

PGDB

• OUR ~~WEDDING~~ REGISTRY. •

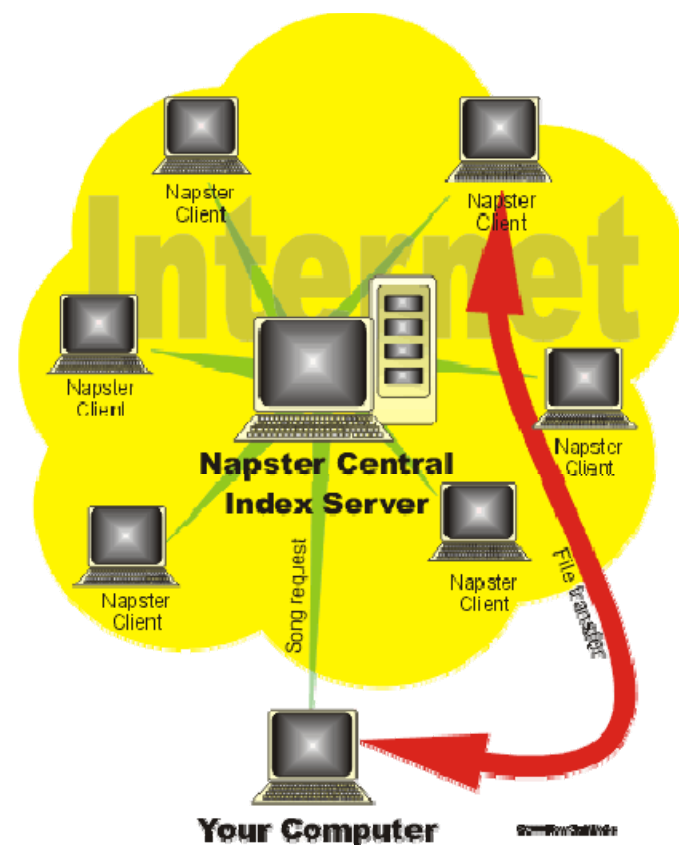
By Ron Caspi



This presentation can be found at
<http://bioinformatics.ai.sri.com/ptools/tutorial/sessions/>

The PGDB Registry

- The PGDB Registry is an Internet-based mechanism for sharing PGDBs among Pathway Tools users.
- The Registry itself is a server operating at SRI that lists the set of available PGDBs. It does not actually contain the PGDBs.
- The PGDBs reside at sites maintained by the users who chose to register them.
- All of the BioCyc PGDBs, plus many more, are available at the Registry



Accessing The Registry



Tools

- Answer List
- Browse PGDB Registry**
- Consistency Checker
- Dead-end Metabolite Finder...
- Chokepoint Reaction Finder...
- Flux Balance Analysis...
- History
- Instant Patch
- Ontology Editor
- Pane
- PathoLogic **CTRL+t**
- Preferences
- Prepare BLAST Reference Data
- Propagate MetaCyc Data Updates
- Publish DBs
- Regulatory Network...
- Search
- Reachability Analysis...
- Upgrade Schema of All DBs

Pathway Genome Database (PGDB) Registry

Find Organism PGDBs:

Organism Subspecies Strain Tier

Type in a search string of at least 3 characters followed by a return ...

Selected PGDBs:

Fetch and Install Selected PGDBs

Cancel

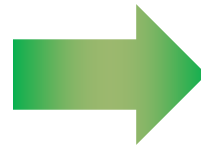
Searching for PGDBs



Pathway Genome Database (PGDB) Registry

Find Organism PGDBs:

| Organism | Subspecies | Strain | Tier |
|--|------------|--------|------|
| <i>Type in a search string of at least 3 characters followed by a return ...</i> | | | |



Pathway Genome Database (PGDB) Registry

Find Organism PGDBs:

Search string **coli** found **170** organism entries:

| Organism | Subspecies | Strain | Tier |
|---------------------------|------------|-----------|------|
| Amycolobicoccus subflavus | | DQS3-9A1 | 3 |
| Amycolobicoccus subflavus | | DQS3-9A1 | 3 |
| Anaerotruncus colihominis | | DSM 17241 | 3 |
| Brachyspira pilosicoli | | 95/1000 | 3 |
| Brachyspira pilosicoli | | B2904 | 3 |
| Brachyspira pilosicoli | | P43/6/78 | 3 |
| Brachyspira pilosicoli | | WesB | 3 |
| Campylobacter coli | | 15-537360 | 3 |
| Campylobacter coli | | 76339 | 3 |
| Campylobacter coli | | JV20 | 3 |
| Escherichia coli | | 042 | 3 |
| Escherichia coli | | 101-1 | |
| Escherichia coli | | 1827-70 | |
| Escherichia coli | | 2362-75 | |
| Escherichia coli | | 3431 | |
| Escherichia coli | | 4_1_47FAA | 3 |
| Escherichia coli | | 536 | 3 |

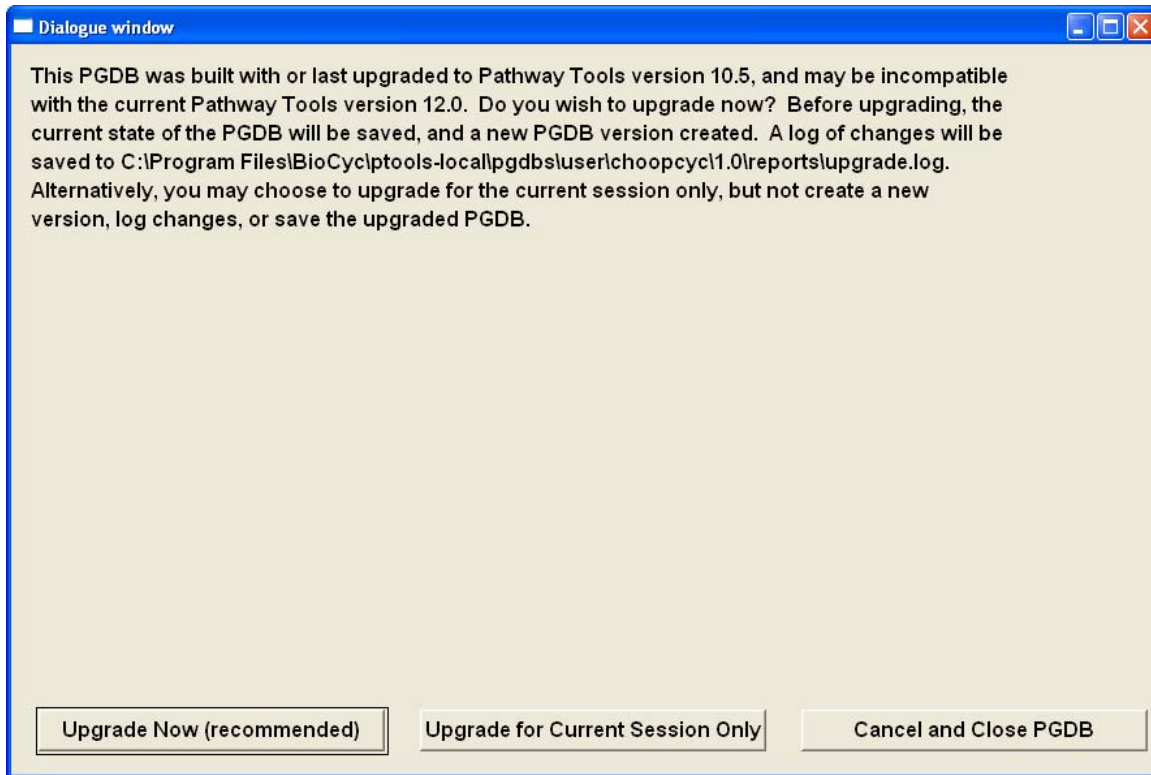
Downloading from The Registry



- Select the desired PGDBs
- Click on the “Fetch & install selected PGDBs” button
- Agree to Terms and Conditions
- Wait...

- The tar.gz file would be downloaded and decompressed, and the uncompressed files will be copied to their destination (ptools-local/pgdbs/registry/dbname)
- Once the process is done, the software will notify you, and you can start using the new PGDB (unless a schema upgrade is required...)

Schema Upgrades



Publishing a PGDB – The Process

The process of publishing a PGDB involves three steps:

- The directories and files that make up the PGDB are packaged and compressed into a single archive file.
- The packaged file is moved to a Web server or an FTP server on a site of your choosing (usually one maintained by your organization) that allows anonymous access for retrieval of stored files.
- The PGDB is registered with the SRI registry server, from which it is visible to Pathway Tools users across the Internet.

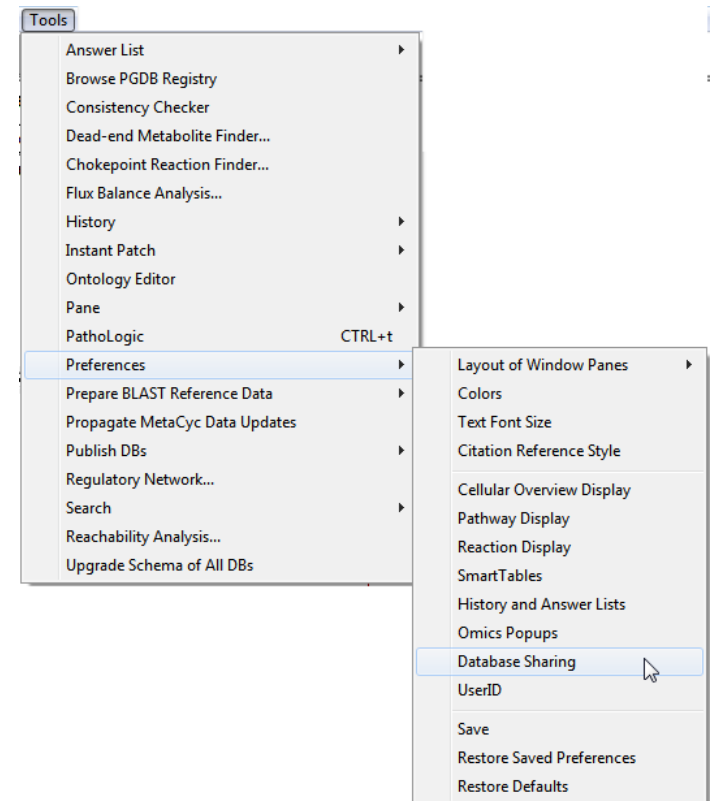


Publishing a PGDB – Preliminary Step

The process of uploading a PGDB to the Registry is largely automated.

However, before this can be done, the user needs to answer some **technical** questions about their FTP/Web server.

Tools → Preferences → Database Sharing



Preliminary Step: Setting Preferences

You will need to answer the following two questions:

Note: if you answer “No” to the first question, you will need to move the packaged files yourself to the location where the files will be available to the public.



Will you be able to use Pathway Tools to upload your archived databases to your FTP site using FTP?

Yes No

For some FTP servers, the directory to which you upload the file is different from the directory from which users will download the file. In that case, the file must be manually moved between directories after uploading is completed. Depending upon file security settings, it may be possible for you to move the file, or you may need to request that your System Administrator move the file.

After uploading, is it necessary to move uploaded files to a different location within the FTP server before the files can be downloaded?

Yes No

Preliminary Step: Setting Preferences

Depending on how you answered these questions, you will see either this (if you answer “Yes” to the first question):

Database sharing settings

NOTE: These settings are relevant only if you intend to publish one or more of your PGDBs using the Pathway Tools database sharing facility. If you do not intend to publish any of your PGDBs, click "Cancel" to exit this dialog.

Enable PGDB sharing functionality

Rerun initial setup

Settings for uploading via FTP:

FTP server to which archive files will be uploaded: localhost

Username for uploading to the FTP server above: ftp

Directory to which archive files will be uploaded: incoming

How remote users will retrieve your archived databases from your server.
Enter in URI format, such as ftp://ftp.orgs-r-us.com/orgs/
or http://www.orgs-r-us.com/orgs/:

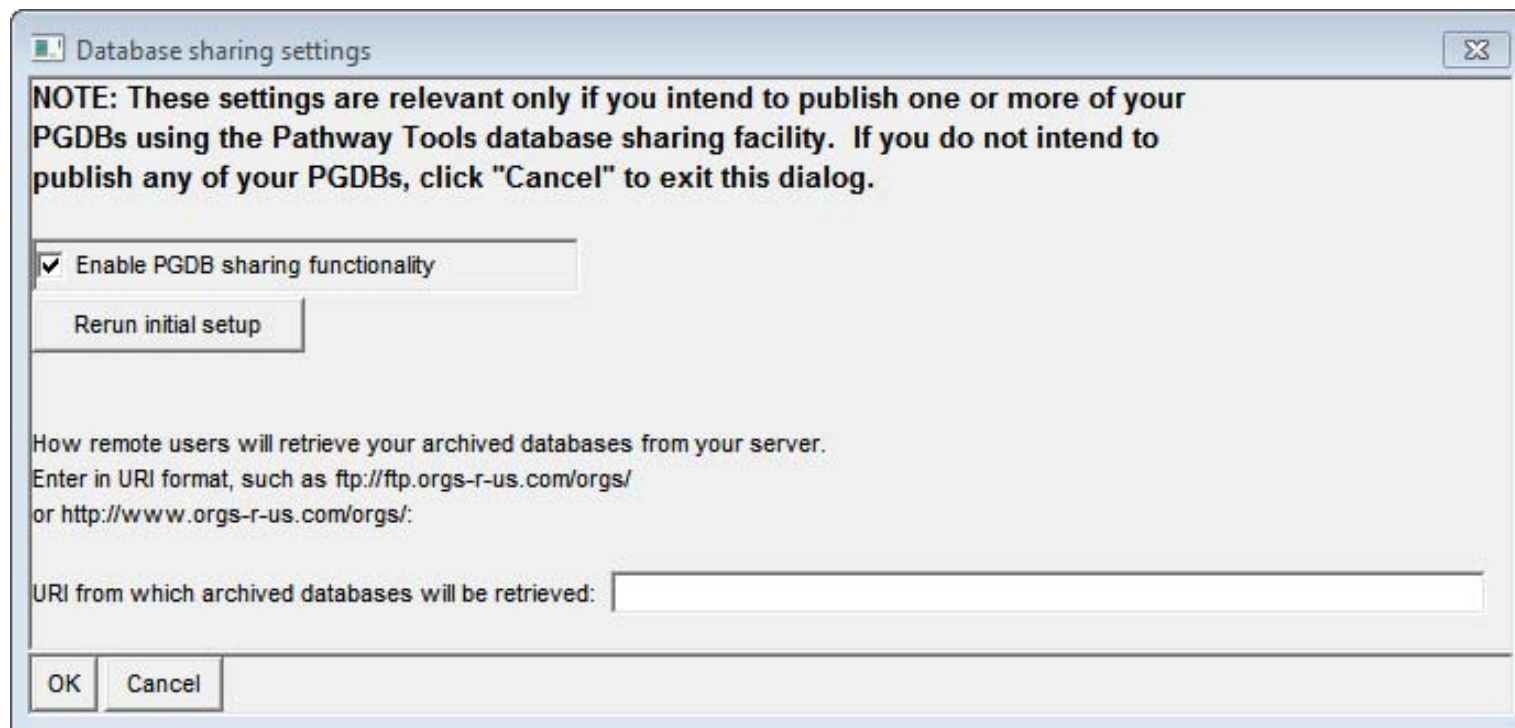
URI from which archived databases will be retrieved:

OK Cancel



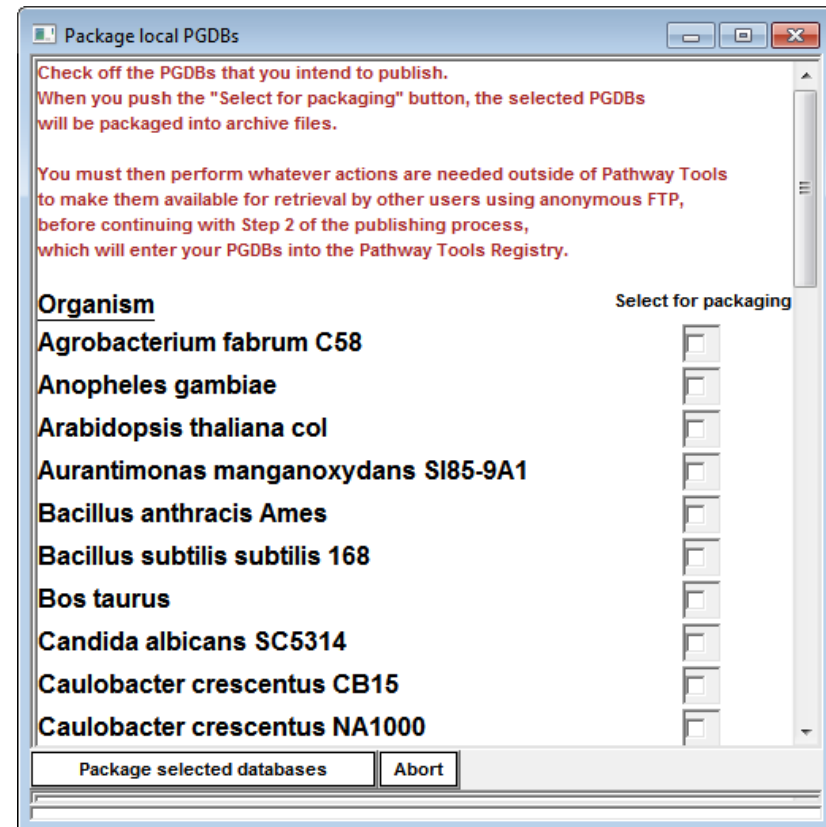
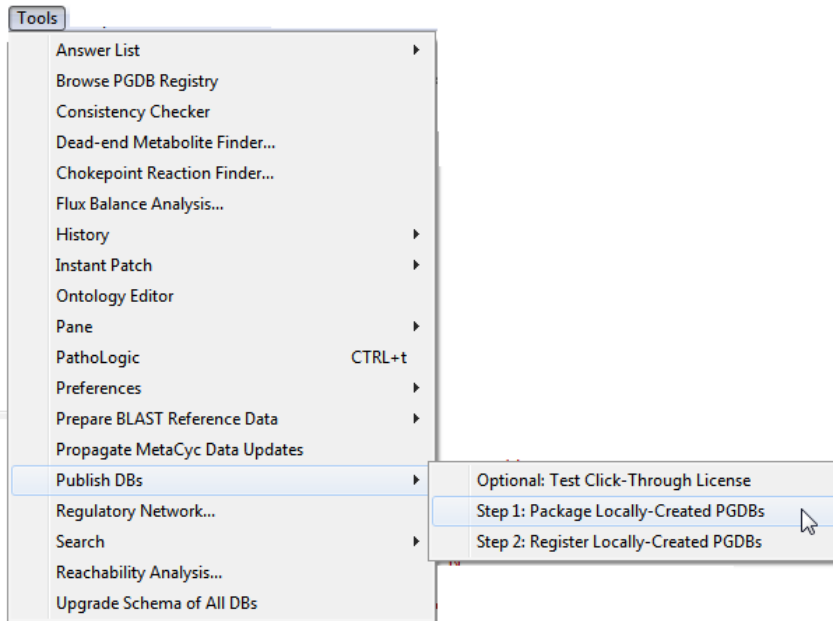
Preliminary Step: Setting Preferences

Or this, if you answer “No” to the first question:



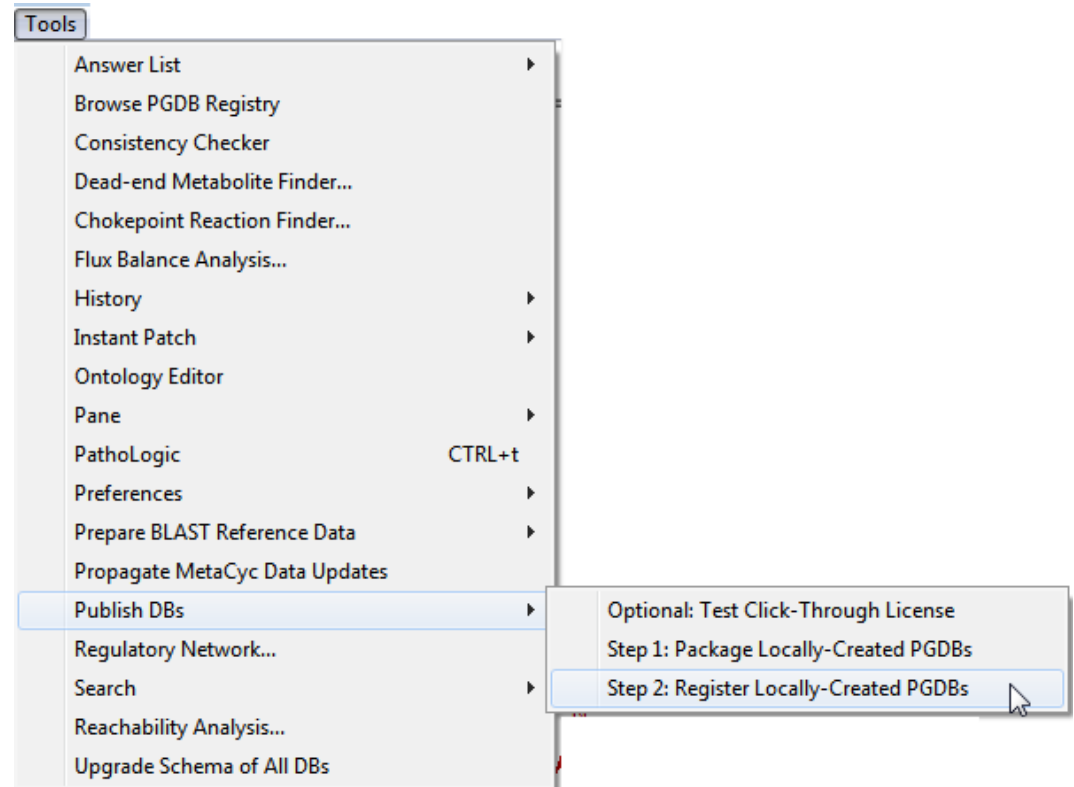
Publishing a PGDB – Packaging

- The process is started by Tools → Publish DBs → Step 1
- Depending on your setup, you may have to manually move the files that are generated during this step to its final location



Publishing a PGDB – Registering

Last step: Registering
PGDBs with the SRI Registry
(Step 2)



See “Publishing PGDBs in the Registry” in the User Guide for more details