

SyMBA: SYstems and Molecular Biology data and metadata Archive

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2: School of Computing Science, Newcastle University

3: School of Computer Science, University of Manchester

November 2007



- ▶ SyMBA is a system that *archives*, stores, and retrieves raw high-throughput data.



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- ▶ SyMBA deals with the technicalities of storing data and the information about that data...



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<http://symba.sourceforge.net>



Data and Metadata

What do we mean by data?

```
OR EPD; EP11223; HS_TP53.  
XX  
FH  Key          Location/Qualifiers  
FH  
FT  source       1..412  
FT  /organism="Homo sapiens"  
FT  /mol_type="genomic DNA"  
FT  /tissue_type="placenta"  
FT  /db_xref="taxon:9606"  
FT  exon          174..396  
FT  /gene="p53"  
FT  /product="phosphoprotein p53"  
FT  /number=1  
XX  
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atgggactg tccagtttg tgccaggcgc ctcgcagggg ttgatggat tggggttttc      240  
ccctcccatg tgctcaagac tggcgctaaa agtttgagc ttctcaaaaag tctagagcca      300  
ccgtccaggg agcaggtagc tgctgggtc cggggacact ttgcgttcgg gctgggagcg      360  
tgcttccac gacggtgaca cgcttccctg gattgggtaa gctcctqact ga             412  
//
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 tgctttccac gacgtgtt
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FT	<u>STRAND</u>	194	199	
FT	<u>STRAND</u>	204	207	
FT	<u>TURN</u>	209	211	
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FT	<u>STRAND</u>	327	334	
FT	<u>HELIX</u>	335	354	
SQ	SEQUENCE	393 AA;	43653 MW;	AD5C149FD8106131 CRC64;
MEEPFQSDPSV	EPPLSQETFS	DLWKLLPENN	VLSPLPSQAM	DDMLLSPDDI EQWFTEDEPGP
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SVTCTYSPAL	NKMFQLAKT	CPVQLWVDST	PPPGRTRVRAM	AIYKQSQHMT EVVRRCPHHE
RCSDSDGLAP	PQHLIRVEGN	LRVEYLDRN	TFRHSVVVPY	EPPEVGSDCT TIHYNYMCNS
SCMGGMNRRP	ILTIITLEDS	SGNLLGRNSF	EVRVACPGR	DRRTEEENLR KKGEPHHELP
PGSTKRALPN	NTSSSPQPKK	KPLDGEYFTL	QIRGRERFEM	FRELNEALEL KDAQAGKEPG
GSRAHSSHLLK	SKKGQSTSRR	KKLMFKTEGP	DSD	

//

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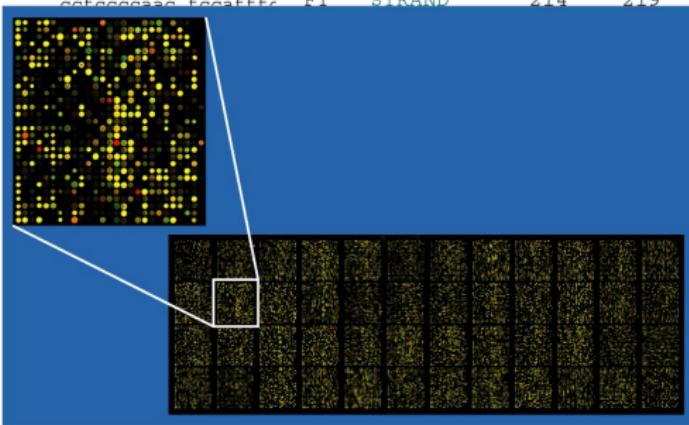
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 FT /organism="Homo sapiens"
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SQ Sequence 412 BP; 76 FT STRAND 194 199
 ggattcctcc aaaatgat FT STRAND 204 207
 ccaccggaaa atgttagt FT TURN 209 211
 cttcccccaac tccattns FT STRAND 214 219



3 MW; AD5C149FD8106131 CRC64;
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 /EYLDDRN TFRHSVVVPY EPPEVGSDCT TIHYNYMCNS
 NLLGRNSF EVRVCACPGR DRRTEEEENLR KKGEPHHELP
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FT source 1..412

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FT /m 100

FT /t 90

FT /d 80

FT exon 17

FT /g 16

FT /p 15

FT /n 14

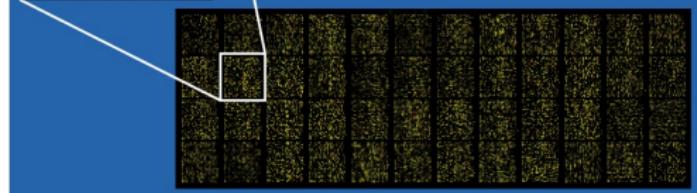
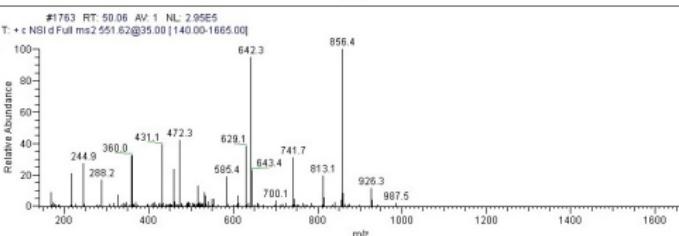
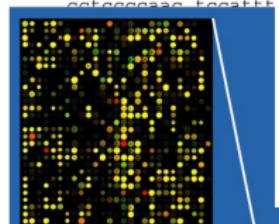
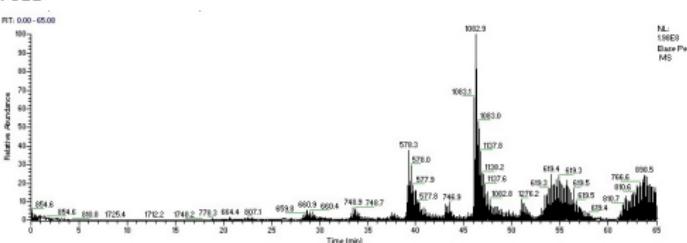
XX

SQ Sequence 412 BP; 7

ggattcctcc aaaatga

ccaccccaaa atgttag

ccatccccaaat tccattt



```
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T: +c NSId Full ms? 551.62@35.00 [140.00-1665.00]
  244.9 288.2 360.0 431.1 472.3 585.4 629.1 642.3 643.4 700.1 741.7 813.1 856.4 926.3 987.5
```

Sequence:

NKLLPENN VLSPLPSQAM DDMLSPDDI EQWFTEDPGP
AAPAPAPS WPLSSSVPSQ KTYQGSYGFR LGFLHSGTAK
VQLWVDST PPPGTRVRAM AIYKQSQHMT EVVRRCPHHE
VEYLDDRN TFRHSVVVPY EPPEVGSDCT TIHYNYMCNS
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FT SOURCE 1 413

FT *Scaree* /Cannan

10 90
15 85

FT / C 83
ET / A

F1
□□ □□ □□

FT exon 17

Page 45

FT / P 8 38

FIT / n 29

XX 654.6

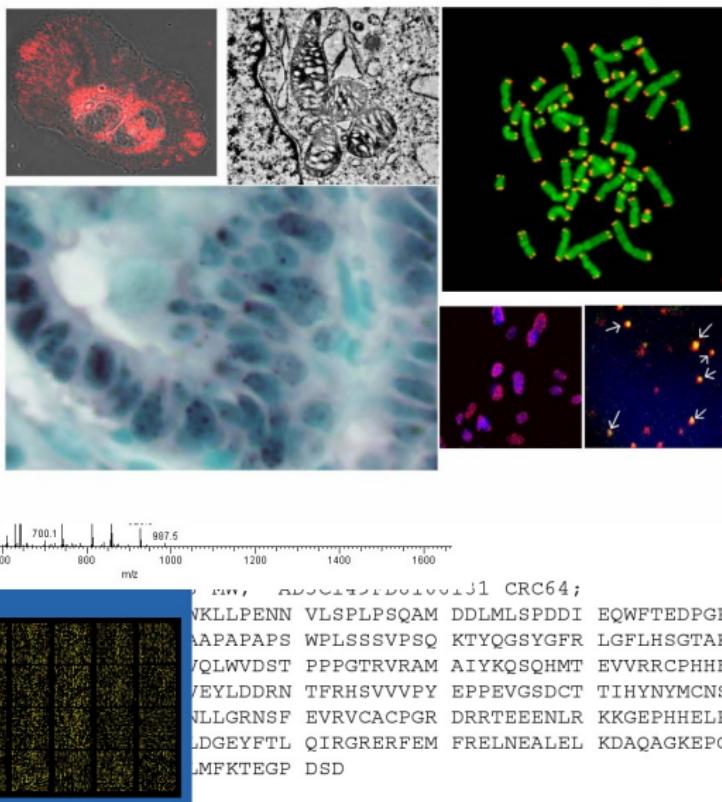
SQ Sequence 412 BP; 7

ggattcctcc aaaatga

ccaccccaaa atgttag T + c NSIdF

catccccccg tcggattt 100-

Volume 30 Number 2 February 2008



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10

FT

FT

FT

FT

FT

ET

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10

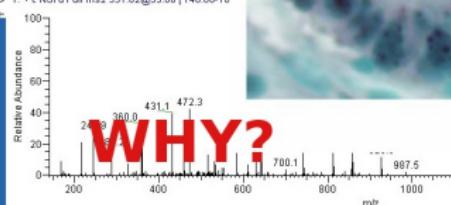
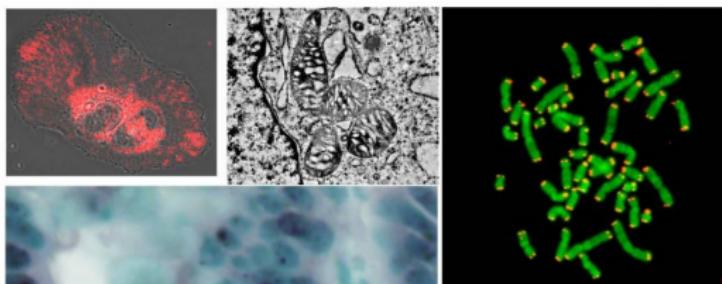
FT

xx

50

WHEN?

WHO?



WHAT? WHERE?
CRC64;
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LWVDST PPPGTRVRAM AIYKQSQHMT EVVRCPHHE
YLDLDRN TFRHSSVVPP EPPEVGSDCT TIHYNYMCNS
LGRNSFS EVRVCACPGR DRRTEEENLR KKGEPHHELP
GEYFTL QIRGRERFETEINAEEDDIOAGLEPG
FKTEGP DSD

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	ccgtccaggg agcaggta	FT	<u>STRAND</u>	251	258
//	tgc ttccac gac ggtga	FT	<u>STRAND</u>	264	274
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What CISBAN needed in a data archive

- ▶ long-term, protected storage for *primary* data



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- ▶ well-organized, easily accessible and searchable



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- ▶ long-term, protected storage for *primary* data
- ▶ well-organized, easily accessible and searchable
- ▶ modification histories for all metadata
- ▶ promote data sharing through the use of standards (e.g. MIBBI)



Which standards and common formats will help with...



Which standards and common formats will help with...

- ▶ choosing metadata to store?



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- ▶ structuring data and metadata?



Which standards and common formats will help with...

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- ▶ simplifying input and retrieval?



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- ▶ choosing metadata to store? - **Minimal Information Reporting Standards**, e.g. MIBBI
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MIAME: what is considered “minimal” for microarrays:

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adapted from <http://www.mged.org/Workgroups/MIAME/miame.html>



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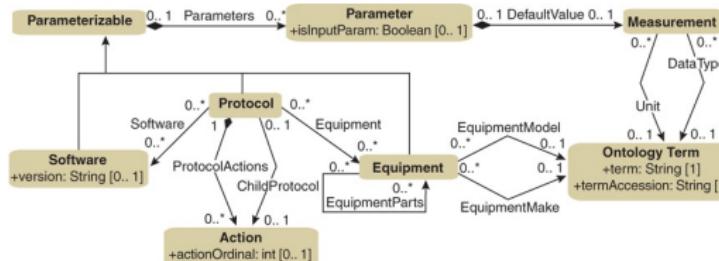
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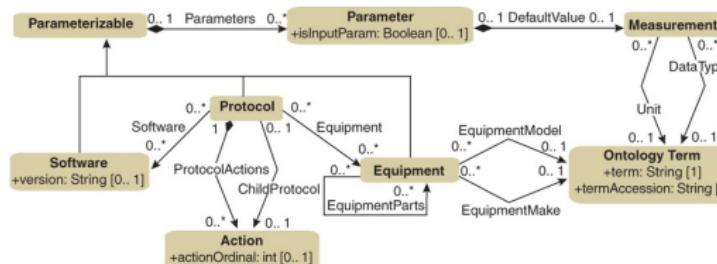
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The Functional Genomics Experiment Object Model & Markup Language (FuGE-OM, FuGE-ML)



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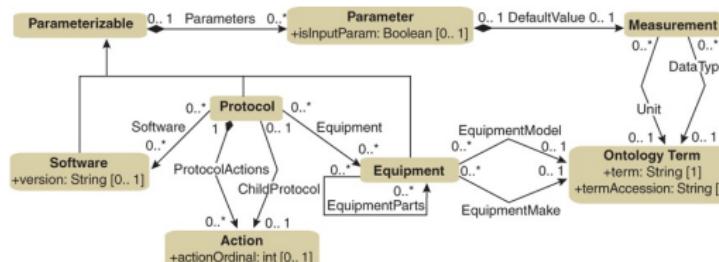


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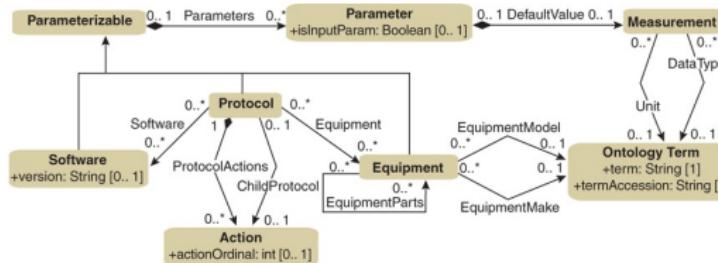


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- ▶ *standardizes* and structures experimental metadata for a range of omics experiments
 - ▶ *models* experimental objects such as samples, protocols, instruments, and software
 - ▶ *provides* extension points for the creation of individual community standards



SyMBA: Data and Metadata Archive



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- ▶ based on the FuGE Object Model



SyMBA: Data and Metadata Archive



- ▶ *based on the FuGE Object Model*
- ▶ *guided by Minimal Information Standards such as MIAME*



SyMBA: Data and Metadata Archive



- ▶ *based on the FuGE Object Model*
- ▶ *guided by Minimal Information Standards such as MIAME*
- ▶ *provides a straightforward method of metadata/data input and retrieval*



How can SyMBA be used?



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- ▶ make use of an existing installation



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 - ▶ production instance
 - ▶ sandbox instance



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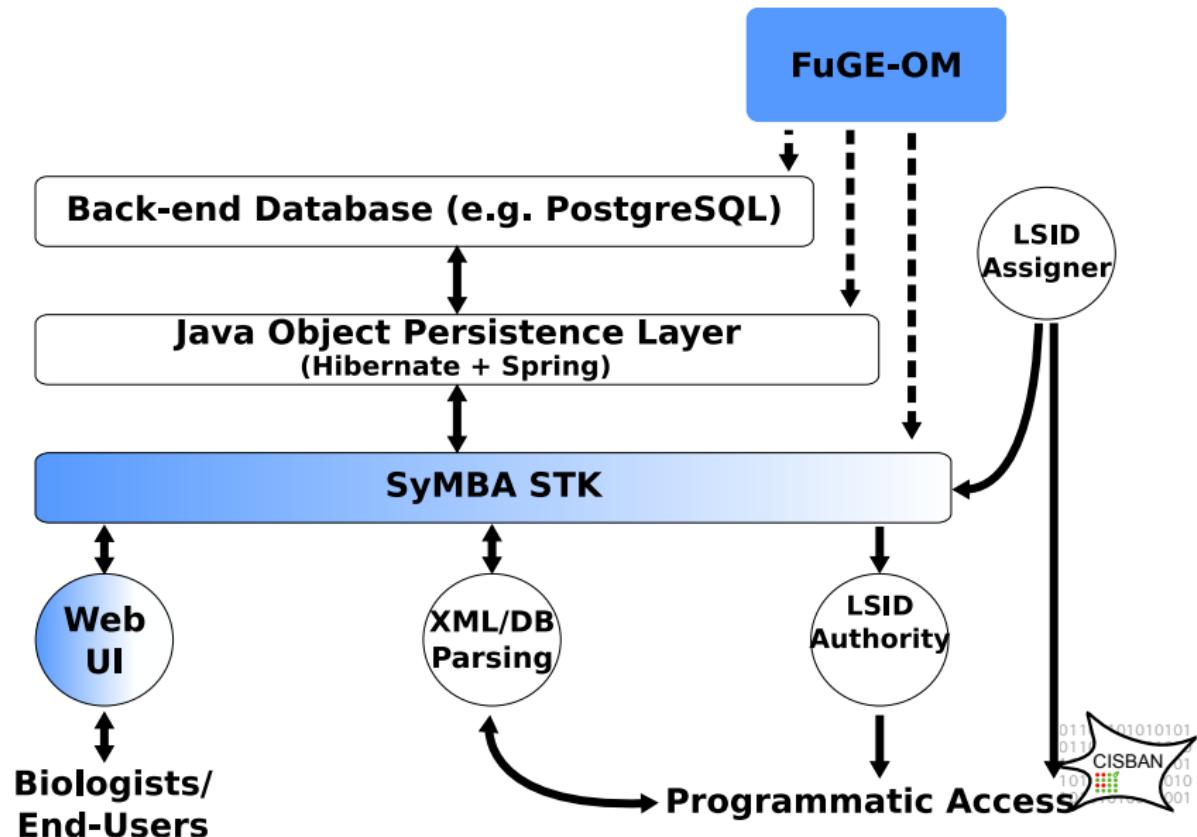
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- ▶ build your own SyMBA



How can SyMBA be used?

- ▶ make use of an existing installation
 - ▶ production instance
 - ▶ sandbox instance
- ▶ build your own SyMBA
- ▶ build & customize your own
 - ▶ propagate your modifications back to the main project





Development and Deployment



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- ▶ all code controlled using Subversion (version control system)
- ▶ a single command each to
 - ▶ build the database
 - ▶ populate the database with people or with protocols
 - ▶ create the web application (a single war file)



Usage

- ▶ SyMBA is used internally within CISBAN



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 - ▶ 2 microarray protocols
 - ▶ 1 proteomics protocol
 - ▶ 1 large-scale robot protocol
 - ▶ 1 live cell imaging protocol



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- ▶ the “sandbox” website contains
 - ▶ 1 example microarray protocol
 - ▶ 1 example proteomics protocol
 - ▶ 1 example live cell imaging protocol
- ▶ more protocols can be added as required
- ▶ each investigation can contain many data files



Usefulness to Researchers



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- ▶ compare aspects of studies such as controls and treatments



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- ▶ a simpler interface than was possible with the original setup at CISBAN



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- ▶ help with preparations for publication



How to Contribute

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How to Contribute

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- ▶ become a developer / tester!



How to Contribute

- ▶ use it!
- ▶ contribute code (e.g. CARMEN Neuroscience Project)
- ▶ become a developer / tester!
- ▶ SourceForge mailing lists and (bug, feature...) trackers



Acknowledgements & Useful URLs

Developers and “Nuts & Bolts” Testers

- ▶ Frank Gibson, Andy Jones, Matt Pocock, Allyson Lister, Olly Shaw, Neil Wipat

Thanks to the Web Testers

- ▶ Steve Addinall, Amanda Greenall, Dominic Kurian, Glyn Nelson, Gabi Saretzki

Useful URLs

- ▶ **SyMBA:** <http://symba.sourceforge.net>
- ▶ **SyMBA Sandbox:** <http://www.cisban.ac.uk/symba-sandbox>
- ▶ **MIAME:**
<http://www.mged.org/Workgroups/MIAME/miame.html>
- ▶ **FuGE:** <http://fuge.sourceforge.net>
- ▶ **Maven:** <http://maven.apache.org>
- ▶ **LGPL:** <http://www.gnu.org/licenses/lgpl.html>





SyMBA (Release 7.10)

SyMBA Home
SyMBA Help
SyMBA Project Home
CISBAN Home
Contact Us
Total Experiments: 1
Total Data Files: 1
Log Off

Welcome, AllysonL

Please select one of the following options: [[Why?](#)]

- Deposit some data (using a new or existing experiment)
- View your saved experiments
- [How to use this site](#)
- Update your personal details

[Return Home](#) :: [View Help](#)

You are currently logged in as AllysonL

If you have any questions or comments, please [contact us](#)



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Acknowledgements



SyMBA (Release 7.10)

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Total Experiments: 1
Total Data Files: 1
Log Off

(1) Introduction -> (2) Attach to an Experiment -> (3) Upload Data -> (4) Select Protocol -> (5) Confirm Your Submission -> (6) Completion and Download

Please enter your data [[Why?](#)]

All submitted files must be of the same data type and belong to the same experiment, large data files may take some time to upload

Investigation:

Type:

Your File:

File 2:

Attach Another File

If your protocol is not here please [contact us](#)

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If you have any questions or comments, please [contact us](#)



Acknowledgements

Description
of File [?]:

Description of the microarray data file.

Please
select your
factor:

Time Point 0

Please
select your
factor:

mutant/WT Microarray Time Series Protocol for the Wild Type Strain

Name/ID of
this
Material
(optional):

Please enter some information about the Material Characteristics, starting with treatment information. There should be a separate box for each treatment performed (optional). *NOTE: All treatments already entered will remain in the system. You may add additional treatments by entering them below.*

Type, Dose
and Length
of
Treatment:

[Add Another Treatment](#)

Next, please choose the correct Material Type.

Please
select
which strain
was used in
the creation
of this data
file.

Wild Type 2

Acknowledgements

Total Experiments: 1
Total Data Files: 1
Log Off

Please check all of your details. Click on any item you wish to modify, which will take you back to the appropriate form page, where you can correct any mistakes.

The experiment you are loading has the following details:

- ◆ Name: **Sample Microarray Experiment**
- ◆ Hypothesis: **A sample hypothesis**
- ◆ Conclusions: **A sample conclusion**

This experiment has the following data file(s) for your **Example mutant/WT Microarray Investigation**:

Information for **Lis_MCA_4697**

- ◆ You have described this file as follows: **Description of the microarray data file**.
- ◆ Your workflow also required that you specify a factor associated with your data file. The factor you have chosen is **Time Point 0**
- ◆ You have also assigned the data file to a particular step in your workflow. The step you have assigned the file to is **mutant/WT Microarray Time Series Protocol for the Wild Type Strain**
- ◆ You have provided information about the material used in the experiment. This material has the following properties
 - ◊ Material Type: **Wild Type 2**

Information for **Lis_MCA_4384**

- ◆ You have described this file as follows: **Description for file 2**
- ◆ Your workflow also required that you specify a factor associated with your data file. The factor you have chosen is **Time Point 0**
- ◆ You have also assigned the data file to a particular step in your workflow. The step you have assigned the file to is **mutant/WT Microarray Time Series Protocol for the Mutant Strain**
- ◆ You have provided information about the material used in the experiment. This material has the following properties
 - ◊ Material Type: **Mutant 1**

Remember, your changes are NOT saved until you click the "Confirm All" button below!

Uploading large files may take several minutes.

[CONFIRM ALL](#)

Acknowledgements

Example mutant/WT Microarray Investigation	Step Containing the mutant/WT Microarray Sample Preparation Protocol	
	Step Containing the mutant/WT Microarray Time Series Protocol for the Wild Type Strain	<p>Time Point 0</p> <p>Wild Type 2 (strain name CV) Lis_MCA_4697</p> <p>Download This File</p> <p>Time Point 60</p> <p>Time Point 90</p> <p>Time Point 120</p> <p>Time Point 150</p> <p>Time Point 180</p> <p>Time Point 210</p> <p>Time Point 240</p> <p>Time Point 270</p>
	Step Containing the mutant/WT Microarray Time Series Protocol for the Mutant Strain	<p>Time Point 0</p> <p>Time Point 60</p> <p>Time Point 90</p> <p>Time Point 120</p> <p>Time Point 150</p>
		<p>01 7 11 10 01</p>