

# PIDs and Cores

CURRENT STATUS AND FUTURE PROGRESS

**Thayumanasamy**

**Somasundaram**

**X-Ray Core Facility**

<https://fla.st/2J0DKH5D>

[tsomasundaram@fsu.edu](mailto:tsomasundaram@fsu.edu)

**FSU**

**INSTITUTE OF  
MOLECULAR BIOPHYSICS**

COLLEGE OF ARTS & SCIENCES

# Persistent identifiers at Cores

- ▶ PID strengths
- ▶ PID issues
- ▶ Missing Piece
- ▶ Adoption
- ▶ Monetization
- ▶ Suggestions
- ▶ PID and a Core
- ▶ Q & A
- ▶ Sci Equip Web Portal



# PID Strengths

- ▶ Ease of finding an asset
- ▶ Implementation
- ▶ Less error prone in identifying an asset
- ▶ Ease of citation
- ▶ Means to get metrics
  - ▶ On usage
  - ▶ Publications
- ▶ Open for future development

# PID Issues

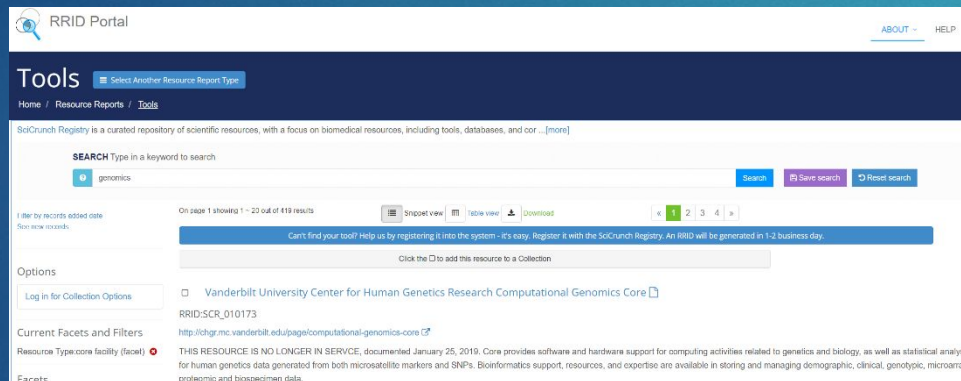
- ▶ Robustness
- ▶ Link Issues
- ▶ Completeness Issues
- ▶ Citation Issues
- ▶ Long term archival
- ▶ Viability



# RRID Robustness

## RRID: Genomics

<https://rrid.site/Genomics>;  
Core Facility

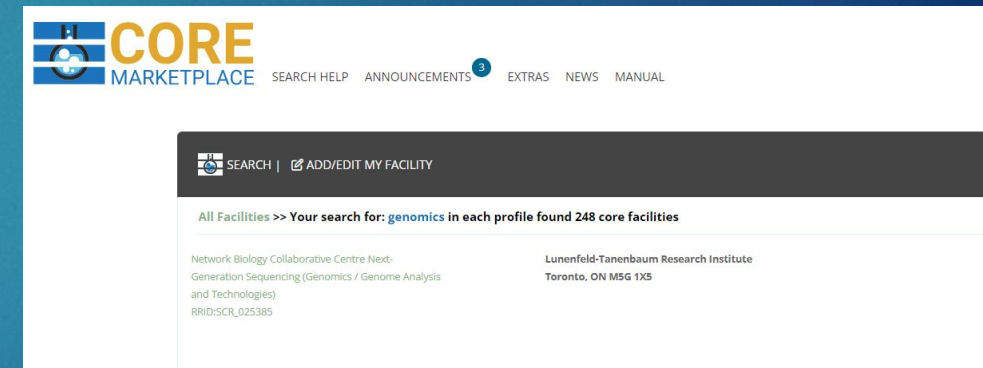


The screenshot shows the RRID Portal search interface. The search bar contains the keyword 'genomics'. Below the search bar, it indicates 'On page 1 showing 1 - 22 out of 419 results'. A blue banner message reads: 'Can't find your tool? Help us by registering it into the system - it's easy. Register it with the SciCrunch Registry. An RRID will be generated in 1-2 business day.' Below this, a search result is displayed for 'Vanderbilt University Center for Human Genetics Research Computational Genomics Core' with the RRID:SCR\_010173. The description states: 'THIS RESOURCE IS NO LONGER IN SERVICE, documented January 25, 2019. Core provides software and hardware support for computing activities related to genetics and biology, as well as statistical analysis for human genetics data generated from both microsatellite markers and SNPs. Bioinformatics support, resources, and expertise are available in storing and managing demographic, clinical, genotypic, microarray proteomic and biospecimen data.'

419 results

## Core Marketplace: Genomics

<https://coremarketplace.org>  
Genomics Core Facility



The screenshot shows the Core Marketplace search interface. The search bar contains the keyword 'genomics'. Below the search bar, it indicates 'All Facilities >> Your search for: genomics in each profile found 248 core facilities'. Below this, two search results are displayed: 'Network Biology Collaborative Centre Next-Generation Sequencing (Genomics / Genome Analysis and Technologies)' with RRID:SCR\_025385, and 'Lunenfeld-Tanenbaum Research Institute' with RRID:SCR\_025385.

248 results

Synchronization  
Single Entity

# RRID Links

RRID: Crystallography

<https://rrid.site/>: Crystallography

Results

<https://rrid.site/>: Results

The screenshot shows the RRID Portal search interface. The search term 'crystallography' has been entered, and the results page displays 118 records. A message indicates that a resource has been added to a collection: 'UNC School of Medicine Macromolecular X-Ray Crystallography Core Facility' with RRID:SCR\_012327. The URL for this resource is provided as <http://www.scienceexchange.com/facilities/macromolecular-x-ray-crystallography-core-facility-2>.

Collections		
Name	Records	Actions
Default Collection	0	
Link_rot	42	
Good_link	56	

[Create New Collection](#)

**Funding Model  
To Support Upkeep**

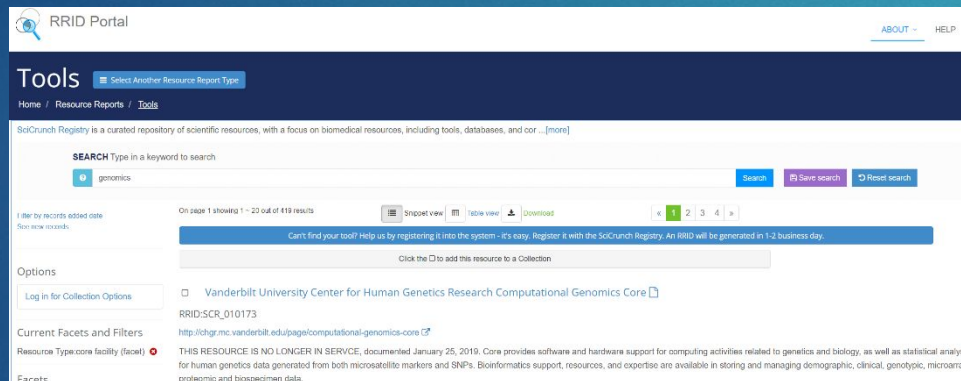
Top 100 results



# RRID Completeness

## RRID: Genomics

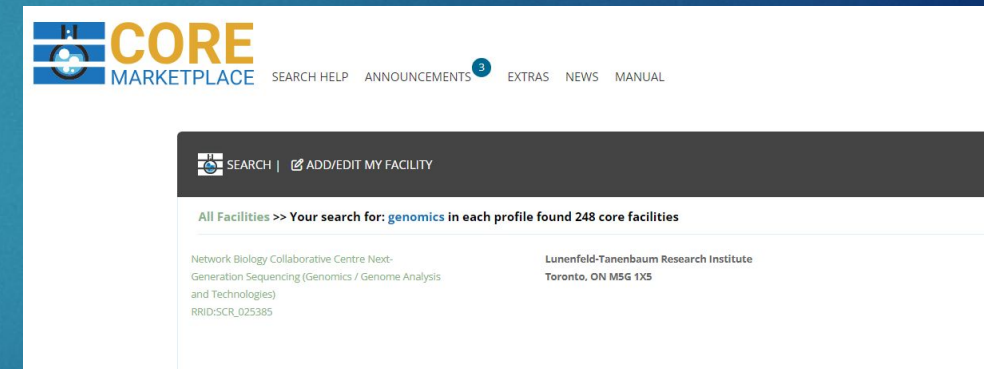
<https://rrid.site/Genomics>;  
Core Facility



100% RRIDed

## Core Marketplace: Genomics

<https://coremarketplace.org>  
Genomics Core Facility



74% RRIDed

Monetization or Funding  
To Support Upkeep

# RRID Citation

## RRID: Genomics

<https://rrid.site/>  
Genomics; Core Facility

”  
“

68.5% Non-zero  
(8.5% Double digit)  
31.5% Zero citation

## RRID: Flow Cytometry

<https://rrid.site/>  
Flow Cytometry; Core Facility

”  
“

66% Non-zero  
(6% Double digit)  
34% Zero citation

**User Awareness**  
**User Adoption**



# RRID Archival

RRID

<https://rrid.site/>

Core Marketplace

<https://coremarketplace.org>

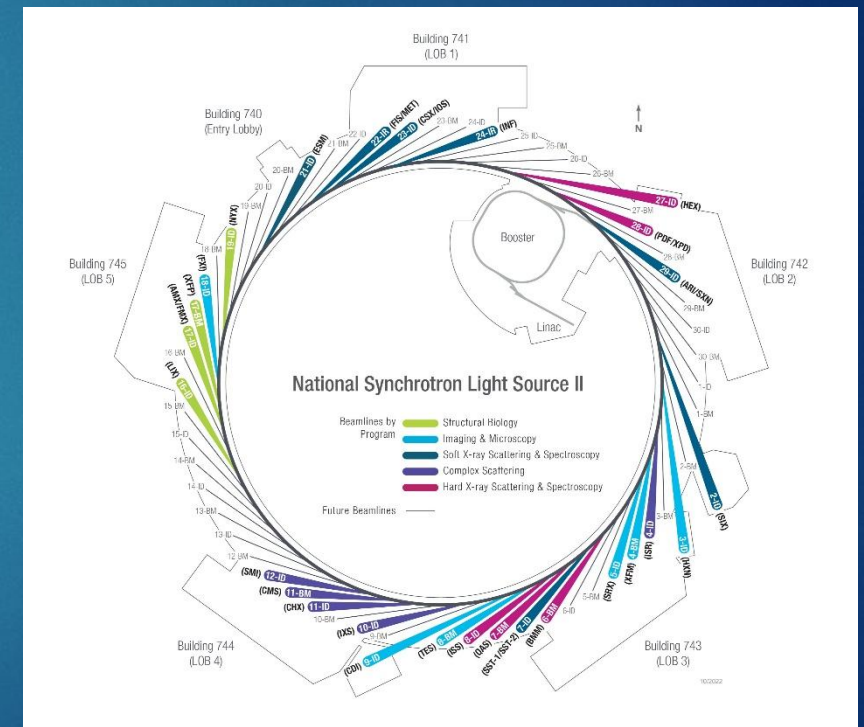
The screenshot shows the RRID Portal interface. At the top, there's a navigation bar with 'Tools' and a dropdown menu for 'Select Another Resource Report Type'. Below this, a search bar contains the keyword 'genomics'. The search results show one entry: 'Vanderbilt University Center for Human Genetics Research Computational Genomics Core' with the RRID:SCR\_010173. A message indicates that the resource is no longer in service, documented on January 25, 2019. The page also includes options for logging in, current facets, and a list of facets.

The screenshot shows the CORE Marketplace interface. At the top, there's a navigation bar with 'CORE MARKETPLACE', 'SEARCH HELP', 'ANNOUNCEMENTS', 'EXTRAS', 'NEWS', and 'MANUAL'. Below this, a search bar contains the keyword 'genomics'. The search results show 248 core facilities. One entry is highlighted: 'Network Biology Collaborative Centre Next-Generation Sequencing (Genomics / Genome Analysis and Technologies)' with the RRID:SCR\_025385. Another entry is 'Lunenfeld-Tanenbaum Research Institute' with the RRID:SCR\_025385.

Archival?  
Manufacturers  
Government Institutions  
Non-profit Consortia

# Missing: National and Regional Centers

- ▶ Brookhaven National Lab: National Synchrotron Light Source II
  - ▶ 32 Beamlines
    - ▶ Structural Biology
    - ▶ Imaging & Microscopy
    - ▶ X-Ray Scattering
    - ▶ X-ray Spectroscopy
  - ▶ Remote & In-person Experience
  - ▶ 1800 users/year
  - ▶ Acknowledgement Requested
  - ▶ RRID should be assigned to these facilities
- ▶ New York Structural Biology Center
  - ▶ NMR Facilities
  - ▶ Cryo EM Facilities
  - ▶ X-Ray Crystallography Facilities





# Missing: National and Regional Centers

- ▶ NHMFL: User Facilities
  - ▶ 7 User Facilities
    - ▶ Structural Biology
    - ▶ Materials Science
    - ▶ Physical and Chemical Sciences
    - ▶ Technique Development
    - ▶ Magnet Technology
  - ▶ Remote & In-person Experience
  - ▶ 1800 users/year
  - ▶ Acknowledgement Requested
  - ▶ RRID should be assigned to these facilities



# Monetization

- ▶ Monetization & Archival
  - ▶ Instrument Manufacturers
    - ▶ Only place to get instrument details
    - ▶ No incentive to keep old data
    - ▶ Information is lost for ever
  - ▶ Government Entities
    - ▶ Rigor and reproducibility
    - ▶ Fund Tracking
    - ▶ Ideal
  - ▶ Non-profit Consortium
    - ▶ All of you here
    - ▶ Another option to archive



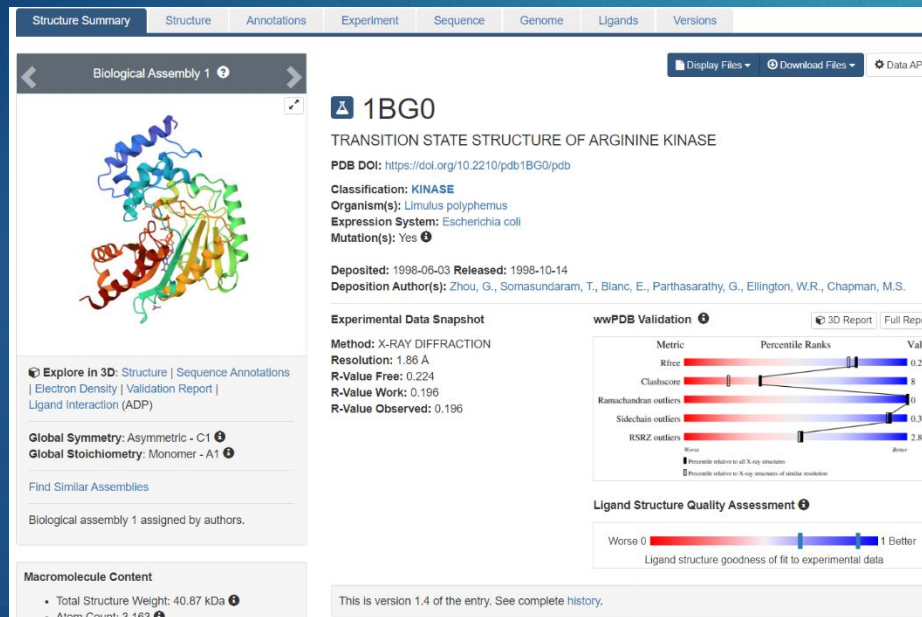
# Journal Usage of RRID

- ▶ Acta Crystallography: A,B,C,D,E, F; not a single mention of RRID 2014-2024
- ▶ Cell (160 Sample RRIDs no Facility RRID;)
- ▶ Biochemistry 2023
  - ▶ 30 Articles
  - ▶ 11 mention Facilities
  - ▶ 18 antibodies/chemicals
- ▶ Antibodies and Chemicals dominate the literature
- ▶ Very little Core Facility mentions despite adoption

# VERSIONING

## PDB Example

<https://www.rcsb.org/structure/1BG0>



Structure Summary | Structure | Annotations | Experiment | Sequence | Genome | Ligands | Versions

Biological Assembly 1

### 1BG0

TRANSITION STATE STRUCTURE OF ARGININE KINASE

PDB DOI: <https://doi.org/10.2210/pdb1BG0/pdb>

Classification: **KINASE**

Organism(s): *Limulus polyphemus*

Expression System: *Escherichia coli*

Mutation(s): Yes

Deposited: 1998-06-03 Released: 1998-10-14

Deposition Author(s): Zhou, G., Somasundaram, T., Blanc, E., Parthasarathy, G., Ellington, W.R., Chapman, M.S.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.86 Å

R-Value Free: 0.224

R-Value Work: 0.196

R-Value Observed: 0.196

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree		0.211
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		2.8%

Ligand Structure Quality Assessment

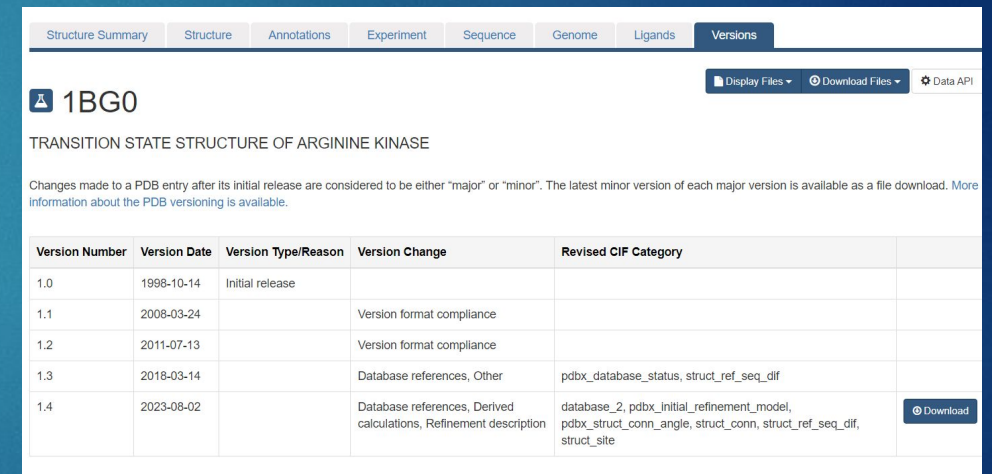
Worse 0 | 1 Better

Ligand structure goodness of fit to experimental data

This is version 1.4 of the entry. See complete history.

## Versioning

<https://www.rcsb.org/versions/1BG0>



Structure Summary | Structure | Annotations | Experiment | Sequence | Genome | Ligands | Versions

### 1BG0

TRANSITION STATE STRUCTURE OF ARGININE KINASE

Changes made to a PDB entry after its initial release are considered to be either "major" or "minor". The latest minor version of each major version is available as a file download. More information about the PDB versioning is available.

Version Number	Version Date	Version Type/Reason	Version Change	Revised CIF Category	
1.0	1998-10-14	Initial release			
1.1	2008-03-24		Version format compliance		
1.2	2011-07-13		Version format compliance		
1.3	2018-03-14		Database references, Other	pdbx_database_status, struct_ref_seq_dif	
1.4	2023-08-02		Database references, Derived calculations, Refinement description	database_2, pdbx_initial_refinement_model, pdbx_struct_conn_angle, struct_conn, struct_ref_seq_dif, struct_site	<a href="#">Download</a>



# VERSIONING

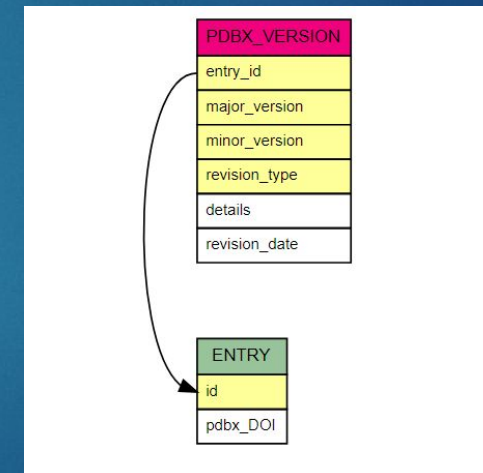
## PDB Example

<https://www.rcsb.org/structure/1BG0>

The screenshot shows the PDB website for entry 1BG0. The main title is "1BG0" and the description is "TRANSITION STATE STRUCTURE OF ARGININE KINASE". The PDB DOI is <https://doi.org/10.2210/pdb1BG0/pdb>. The classification is KINASE, and the organism is Limulus polyphemus. The expression system is Escherichia coli. The deposition date is 1998-06-03 and the release date is 1998-10-14. The deposition author(s) are Zhou, G., Somasundaram, T., Blanc, E., Parthasarathy, G., Ellington, W.R., Chapman, M.S. The experimental data snapshot shows the method as X-RAY DIFFRACTION, resolution as 1.86 Å, R-Value Free as 0.224, R-Value Work as 0.196, and R-Value Observed as 0.196. The wwPDB Validation section shows a bar chart of metrics: R-fact, Clashscore, Ramachandran outliers, Sidechain outliers, and BSRZ outliers. The Ligand Structure Quality Assessment section shows a bar chart of ligand structure goodness of fit to experimental data.

## Versioning

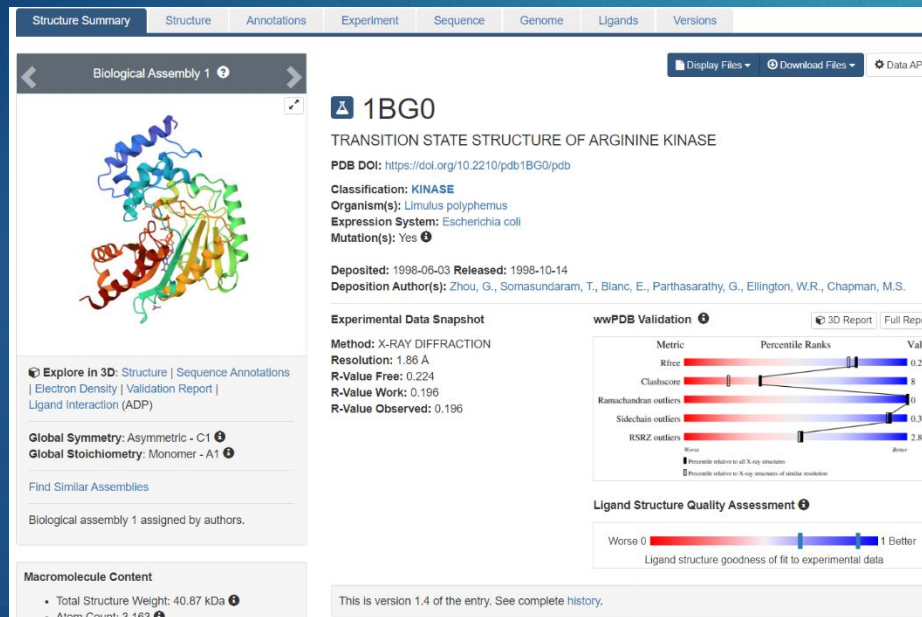
<https://www.rcsb.org/versions/1BG0>



# EXTENSION

## PDB Example

<https://www.rcsb.org/structure/1BG0>



The screenshot displays the PDB entry page for 1BG0. The main title is "1BG0" with the subtitle "TRANSITION STATE STRUCTURE OF ARGININE KINASE". The PDB DOI is <https://doi.org/10.2210/pdb/1BG0/pdb>. The classification is KINASE, the organism is Limulus polyphemus, and the expression system is Escherichia coli. The entry was deposited on 1998-06-03 and released on 1998-10-14. The authors are Zhou, G., Somasundaram, T., Blanc, E., Parthasarathy, G., Ellington, W.R., and Chapman, M.S. The experimental data snapshot shows X-RAY DIFFRACTION with a resolution of 1.86 Å, R-Value Free of 0.224, R-Value Work of 0.196, and R-Value Observed of 0.196. The wwPDB Validation section includes a bar chart for Percentile Ranks and a Ligand Structure Quality Assessment section.

Metric	Percentile Ranks	Value
Rfree		0.211
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.3%
RSRZ outliers		2.8%

Worse	0	1	Better
Ligand structure goodness of fit to experimental data			

## Extension

<https://www.rcsb.org/extension>

### Extended PDB accession codes

To plan for future growth of the PDB archive and to more closely conform with the "Findability" principle of the FAIR data management, we have extended the PDB accession codes from the familiar four character style to 8 characters prefixed with "pdb". For example, PDB accession code for entry `1abc` becomes `pdb_00001abc`. This new format of PDB accession codes will be included in the coordinate files at a later date. The versioned FTP tree uses the extended PDB accession codes in file naming.



# PID Core Example: IMB XRF

- ▶ IMB XRF
  - ▶ Established in 1993
  - ▶ RRID: SCR\_01792 (For the Facility) ~2020 or 2021
  - ▶ Multiple Core Instruments
    - ▶ Generators, Monochromators, Detectors, Cryo adaptors, Table Extensions, Safety enclosures, Helium tunnels, etc.,
  - ▶ Some stayed the same since 1993
  - ▶ Many had additions and modifications
    - ▶ How to handle it? Versioning; Won't it complicate the simplicity?
  - ▶ Several accessories
    - ▶ Newer, older, surplus; How to handle decrepit devices?
  - ▶ What the RRID signifies?
    - ▶ Facility: Simple but not accurate or complete
    - ▶ Instruments: Multiple but accurate
  - ▶ Adoption
  - ▶ Calibration

# PIDs and Cores

QUESTIONS?

**Thayumanasamy**

**Somasundaram**

<https://fla.st/2J0DKH5D>

[tsomasundaram@fsu.edu](mailto:tsomasundaram@fsu.edu)

**FSU** | **INSTITUTE OF**  
**MOLECULAR BIOPHYSICS**  
COLLEGE OF ARTS & SCIENCES





# Simple and Clean Web Interface

The screenshot displays the 'SCIENTIFIC EQUIPMENT' portal. At the top, there is a search bar with the text 'Search Scientific Equipment' and a magnifying glass icon. To the right of the search bar are links for 'View All' and 'Reset'. Below the search bar, the word 'OR' is centered. There are three dropdown menus for filtering: 'Group' (set to 'Any'), 'Facility' (set to 'Any'), and 'Department' (set to 'Any'). A red 'GO!' button is positioned to the right of these filters. Below the filters, a list of equipment items is displayed in three columns. The first column lists various pieces of equipment, the second lists facilities, and the third lists departments.

Group	Facility	Department
AUTOCLAVE	ANALYTICAL LAB (BIO)	Biological Science
BALANCE	BIO CORE FACILITIES	Chemical Engineering
BATTERY TESTER	BIOLOGICAL SCIENCE IMAGING RESOURCE	Chemistry & Biochemistry
BIKE	CHEMISTRY NMR LAB	College of Medicine MRI
BINDING ASSAY	CONDENSED MATTER & MATERIALS PHYSICS	
BIOANALYZER	CONFOCAL MICROSCOPY LABORATORY	
BODY COMPOSITION TESTER	DNA SEQUENCING LAB (BIO)	
CALORIMETER	FLOW CYTOMETRY LAB (COM)	
CAMERA	HIGH PERFORMANCE MATERIALS INSTITUTE (HPMI)	
CARBON COATER	IMB COMMON LAB	
CELL CLUSTER GENERATOR	MASS SPEC LAB (CHEM)	
CELL FRENCH PRESS		
CELL STORAGE		
CENTRIFUGE		

© Florida State University  
Tallahassee, FL 32306

FSU Directory Assistance  
Questions or Comments

Privacy Policy  
Copyright

Facebook, Instagram, Twitter, YouTube, LinkedIn, Plus icons



Description and keywords

Name, model number

View images

Make a suggestion

**Title:** CRYSTALLIZATION INCUBATOR 400L

✓ Active

**Group:** INCUBATOR

**Location:** KASHA LABORATORY 0412

**Manufacturer:** MOLECULAR DIMENSIONS

**Availability:** ALL DAY

**Department:** Inst of Molecular Biophysics

**Contact Name:** THAYUMANASAMY SOMASUNDARAM

**Facility:** X-RAY CRYSTALLOGRAPHY FACILITY

**Keyword(s):** INCUBATOR, CRYSTALS, VIBRATION FREE

**Description:** VIBRATION-FREE INCUBATOR SUITABLE FOR CRYSTAL GROWTH. 400 L CAPACITY. ONLINE ACCESS.



More

**Title:** CRYSTALLIZATION ROBOT

✓ Active

**Group:** X-RAY DIFFRACTION

**Location:** KASHA LABORATORY 0412

**Manufacturer:** ART ROBBINS

**Availability:** SCHEDULED

**Department:** Inst of Molecular Biophysics

**Contact Name:** THAYUMANASAMY SOMASUNDARAM

**Facility:** X-RAY CRYSTALLOGRAPHY FACILITY

**Keyword(s):** CRYSTALLIZATION, ARI, GRYPHON, AUTOMATED, LIQUID SYSTEM

**Description:** AUTOMATED ARI GRYPHONCRYSTALLIZATION ROBOT



More

**Title:** FORMULATOR 16 W/PUMP BOX

✓ Active

**Group:** FORMULATOR

**Location:** KASHA LABORATORY 0412

**Manufacturer:** FORMULATRIX

**Availability:** SCHEDULED

**Department:** Inst of Molecular Biophysics

**Contact Name:** THAYUMANASAMY SOMASUNDARAM

**Facility:** X-RAY CRYSTALLOGRAPHY FACILITY

**Keyword(s):** CUSTOM BUFFERS, NEW FORMULATIONS, CRYSTALLIZATION

**Description:** CUSTOM BUFFER PREPARATION FORMULATOR



More

# Equipment Details

# Search Results





## Data

Example of raw data from controller														
TAG_NUMBE	Descr	Acq Date	DeptID	Dept Desc	Fund	Project	Cost	Accur	NBV	Asset ID	Long Descr	Location	Loc Descr	Building
492000431586	Air Permeability Tester	7/26/2018	134000	Dept Retail	110		20868.890	#####	11130.07	000000097522	Air Permeabil	01350307	SANDELS BUIL	0069
492000433268	TruBurst4 1440 Strength Tester	8/19/2021	625000	Moran Col	140		23261.000	#####	18996.48	000000100958	TruBurst4 144	01350307	SANDELS BUIL	9021
492000431166	Instron 5965 Tensile Testing	3/27/2018	625000	Moran Col	110		46702.540	#####	22183.71	000000096681	Instron 5965 T	01350307	SANDELS BUIL	6046
492000414965	MARTINDALE ABRASION & P-TESTER	4/18/2008	134000	Dept Retail	140		12439.000	#####	0.00	000000073812		01350307	SANDELS BUIL	0069
Example rearranged data														
ASSET_TAG	DESCRIPTION	ASSET_TYPE	ASSET_GROUP	STATUS	TAG_NUMBER	REGION_CODE	FAC_ID	BLDG	LOCATION_CODE	MANUFACTURE_CODE	MODEL_NO	SERIAL_NO	EXTRA_DESC	PURCHASE_PRICE
000000097522	SDL Atlas Air Permeability Tester	SCI_RESEARCH	Air Permeability	In Service	492000431586	TALL	MAIN CAMPUS	0135	0307	ATLAS	M021A	021Q0004		\$20,868.89
000000100958	James Heal Bursting Strength Tester	SCI_RESEARCH	Strength Tester	In Service	492000433268	TALL	MAIN CAMPUS	0135	0307	PPT Group Corp / James Heal	1440	1440/21/1257		\$23,261.00
000000096681	Instron 5965 Tensile Testing	SCI_RESEARCH	Tensile Tester	In Service	492000431166	TALL	MAIN CAMPUS	0135	0307	Instron		5965B15859		\$46,702.54
000000073812	MARTINDALE ABRASION & TESTER	SCI_RESEARCH	Abrasion Tester	In Service	492000414965	TALL	MAIN CAMPUS	0135	0307	ATLAS		NONE		\$12,439.00



## Simple Goal

- Create and maintain a searchable FSU-Wide Shared Equipment Database
- Assist Faculty, Students, Staff to find local resources
- Connect Core Facility Experts with users
- 550 Shared Equipment listed
- Minimal cost: 20 weeks/per year, 10 h/week, \$20/h; \$4000/year
- Four undergrads since 2017
- Update to date since 2016 - Summer 2024
- Provost and VP-R have funded it since 2016