

How to Administer a PGDB

Getting Ready to Release

- **Decide on release frequency**
 - Don't wait until it's perfect to release it!
- **Run consistency checker**
 - Also updates organism-summary statistics
- **Update publications, authors in organism frame**
 - Right-click on organism, Edit->Frame Editor
- **Update Overview**
- **Deposit PGDB in SRI PGDB registry**
 - Will allow SRI to include it in BioCyc
- **Create new version of PGDB**
 - Edit against the new version, old version visible through web site
 - How to ensure web server sees right version?
- **Author release notes**

Administering the Web Server

- Web server is written entirely in Lisp!
- May need to restart server periodically
- We use website monitor to page admin when site is down
- <http://xyzcyc.org/load-patches>
- <http://xyzcyc.org/purge-cache>
- **When an error occurs:**
 - (setf cwest::*debug?* t) to enter debugger

Using RDBMS for Storage

- **Either Oracle or MySQL**
- **Enable concurrent multi-user updates**
- **Backup KB to File command from Pathologic**
- **Show Changes**
 - Lists all changes for a particular database object in reverse chronological order
 - Internal Ocelot representation of changes

Show Changes

History of changes to PRTRANS-RXN

The log contains the following operations on the frame PRTRANS-RXN.

| User Id | TID | Merge time | Operation |
|---------|-------|-----------------------|--|
| paley | 18246 | 05/03/2006 @ 17:24:08 | (PUT-SLOT-VALUES PRTRANS-RXN RIGHT (ANTHRANILATE PRPP) :SLOT-TYPE :AUTO) |
| paley | 18246 | 05/03/2006 @ 17:24:08 | (PUT-SLOT-VALUES PRTRANS-RXN LEFT (N-(5-PHOSPHORIBOSYL)-ANTHRANILATE PPI) :SLOT-TYPE :AUTO) |
| kr | 12632 | 04/07/2005 @ 17:10:56 | (PUT-SLOT-VALUE PRTRANS-RXN BALANCE-STATE :BALANCED :SLOT-TYPE :AUTO) |
| caspi | 12212 | 02/24/2005 @ 17:16:37 | (REMOVE-SLOT-VALUE PRTRANS-RXN IN-PATHWAY |

Dismiss

Update Propagation

- **New version of Pathway Tools includes updates to MetaCyc**
 - New/updated compound structures, names, synonyms
 - Updated reaction substrates, EC numbers
 - Updated pathways
 - ◆ names, reactions, layout
 - ◆ pathways may be split into sub-pathways
 - New pathways, reactions, compounds
 - Duplicate reactions, compounds merged
- **Automated schema upgrade does not propagate any of these changes**

Update Propagation

- **(propagate-updates-from-metacyc orgids)**
 - Internal tool – not user-tested!
 - Assumes any differences are due to changes in MetaCyc
 - Propagates only selected slots
 - Logs all changes, suggested changes – check results carefully!
 - Updates compounds, reactions
 - Updates pathway names, but not topology
 - Reports on differences in topology
 - Does not infer any new pathways
 - Work in progress!