Simple Usage
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Chapter 1  Introduction

We developed an open source laboratory information management system for 2-D gel electrophoresis-based proteomics workflow. The software development project is served by Proteomics Collaboration Research Group members, Tokyo Metropolitan Institute of Gerontology. This new LIMS is licensed under GNU Lesser General Public License. The LIMS is carried out as PostgreSQL-PHP-apache system on Linux OS. We explain how to use the LIMS.

In order to begin with this program, open the Proteomics LIMS module window of your PC. This Proteomics LIMS system can be used only by a registered user inputting “User name” and “Password”. This is the system which creates a synthetic analysis by inputting user's research data and related information to each unit.

Chapter 2  Add 1&2DE-gel data, Digestion plate data, MS plate and 2DEPAGE map data

Open the window of “Home” including “Add or update 1&2DE-gel data”, “Add or update digestion plate data”, “Add or update MS plate data” and “Add or update 2DPAGE map data”.

At first, enter the User name (ex. morisawa), Password (****) and 1&2-gel ID (ex. mori_test) in each box, and click on “Go” button (Fig.1). Then the window of “Add 1&2DE-gel data of mori_test” appears. In this window, enter “1&2DE-gel name (ex. mori_test gel)”, and click on “Add new gel data” button (Fig.2). Then the window of “Saved data is OK!” appears, and click on “Upload gel image file or gel image icon file”
link button (Fig.3). Then the window of “Update or delete 2DE-gel data of mori_test” appears. In this window, input experimental data to each item, and upload 2DE-gel image and 2DE-gel icon. 2DE-gel icon (width:120 pixel) must be prepared by users. Uploading a TIFF image instead of a JPEG image causes an error. Check the uploaded gel image and gel icon (Fig.4).
Secondly in the “Home” window, enter the User name (ex. morisawa), Password (****) and Digestion plate ID (ex. mori_test) in each box, and click on “Go” button (Fig.1). Then the window of “Add digestion plate data of mori_test” appears. In this window, enter each item, and click on “Add digestion plate data” button (Fig.5). Then the window of “Digestion plate map of mori_test” appears (Fig.6).
Thirdly in the “Home” window, enter the User name (ex. morisawa), Password (****) and MS plate ID (ex. mori_test) in each box, and click on “Go” button (Fig.1). Then the window of “Add MS plate data of mori_test” appears. In this window, enter the each item, and click on “Add MS plate data” button (Fig.7). Then the window of “MS plate map of mori_test” appears (Fig.8).
Finally in the “Home” window, enter the User name (ex. morisawa), Password (****) and 2DEPAGE map ID (ex. mori_test) in each box, and click on “Go” button (Fig.1). Then the window of “Add Header and Map data” appears. In this window, input experimental data to each item, and click on “Add header and map data of 2DEPAGE” button (Fig.9). Then the window of “The addition of header data is OK! The addition of map data is OK!” appears. In this window, click on “Update the header of 2DPAGE map” link button (Fig.10). Then the window of “Update header data of 2DPAGE map: mori_test” appears. In this window, enter the each item, and upload 2DE-gel image and 2DE-gel icon. Moreover, copy 2DE-Gel data by gel ID and 2DE-Gel data by analysis set ID. Check the uploaded gel image and gel icon (Fig.11).
Fig. 9

Fig. 10
Fig. 11
Chapter 3  Add and update protocol data

Open the window of "Protocol home" including "Add or update material data", "Add or update gel method data" and "Add or update analysis method data".

![Fig.12](image1.png)

At first, enter the User name (ex. morisawa), Password (****) and Material ID (ex. mori_test) in each box, and click on "Go" button (Fig.12). Then the window of "Add material data of mori_test" appears. In this window, enter the each item, and click on "Add material data" button (Fig.13). Then the window of "The insert of data is OK!" appears. In this window, click on "Material list" link button. Then the window of "Material list" appears.

![Fig.13](image2.png)
In this window, click on “Material ID (ex. Mat_Astro)” link button (Fig.14). Then the window of “Login for material” appears. Enter the Password (****), and click on “Update or delete material data “ button (Fig.15). Then the window of “Update or delete material data” appears. In this window, input experimental material data in each box, and update or delete material data (Fig.16). In addition, click on “Insert in 2DEPAGE map data” button, and then “2DPAGE map list” appears. In this window, click on the user’s gel icon (ex. Mat_Astro) (Fig.17). Then the window of “Login for 2DPAGE map (the insert of material data)” appears. Enter the Password (****), and click on “Update 2DPAGE map data (the insert of material data)” button (Fig.18). Then the window of “Update Map Data of Mat_Astro” appears. Input the data in each box, and click on “Update 2DPAGE map data” (Fig.19).
Secondly in the “Protocol home” window, enter the User name (ex. morisawa), Password (****) and Gel method ID (ex. mori_test) in each box, and click on “Go” button (Fig.12). Then the window of “Add gel method data of mori_test” appears. In this window, enter the each item, and click on “Add gel method data” button (Fig.20). Then the window of “The insert of data is OK!” appears. In this window, click on “Gel method list” link button. Then the window of “Gel method list” appears.

In the window, click on “Gel method ID (ex. Standard_2DE)” link button (Fig.21). Then
the window of “Login for gel method” appears. Enter the Password (****), and click on “Update or delete gel method data” button (Fig.22). Then the window of “Update or delete gel method data” appears. In this window, input experimental gel method data in each box, and update or delete gel method data (Fig.23). In addition, click on “Insert in 2DEPAGE map data” button, and then “2DEPAGE map list” appears. In this window, click on the user’s gel icon (ex. Mat_Astro) (Fig.24). Then the window of “Login for 2DEPAGE map (the insert of gel method data)” appears. Enter the Password (****), and click on “Update 2DEPAGE map data (the insert of gel method data)” button (Fig.25). Then the window of “Update Map Data of Mat_Astro” appears. Input the data in each box, and click on “Update 2DEPAGE map data” (Fig.26).
Finally in the “Protocol home” window, enter the User name (ex. morisawa), Password (****) and Analysis method ID (ex. mori_test) in each box, and click on “Go” button (Fig.12). Then the window of “Add analysis method data of mori_test” appears. In this window, enter the each item, and click on “Add analysis method data” button (Fig.27). Then the window of “The insert of data is OK!” appears. In this window, click on “Analysis method list” link button. Then the window of “Analysis method list” appears.

In the window, click on “Analysis method ID (ex. Toda_org)” link button (Fig.28). Then the window of “Login for analysis method” appears. Enter the Password (****), and click
on “Update or delete analysis method data” button (Fig. 29). Then the window of “Update or delete analysis method data” appears. In this window, input experimental analysis method data in each box, and update or delete analysis method data (Fig. 30). In addition, click on “Insert in 2DEPAGE map data” button, and then “2DPAGE map list” appears. In this window, click on the user’s gel icon (ex. Mat_Astro) (Fig. 31). Then the window of “Login for 2DPAGE map (the insert of analysis method data)” appears. Enter the Password (****), and click on “Update 2DPAGE map data (the insert of analysis method data)” button (Fig. 32). Then the window of “Update Map Data of Mat_Astro” appears. Input the data in each box, and click on “Update 2DPAGE map data” (Fig. 33).
Chapter 4  Component parts

4-1.  Home
The window of “Home” including “Add or update 1&2DE-gel data”, “Add or update digestion plate data”, “Add or update MS plate data” and “Add or update 2DPAGE map data”.
# Enter “User name”, “Password” and “ID number (1&2DE-gel ID, digestion plate, MS plate or 2DPAGE Map)”, and click on “Go” button.

4-2.  Keyword search
The window of “Keyword search” including “Search 1 & 2DE-gels for spot data”, “Search digestion plates for well data”, “Search MS plates for well data”, “Search 2DPAGE database for spot data” and “Search 2DPAGE database for spot data (graph of protein expression)”.  
# Search by terms. Enter the term in each box, and click on “Search” button (Fig.34).

4-3.  Editing workflow data
4-3-1. The window of “1&2DE-gel list” including “User name”, “1&2DE-gel ID”, 1&2DE-gel name”, “Date” and “Image” (Fig.35). If you select the 1&2DE-gel ID such as “Mat_Astro”, the window of “Login for 1&2DE-gel” will appear (Fig.36).
# Enter the Password for “Add, update or delete 1&2DE-gel spot data”, and then the window of “1&2DE-gel map of Mat_Astro” appears (Fig.37). When you want to make the new position on this window, detect the spot position by moving a pointing mouse cursor, and click on “Detect the spot position” button. Rectangular width can be changed in accordance with the size of the spot. Then the window of “Add spot data in 1&2DE-gel” appears, and input the data in each box (Fig.38). If you select the SSP number such as “2201” by moving a pointing mouse cursor, the window of “Update or delete spot data of 1&2DE-gel” will appear (Fig.39).
# Enter the Password for “Update or delete 1&2DE-gel data” (Fig.36). Then the window of “Update or delete 1&2DE-gel data of Mat_Astro” appears.
4.3.2. The window of “Digestion plate list” including “User name”, “Digestion plate ID”, “Digestion plate name” and “Date” (Fig.40). If you select the Digestion plate ID such as “Mat_Astro”, the window of “Login for digestion plate” will appear (Fig.41).
# Enter the Password for “Add, update or delete well data of digestion plate”, and then the window of “Digestion plate map of: Mat_Astro” appears (Fig.42). When you want to make the new position on this window, detect the well position by moving a pointing mouse cursor, and click on “Detect the well position” button. Then the window of “Add well data of digestion plate” appears, and enter the corresponding 1&2DE-gel ID and SSP number (Fig.43). If you select a Well ID such as “D5” by moving a pointing mouse cursor, the window of “Update or delete well data of digestion plate” will appear (Fig.44).

# Enter the Password for “Update or delete digestion plate data” (Fig.41). Then the window of “Update or delete digestion data of Mat_Astro” appears.
4.3.3. The window of “MS plate list” including “User name”, “MS plate ID”, “MS plate name” and “Date” (Fig.45). If you select the MS plate ID such as “Mat_Astro”, the window of “Login for MS plate” will appear (Fig.46).
# Enter the Password for “Add, update or delete well data of MS plate”, and then the window of “MS plate map of Mat_Astro” appears (Fig.47). When you want to make the new position on this window, detect the well position by moving a pointing mouse cursor, and click on “Detect the well position” button. Then the window of “Add well data of MS plate” appears, and enter the corresponding digestion plate ID and well ID (Fig.48). If you select the Well ID such as “D23” by moving a pointing mouse cursor, the window of “Update or delete well data of MS plate” will appear (Fig.49).

# Enter the Password for “Update or delete MS plate data” (Fig.41). Then the window of “Update or delete MS plate data of Mat_Astro” appears.
4-3-4. The window of “2D-PAGE map list” (Fig. 50). If you select 2DPAGE map such as “Mat_Astro”, the window of “Login for 2DPAGE map” will appear.
# Enter the Password for “Add, update or delete spot data of 2DPAGE map” (Fig.51). Then the window of “2DPAGE map : Mat_Astro” appears (Fig.52). In this window, click on “Disp spot number” link button, the spot numbers appear. When you want to make the new position on this window, detect the spot position by moving a pointing mouse cursor, and click on “Detect the spot position” button. Rectangular width can be changed in accordance with the size of the spot. Then the window of “Add spot data in 2DPAGE
map” appears, and enter the corresponding MS plate ID, well ID and other data in each box (Fig.53). If you select the spot number such as “2201” by moving a pointing mouse cursor, the window of “Update or delete spot data of 2DPAGE map” will appear (Fig.54). When you click on “Detect Well (digestion plate)” link button, the window of “Well data in digestion plate” appears (Fig.55). Cross mark shows the well of “A2”.

# Enter the Password for “Update or delete header data of 2DPAGE map” or “Update map data of 2DPAGE map” (Fig.51). Then the window of “Update header data of 2DPAGE map” or “Update Map data of Mat_Astro” appears.
4.4. Protocol data

4.4.1. The window of “Protocol Home” including “Add or update material data”, “Add or update gel method data” and “Add or update analysis method data”.
   # Enter ”User name”, ”Password” and ”ID number (material ID, method ID or analysis ID) ”, and then click on “Go” button (Fig.12).

4.4.2. The window of “Keyword search for protocol” including “Search material data by keyword”, “Search gel method data by keyword” and “Search analysis method by keyword”
   # Search by terms. Enter the term in each box, and click on “Search” button (Fig.56).
4-4-3. The window of “Material list” including “User name”, “Material ID”, “Material name” and “Date”.
# If you select the Material ID such as “Mat_Astro”, the window of “Login for Material” will appear. Enter the Password, and then the window of “Update and delete material data of Mat_Astro” appears.

4-4-4. The window of “Gel method list” including “User name”, “Method ID”, “Gel method name” and “Date”.
# If you select the Method ID such as “Standard_2DE”, the window of “Login for gel method” will appear. Enter the Password, and then the window of “Update and delete gel method data of Standard_2DE” appears.

4-4-5. The window of “Analysis method list” including “User name”, “Analysis ID”, “Analysis method name” and “Date”.
# If you select the Method ID such as “Toda_org”, the window of “Login for analysis method” will appear. Enter the Password, and then the window of “Update or delete analysis method data” appears.

4-5. Change user password
When you need to change “User Password”, enter “User name” and “Password”, and click on “Enter user name & password” button (Fig.57). Then the window of “Enter new password” appears. In this window, enter “New password” in each box.
4-6. Administrator only
Only the administrator is allowed to use the window of “Add or delete user” (Fig.58). A new user is also able to be registered on this window (Fig.59).
Proteomics LIMS module

Add or update user

User Name
Password
Re password
Affiliation
Note
Add or update user

Delete user

User Name
Delete user
Chapter 5. Installation

5-1 Setup

Software requirements: Apache revision 1.3.34 or later, PostgreSQL revision 7.4.3 or later, PHP revision 4.3.7 or later, GD library revision 2.0.27 or later. Please install them in advance.

And please set up as follows.

Please edit /usr/local/lib/php.ini

```
register_globals = On
#tar xvzf LIPAGE_****.tar.gz
#mv LIMS /usr/local/apache/htdocs
#cd /usr/local/apache/htdocs/LIMS
#su postgres
$createdb proteomedb
```

Please create and edit the first line in limsuser.back.

admin(Input as a word)

[ Using an example of user data:
```
#cp limsuser.euc limsuser.back
    Usernames of the LIMS are toda and hmorisawa. The passwords are bmc27info and bmc36info.
```
]

$psql -f createlimstable.sql proteomedb
The top page of the LIMS is http://servername/LIMS/lims.html.

5-2 Apache-PHP-PostgreSQL installation instruction using source files

The following description is applicable to Fedora Core 5.

Please install rpm packages of gcc and environments for developments, first.
Please download each source files of apache_1.3.35.tar.gz, php_5.1.2.tar.gz, gd_2.0.33.tar.gz, jpegsrc.v6b.tar.gz, libpng-1.2.6rc5.tar.gz and postgresql-8.1.3.tar.gz from the internet.

The download sites in the Internet
```
http://www.apache.org/
http://www.php.net/
http://www.boutell.com/gd/
ftp://ftp.uu.net/graphics/jpeg/
http://www.libpng.org/pub/png/libpng.html
http://www.postgresql.org/
```
[Apache installation]

#tar xvzf apache_1.3.35.tar.gz
#cd apache_1.3.35
#OPTIM="-O2" ./configure --enable-module=so
#make
#make install
#vi /usr/local/apache/conf/httpd.conf

    ServerName **********                  ( Enter a right name of server )

#vi /etc/rc.d/rc.local

    /usr/local/apache/bin/apachectl start          ( The line is added )

[PostgreSQL installation]

#adduser postgres
#passwd postgres
#mkdir /usr/local/src/postgresql-8.1.3
#chown postgres /usr/local/src/postgresql-8.1.3
#chown postgres /usr/local/src/postgresql-8.1.3
#mkdir /usr/local/pgsql
#chown postgres /usr/local/pgsql
#su postgres
$cd /usr/local/src
$tar xvfz postgresql-8.1.3.tar.gz
$cd /usr/local/src/postgresql-8.1.3
$./configure
$make
$make install

$vi /home/postgres/.bashrc

    PATH="$PATH":/usr/local/pgsql/bin
export POSTGRES_HOME=/usr/local/pgsql
export PGLIB=$POSTGRES_HOME/lib
export PGDATA=$POSTGRES_HOME/data
export MANPATH="$MANPATH":$POSTGRES_HOME/man
export LD_LIBRARY_PATH="$LD_LIBRARY_PATH":"PGLIB"

$source ~/.bashrc
$initdb
$ cd /usr/local/pgsql/data
$chmod 600 pg_hba.conf
$vi pg_hba.conf
    #host    all    all    ::1/128    ident sameuser   (Add #)
    host    all    0.0.0.0    0.0.0.0    trust             (The line is added)
$su -
#vi /etc/rc.d/rc.local

    rm /tmp/.s.PGSQL.* (The line is added)
    su · postgres ·c “postmaster ·S ·i” (The line is added)

    [zlib installation]
    #tar xvzf zlib-1.2.1.tar.gz
    #cd zlib-1.2.2
    #./configure ·-shared
    #make
    #make install

    [JPEG-6b installation]
    #tar xvzf jpegsrc.v6b.tar.gz
    #cd src/jpeg-6b
    #./configure ·-enable-shared ·-enable-static
    #make
    #make install

    [libpng installation]
    #tar zxf libpng-1.2.6rc5.tar.gz
    #cd libpng-1.2.6rc5
    #cp scripts/makefile.linux makefile
    #vi makefile
        ZLIBLIB=/usr/local/lib (The line is added)
        ZLIBINC=/usr/local/include (The line is added)
        #ZLIBLIB=../zlib (Add #)
        #ZLIBINC=../zlib (Add #)
    #make
    #make install

    [GD installation]
    #tar xvzf gd-2.0.28.tar.gz
    #cd gd-2.0.28
    #./configure
    #make
    #make install

    [PHP installation]
    #tar xvzf php-5.1.2.tar.gz
    #cd php-5.1.2./configure ·-with-pgsql ·-with-apxs=/usr/local/apache/bin/apxs
    ·-enable-mbstr-enc-trans ·-enable-mbstring ·-enable-mbregex ·-enable-versioning
    ·-with-zlib·dir=/usr/local/lib ·-with·gd ·-with·jpeg·dir=/usr/local/lib
    #make
    #make install
#cp php.ini-dist /usr/local/lib/php.ini  
#vi /usr/local/apache/conf/mime.types

```
application/x-httpd-php php ( The line is added )
application/x-httpd-source phps ( The line is added )
```

#cd ext/pgsql  
#phpize  
#aclocal  
#./configure  
#make  
#make EXTENSION_DIR=/usr/local/lib/php/extensions install  
#vi /usr/local/lib/php.ini

```
extension_dir = /usr/local/lib/php/extensions ( <- extension_dir = / )
extension = pgsql.so ( The line is added )
register_globals = On ( The line is added )
```

----------

#tar xzvf LIPAGE_****.tar.gz  
#mv LIMS /usr/local/apache/htdocs  
#cd /usr/local/apache/htdocs/LIMS  
#cp limsuser.euc limsuser.back  
#su postgres  
$createdb proteomedb  
$createuser nobody

[ Using an example of user data:  
  #cp limsuser.euc limsuser.back  
  Usernames of the LIMS are toda and hmorisawa. The passwords are bmc27info and bmc36info. ]

$psql -f createlimstable.sql proteomedb
The setup finished. The top page of the LIMS is http://servername/LIMS/lims.html.

5-3  Apache·PHP·PostgreSQL installations instruction  
using rpm packages on Fedora Core 4 and 5

The following description is applicable to Fedora Core 4 and 5.  
Please select workstation install in installation type on Fedora Core 4 or 5

Please set up as follows.  
#yum -y install httpd php php-gd php-pgsql  
#yum -y install postgresql postgresql-server  
#chkconfig httpd on  
#chkconfig postgresql on
Please configure the three following files.

vi /etc/httpd/conf/httpd.conf
  User nobody          (← User apache  )
  Group nobody         (← Group apache  )

vi /etc/php.ini
  register_globals = On      (← register_globals = Off)

vi /var/lib/pgsql/data/pg_hba.conf
  #host     all    all     ::1/128      ident sameuser       (Add # )
  host      all    all     0.0.0.0    0.0.0.0  trust         (The line is added )

Please reboot.

-------------

Please set up as follows.

#tar xvzf LIPAGE_****.tar.gz
#mv LIMS /var/www/html
#cd /var/www/html/LIMS
#cp limsuser.euc limsuser.back
#su postgres
$createdb proteomedb
$createuser nobody

[  Using an example of user data:
    #cp limsuser.euc limsuser.back
    Usernames of the LIMS are toda and hmorisawa. The passwords are bmc27info
    and bmc36info. ]

$psql -f createlimstable.sql proteomedb
The setup finished. The top page of the LIMS is http://servername/LIMS/lims.html.