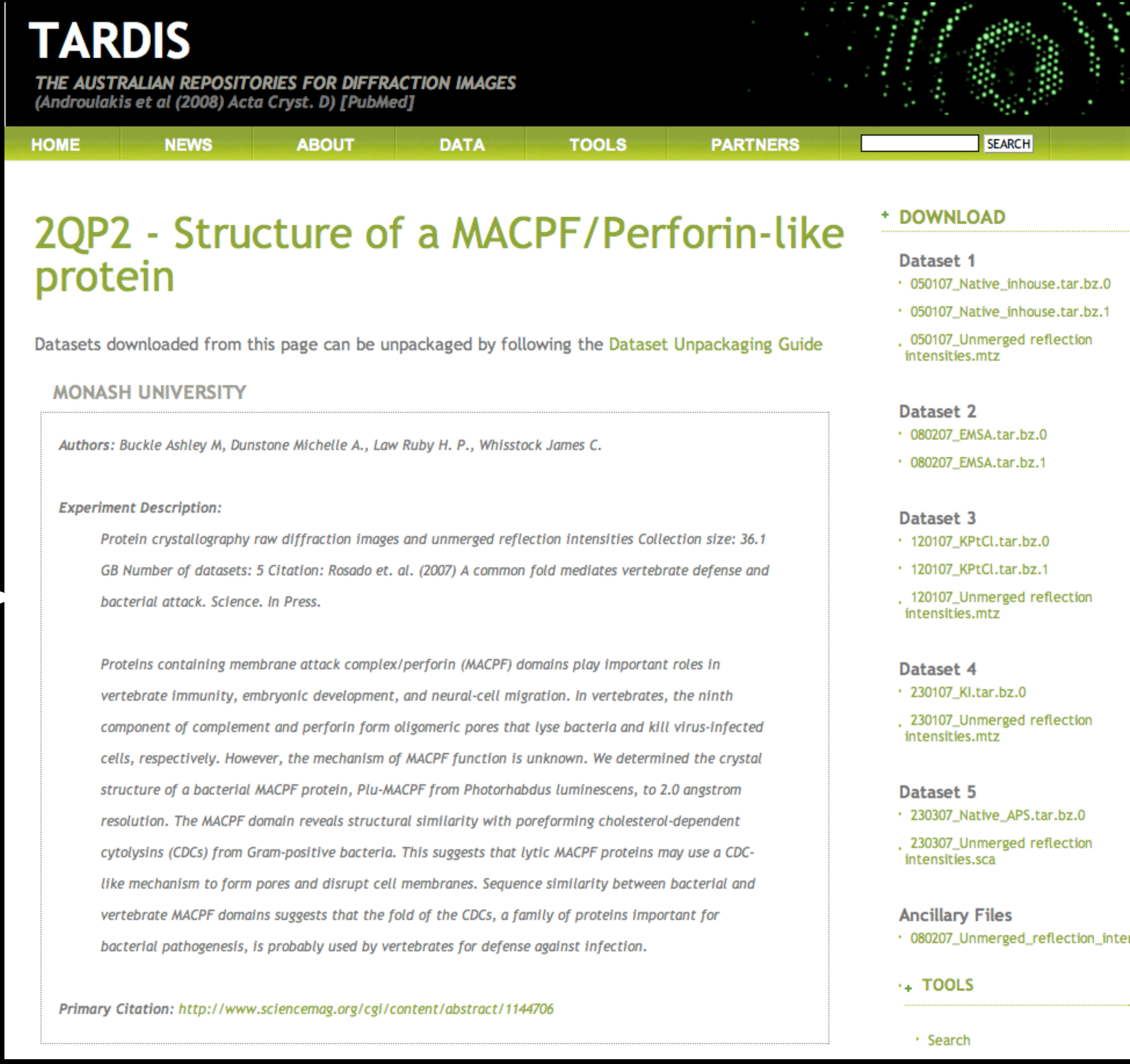
TOOLS

- Search
- Index
- Dataset Unpackaging Guide

Federated approach

Institutional Repositories





TARDIS

THE AUSTRALIAN REPOSITORIES FOR DIFFRACTION IMAGES
(Androulakis et al (2008) Acta Cryst. D) [PubMed]

2QP2 - Structure of a MACPF/Perforin-like protein

Datasets downloaded from this page can be unpackaged by following the Dataset Unpackaging Guide

MONASH UNIVERSITY

Authors: *Buckle Ashley M, Dunstone Michelle A., Law Ruby H. P., Whisstock James C.*

Experiment Description:

Protein crystallography raw diffraction images and unmerged reflection intensities Collection size: 36.1 GB Number of datasets: 5 Citation: Rosado et. al. (2007) A common fold mediates vertebrate defense and bacterial attack. Science. In Press.

Proteins containing membrane attack complex/perforin (MACPF) domains play important roles in vertebrate immunity, embryonic development, and neural-cell migration. In vertebrates, the ninth component of complement and perforin form oligomeric pores that lyse bacteria and kill virus-infected cells, respectively. However, the mechanism of MACPF function is unknown. We determined the crystal structure of a bacterial MACPF protein, Plu-MACPF from Photorhabdus luminescens, to 2.0 angstrom resolution. The MACPF domain reveals structural similarity with poreforming cholesterol-dependent cytolysins (CDCs) from Gram-positive bacteria. This suggests that lytic MACPF proteins may use a CDC-like mechanism to form pores and disrupt cell membranes. Sequence similarity between bacterial and vertebrate MACPF domains suggests that the fold of the CDCs, a family of proteins important for bacterial pathogenesis, is probably used by vertebrates for defense against infection.

Primary Citation: *http://www.sciencemag.org/cgi/content/abstract/1144706*

+ DOWNLOAD

Dataset 1
- 050107_Native_inhouse.tar.bz.0
- 050107_Native_inhouse.tar.bz.1
- 050107_Unmerged reflection intensities.mtz

Dataset 2
- 080207_EMSA.tar.bz.0
- 080207_EMSA.tar.bz.1

Dataset 3
- 120107_KPtCl.tar.bz.0
- 120107_KPtCl.tar.bz.1
- 120107_Unmerged reflection intensities.mtz

Dataset 4
- 230107_KI.tar.bz.0
- 230107_Unmerged reflection intensities.mtz

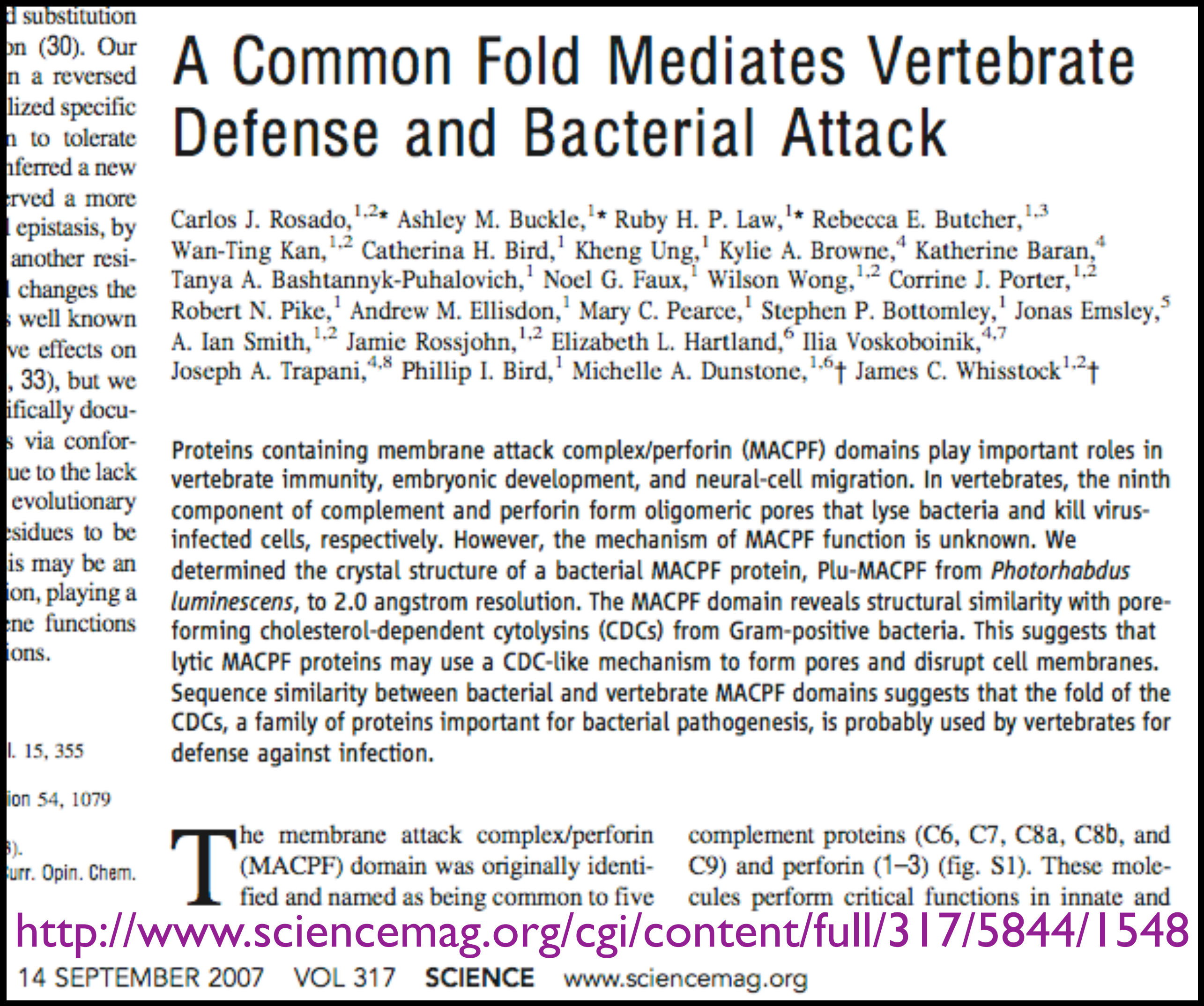
Dataset 5
- 230307_Native_APS.tar.bz.0
- 230307_Unmerged reflection intensities.sca

Ancillary Files
- 080207_Unmerged_reflection_inte

+ TOOLS

- Search

Publication of raw data alongside publication of paper and coordinates



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ion 54, 1079

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urr. Opin. Chem.

A Common Fold Mediates Vertebrate Defense and Bacterial Attack

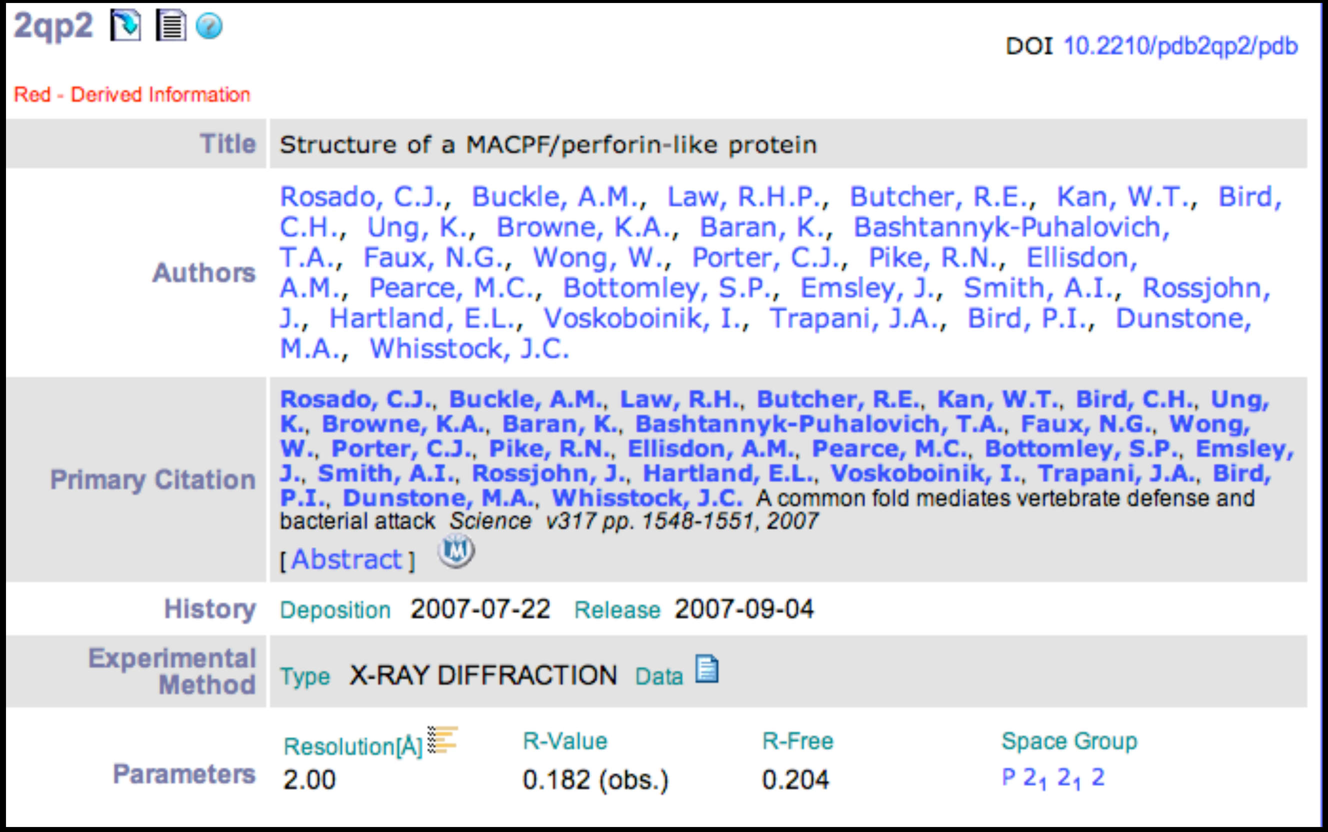
Carlos J. Rosado,[1,2*] Ashley M. Buckle,[1*] Ruby H. P. Law,[1*] Rebecca E. Butcher,[1,3] Wan-Ting Kan,[1,2] Catherina H. Bird,[1] Kheng Ung,[1] Kylie A. Browne,[4] Katherine Baran,[4] Tanya A. Bashtannyk-Puhalovich,[1] Noel G. Faux,[1] Wilson Wong,[1,2] Corrine J. Porter,[1,2] Robert N. Pike,[1] Andrew M. Ellisdon,[1] Mary C. Pearce,[1] Stephen P. Bottomley,[1] Jonas Emsley,[5] A. Ian Smith,[1,2] Jamie Rossjohn,[1,2] Elizabeth L. Hartland,[6] Ilia Voskoboinik,[4,7] Joseph A. Trapani,[4,8] Phillip I. Bird,[1] Michelle A. Dunstone,[1,6]† James C. Whisstock[1,2]†

Proteins containing membrane attack complex/perforin (MACPF) domains play important roles in vertebrate immunity, embryonic development, and neural-cell migration. In vertebrates, the ninth component of complement and perforin form oligomeric pores that lyse bacteria and kill virus-infected cells, respectively. However, the mechanism of MACPF function is unknown. We determined the crystal structure of a bacterial MACPF protein, Plu-MACPF from *Photorhabdus luminescens*, to 2.0 angstrom resolution. The MACPF domain reveals structural similarity with pore-forming cholesterol-dependent cytolysins (CDCs) from Gram-positive bacteria. This suggests that lytic MACPF proteins may use a CDC-like mechanism to form pores and disrupt cell membranes. Sequence similarity between bacterial and vertebrate MACPF domains suggests that the fold of the CDCs, a family of proteins important for bacterial pathogenesis, is probably used by vertebrates for defense against infection.

The membrane attack complex/perforin (MACPF) domain was originally identified and named as being common to five complement proteins (C6, C7, C8a, C8b, and C9) and perforin (1–3) (fig. S1). These molecules perform critical functions in innate and

http://www.sciencemag.org/cgi/content/full/317/5844/1548

14 SEPTEMBER 2007 VOL 317 **SCIENCE** www.sciencemag.org



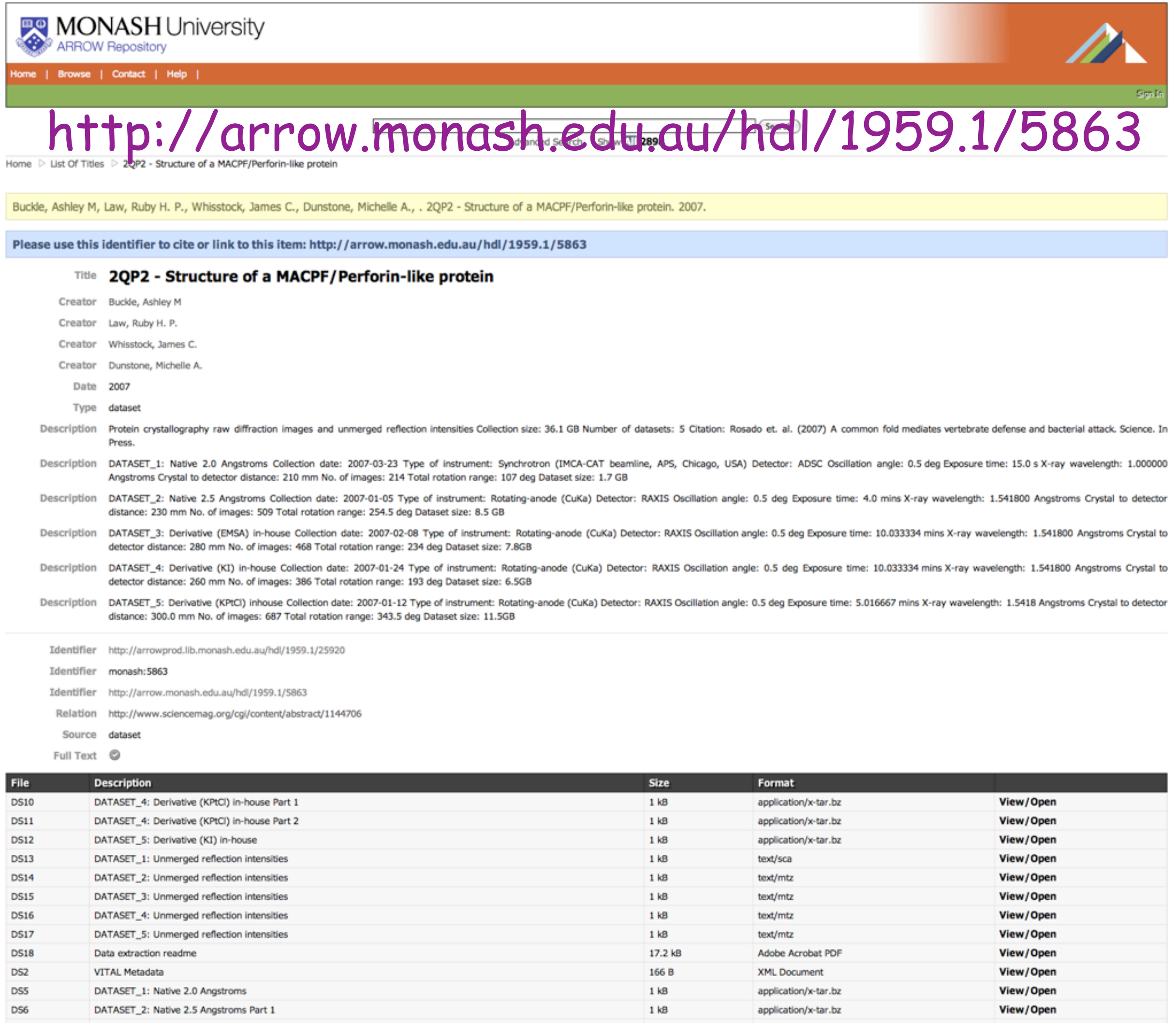
2qp2

DOI 10.2210/pdb2qp2/pdb

Red - Derived Information

Title	Structure of a MACPF/perforin-like protein
Authors	Rosado, C.J., Buckle, A.M., Law, R.H.P., Butcher, R.E., Kan, W.T., Bird, C.H., Ung, K., Browne, K.A., Baran, K., Bashtannyk-Puhalovich, T.A., Faux, N.G., Wong, W., Porter, C.J., Pike, R.N., Ellisdon, A.M., Pearce, M.C., Bottomley, S.P., Emsley, J., Smith, A.I., Rossjohn, J., Hartland, E.L., Voskoboinik, I., Trapani, J.A., Bird, P.I., Dunstone, M.A., Whisstock, J.C.
Primary Citation	**Rosado, C.J., Buckle, A.M., Law, R.H., Butcher, R.E., Kan, W.T., Bird, C.H., Ung, K., Browne, K.A., Baran, K., Bashtannyk-Puhalovich, T.A., Faux, N.G., Wong, W., Porter, C.J., Pike, R.N., Ellisdon, A.M., Pearce, M.C., Bottomley, S.P., Emsley, J., Smith, A.I., Rossjohn, J., Hartland, E.L., Voskoboinik, I., Trapani, J.A., Bird, P.I., Dunstone, M.A., Whisstock, J.C.** A common fold mediates vertebrate defense and bacterial attack *Science v317 pp. 1548-1551, 2007* [Abstract]
History	Deposition 2007-07-22 Release 2007-09-04
Experimental Method	Type X-RAY DIFFRACTION Data

	Resolution[Å]	R-Value	R-Free	Space Group
Parameters	2.00	0.182 (obs.)	0.204	P 2_1 2_1 2



http://arrow.monash.edu.au/hdl/1959.1/5863

Home ▷ List Of Titles ▷ 2QP2 - Structure of a MACPF/Perforin-like protein

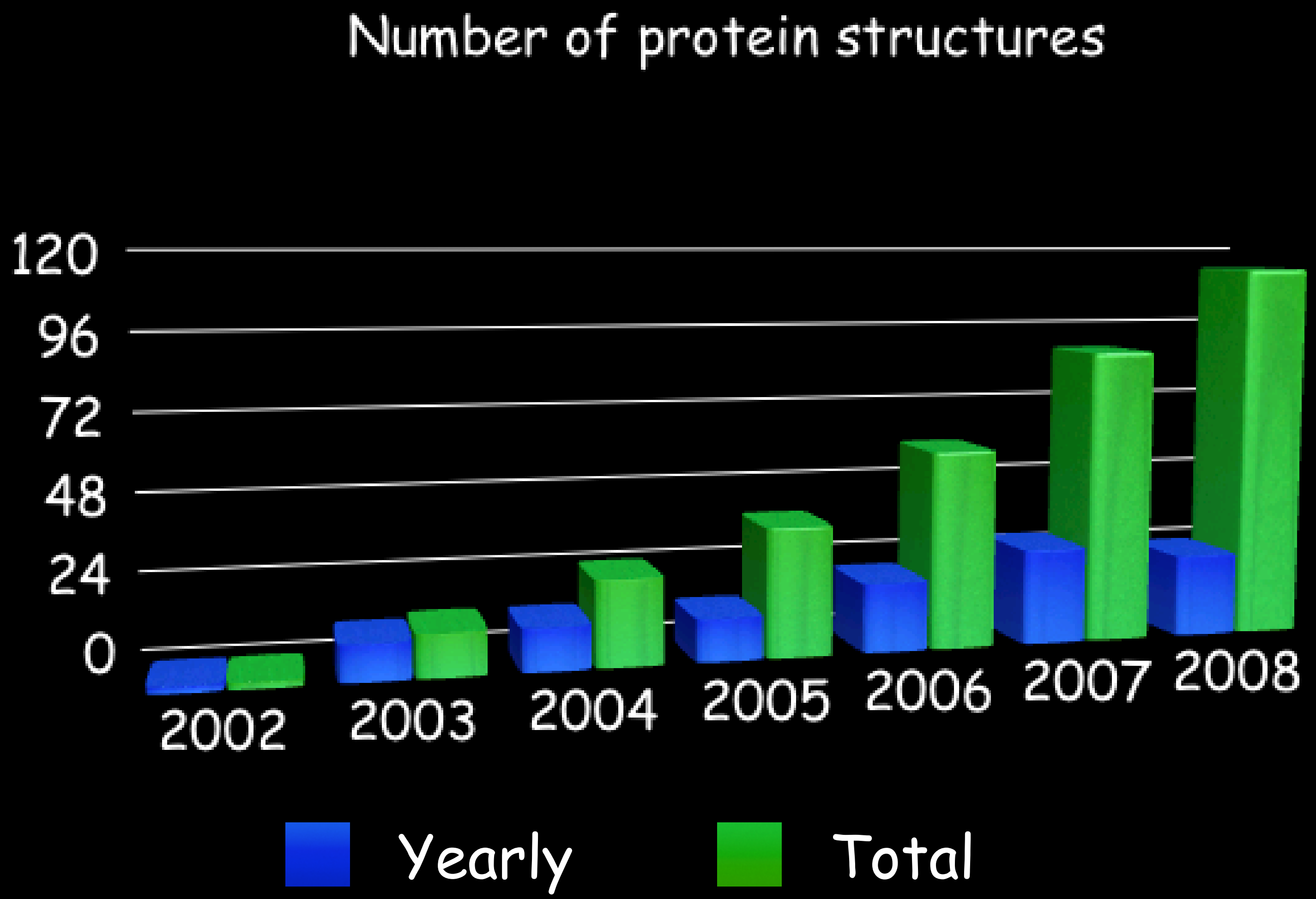
Buckle, Ashley M, Law, Ruby H. P., Whisstock, James C., Dunstone, Michelle A., . 2QP2 - Structure of a MACPF/Perforin-like protein. 2007.

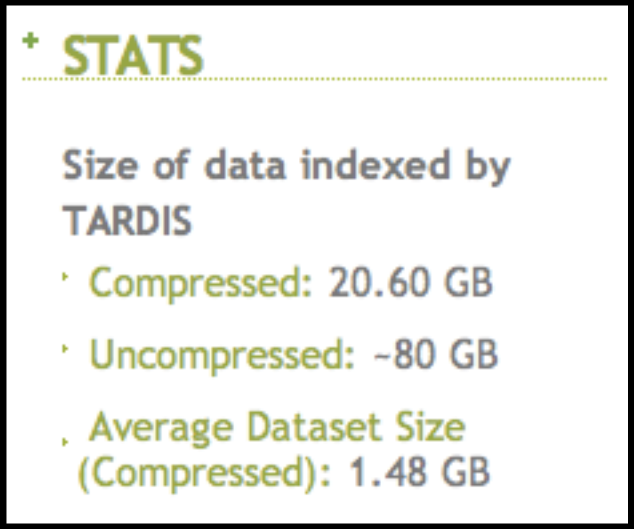
Please use this identifier to cite or link to this item: http://arrow.monash.edu.au/hdl/1959.1/5863

Title	**2QP2 - Structure of a MACPF/Perforin-like protein**
Creator	Buckle, Ashley M
Creator	Law, Ruby H. P.
Creator	Whisstock, James C.
Creator	Dunstone, Michelle A.
Date	2007
Type	dataset
Description	Protein crystallography raw diffraction images and unmerged reflection intensities Collection size: 36.1 GB Number of datasets: 5 Citation: Rosado et. al. (2007) A common fold mediates vertebrate defense and bacterial attack. Science. In Press.
Description	DATASET_1: Native 2.0 Angstroms Collection date: 2007-03-23 Type of instrument: Synchrotron (IMCA-CAT beamline, APS, Chicago, USA) Detector: ADSC Oscillation angle: 0.5 deg Exposure time: 15.0 s X-ray wavelength: 1.000000 Angstroms Crystal to detector distance: 210 mm No. of images: 214 Total rotation range: 107 deg Dataset size: 1.7 GB
Description	DATASET_2: Native 2.5 Angstroms Collection date: 2007-01-05 Type of instrument: Rotating-anode (CuKa) Detector: RAXIS Oscillation angle: 0.5 deg Exposure time: 4.0 mins X-ray wavelength: 1.541800 Angstroms Crystal to detector distance: 230 mm No. of images: 509 Total rotation range: 254.5 deg Dataset size: 8.5 GB
Description	DATASET_3: Derivative (EMSA) in-house Collection date: 2007-02-08 Type of instrument: Rotating-anode (CuKa) Detector: RAXIS Oscillation angle: 0.5 deg Exposure time: 10.033334 mins X-ray wavelength: 1.541800 Angstroms Crystal to detector distance: 280 mm No. of images: 468 Total rotation range: 234 deg Dataset size: 7.8GB
Description	DATASET_4: Derivative (KI) in-house Collection date: 2007-01-24 Type of instrument: Rotating-anode (CuKa) Detector: RAXIS Oscillation angle: 0.5 deg Exposure time: 10.033334 mins X-ray wavelength: 1.541800 Angstroms Crystal to detector distance: 260 mm No. of images: 386 Total rotation range: 193 deg Dataset size: 6.5GB
Description	DATASET_5: Derivative (KPtCl) inhouse Collection date: 2007-01-12 Type of instrument: Rotating-anode (CuKa) Detector: RAXIS Oscillation angle: 0.5 deg Exposure time: 5.016667 mins X-ray wavelength: 1.5418 Angstroms Crystal to detector distance: 300.0 mm No. of images: 687 Total rotation range: 343.5 deg Dataset size: 11.5GB
Identifier	http://arrowprod.lib.monash.edu.au/hdl/1959.1/25920
Identifier	monash:5863
Identifier	http://arrow.monash.edu.au/hdl/1959.1/5863
Relation	http://www.sciencemag.org/cgi/content/abstract/1144706
Source	dataset
Full Text	●

File	Description	Size	Format	
DS10	DATASET_4: Derivative (KPtCl) in-house Part 1	1 kB	application/x-tar.bz	**View/Open**
DS11	DATASET_4: Derivative (KPtCl) in-house Part 2	1 kB	application/x-tar.bz	**View/Open**
DS12	DATASET_5: Derivative (KI) in-house	1 kB	application/x-tar.bz	**View/Open**
DS13	DATASET_1: Unmerged reflection intensities	1 kB	text/sca	**View/Open**
DS14	DATASET_2: Unmerged reflection intensities	1 kB	text/mtz	**View/Open**
DS15	DATASET_3: Unmerged reflection intensities	1 kB	text/mtz	**View/Open**
DS16	DATASET_4: Unmerged reflection intensities	1 kB	text/mtz	**View/Open**
DS17	DATASET_5: Unmerged reflection intensities	1 kB	text/mtz	**View/Open**
DS18	Data extraction readme	17.2 kB	Adobe Acrobat PDF	**View/Open**
DS2	VITAL Metadata	166 B	XML Document	**View/Open**
DS5	DATASET_1: Native 2.0 Angstroms	1 kB	application/x-tar.bz	**View/Open**
DS6	DATASET_2: Native 2.5 Angstroms Part 1	1 kB	application/x-tar.bz	**View/Open**

How much data?



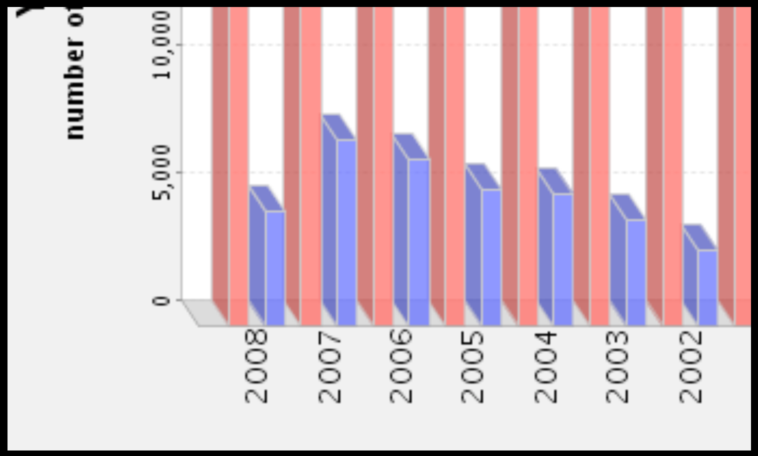


STATS

Size of data indexed by TARDIS

- Compressed: 20.60 GB
- Uncompressed: ~80 GB
- Average Dataset Size (Compressed): 1.48 GB

15 datasets
= 21 Gb
20 structures/year growth
= 30 Gb / year



if PDB growth = 10000 / year
=15 Tb / year

3302 records in the Monash repository
(PhD thesis, images etc)
= 140 Gb
58% is crystallographic raw data
(uncompressed)

Benefits to making raw data available

- Data is stored safely !
- Experiment reproducibility/validation
- Methods development
- Re-refinement of published structures with new methods
- Some data cannot be processed!

Future

- Engagement
  - community
  - wwPDB
  - Journals
  - IUCR
- Data format/standardisation - eg imgCIF/CBF

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