

MASCOT *Integra*

How Mascot Integra helps
run a Core Lab

MASCOT :How Mascot Integra helps run a Core Lab

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Areas where a database can help a core lab

- Project, experiment and sample tracking
- Flexibility in experiment design
- Role based security
- Automation
- Custom results formatting
- Reporting to publication standards
- Accounting and billing
- Customer interface
- Instrument usage, success rates and other metrics

I will be covering each of these areas in more detail as I go through the presentation. For most of the examples I will be using information from a core service that I worked for some years ago.

Project, experiment and sample tracking

Project List Return Add Edit View Delete Import

Hide Search Bar

Search Bar Search Close Refresh **Status Active**

Group by Columns:
 Status OK

Search within the Id/Desc: OK

Search by a Query:
[ActiveProjects](#)
[AllProjects](#)
[ClosedProjects](#)
[CompleteProjects](#)
[Confidential Project](#)
[Non-confidentialPro](#)

ID	Description	Focus	Status	Start Date
<input type="checkbox"/> P-070900048	P element transposase phosphorylation		Active	5/2/01 12:58 PM
<input type="checkbox"/> P-070900050	2D gel Rio Protein ID		Active	5/2/01 1:02 PM
<input type="checkbox"/> P-070900058	Analysis of the S. cerevisiae condensin complex		Active	8/23/01 2:44 PM
<input type="checkbox"/> P-070900060	Neuropeptide identification from the egl-21 Carboxypeptidase mutant		Active	12/13/01 2:53 PM
<input type="checkbox"/> P-070900061	Visualization of RanGTP gradient		Active	12/4/01 2:56 PM

Status Complete

ID	Description	Focus	Status	Start Date
<input type="checkbox"/> P-070900047	HIM		Complete	4/26/01 12:56 PM
<input type="checkbox"/> P-070900049	Protein ID		Complete	5/1/01 12:59 PM
<input type="checkbox"/> P-070900051	Aminopeptidase Protein ID		Complete	5/9/01 1:03 PM
<input type="checkbox"/> P-070900052	Test Samples and standards		Complete	5/22/01 1:04 PM
<input type="checkbox"/> P-070900053	Identification of a host cytosolic receptor for bacteria		Complete	6/14/01 1:08 PM
<input type="checkbox"/> P-070900054	Function and regulation of the human Arp2/3 complex		Complete	6/29/01 2:37 PM
<input type="checkbox"/> P-070900055	Sec16p binding proteins		Complete	7/30/01 2:38 PM

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One of the most important tasks in a core lab is keeping track of all the collaborations, samples and results. Here I am showing the Integra view of the projects that are active and in progress or that have been completed by the core lab. I can filter and sort the projects with the controls in the left hand search bar. The filters that are displayed depends on what information you are viewing and they are extendable.

Sample tracking

The screenshot displays the Mascot sample tracking interface. At the top, there is a navigation bar with buttons for Return, Add, Edit, View, Delete, Find Mascot hits, History, and Find Child Samples. Below this is a search bar with a dropdown menu set to 'Sample Type' and an 'OK' button. To the right of the search bar, there are checkboxes for 'Select All' and 'Collapse All', and a text input field with the placeholder 'Show child samples of the selected sample(s)'. The main content area features a table with the following columns: ID, Description, Sample Type, Sub Type, Process, Content, and Units. A single row is visible with the ID 'S-071018-00002', description 'gel 1 sample', and a value of '0' in the 'Content' column. On the left side, there is a 'Search by a Query:' section with links for 'AllSamples', 'AvailableSamples', 'By Project', 'MySamples', and 'TodaysSamples'. Below this, there is a 'Project Description' section with the text 'Sec16p biding proteins' and a 'Search Now' button. The footer of the page contains the Mascot logo, the tagline ':How Mascot Integra helps run a Core Lab', the copyright notice '© 2008 Matrix Science', and the Matrix Science logo.

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I can also track individual samples by project as I am doing here in this screen shot, or by type or date, again controlled by the standardized search bar on the left.

Child sample tree for [S-071018-00002 gel 1 sample](#) [Return](#)

[S-071018-00002](#) - gel 1 sample - Sample

[gel-10200700186-A-01](#) - - GelLane

[gs-102007-00001](#) - - GelSpot

[S-071018-00007](#) - 1 - Sample

[S-071018-00045](#) - 1 (derivitised) - Sample

[S-071018-00083](#) - 1 (derivitised) (derivitised) - Sample

[S-071018-00121](#) - 1 (derivitised) (derivitised) (digest) - Sample

[S-071018-00159](#) - Purified from 1 (derivitised) (derivitised) (digest) - Sample

ms_filesample [msf-18102007-0012469](#) - : \\shark\MSDData2\RJJ data\UCB\Bruker samples\P-070800055 Sec16\M011107002\1Ref\Fid -

[msf-19102007-0012511](#) - Mascot results object from ../data/20071019/F029540.dat - ms_filesample

[mss-19102007-00028](#) - fid Gel 1 Sec16p biding proteins (task EXP-071000356-1592) Sprot 100ppm IAM MetOx NAc Pro PyroGly Integra (E:\MSData2\RJJ data\UCB\Bruker samples\P-070800055 Sec16\M011107002\1Ref) - ms_srch

Search contains 2 protein hits.

[gs-102007-00002](#) - - GelSpot

[S-071018-00008](#) - 2 - Sample

[S-071018-00046](#) - 2 (derivitised) - Sample

[S-071018-00084](#) - 2 (derivitised) (derivitised) - Sample

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For any sample I can look up the child samples all the way down to the search results. I can also go from a search result and map the sample relationships all the way back up the tree to the original sample too.

Flexibility in experiment design

- **45 experimental tasks**

- Can model simple to complex experiments



- **Save templates for your standard protocols**
- **No software customization needed to support new experiment designs**

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Each core service has a unique mixture of instrumentation and protocols in use. Methods are continually refined and new protocols are introduced to support requests by customers. Methods are built up from the 45 predefined tasks in the system. Here are the icons from some of the tasks that are available. If you have a standardized protocol that is used for say MudPIT experiments then you can save the experiment design to a template. The flexible experiment design interface in Integra means that no costly software customization is needed each time a new protocol is implemented, or instrument is purchased.

Edit Experiment EXP-071000356

Return Save Reset Edit Exp. Plan Start Exp. Review Exp.

Experiment

ID: EXP-071000356

Description: Gel 1 Sec16p biding proteins

Status: In-progress Last Task: EXP-071000356-1591

Study: S-071000066

Study description: Sec16p biding proteins

Notes

Experimental Plan

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Here is an example of an experiment design built from the different tasks for protein identification from multiple bands from a 1D gel.

Experiment templates

Library Type Templates			
<input type="checkbox"/>	ID	Image	Description
<input type="checkbox"/>	LG-070400087		MudPIT
<input type="checkbox"/>	LG-070400088		LCMSMS
<input type="checkbox"/>	LG-070900095		1Dgel
<input type="checkbox"/>	LG-070600090		LTQ LCMSMS
<input type="checkbox"/>	LG-070700091		Raw MS data
<input type="checkbox"/>	LG-070700092		Peaklist
<input type="checkbox"/>	LG-071000097		Core service gel
<input type="checkbox"/>	LG-071000098		Core services ingel digest

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Such an experiment protocol can be saved as a template with all the default run time parameters, volumes of solutions and HPLC conditions etc, for each different step pre-assigned. These templates are available to all the other Integra users.

Role based security

User Maintenance

tech

User Id	tech	User Type	Concurrent Named User
Description	Tech Nician		
Password	*****		
Password Confirm	*****	Expiry Date	<input type="text"/>
Force Change Password	<input type="checkbox"/>	Status	Active
Disabled Reason	<input type="text"/>		

Roles

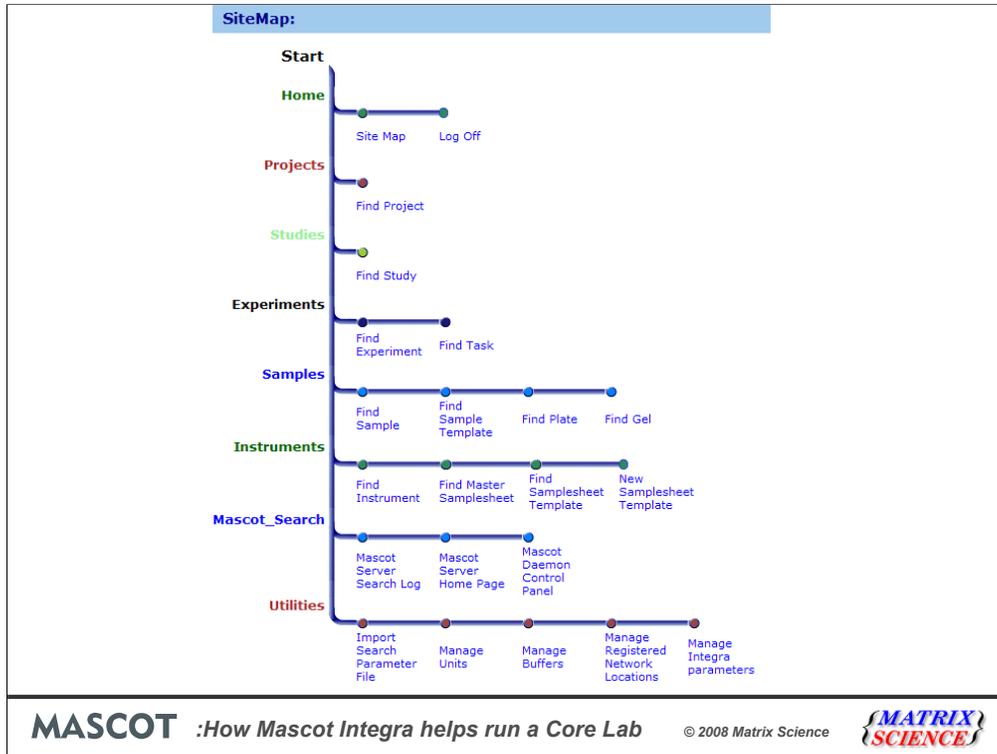
<input type="checkbox"/> Administrator	<input type="checkbox"/> Analyst	<input type="checkbox"/> CertificationOverid
<input checked="" type="checkbox"/> Gel Technician	<input type="checkbox"/> Inventory Manager	<input type="checkbox"/> LabManager
<input checked="" type="checkbox"/> MS Technician	<input type="checkbox"/> ManagerApproval	<input checked="" type="checkbox"/> Prep Technician
<input type="checkbox"/> Preparation	<input type="checkbox"/> Project Manager	<input type="checkbox"/> QA
<input type="checkbox"/> Receipt	<input type="checkbox"/> Reference	<input type="checkbox"/> Sample Manager
<input type="checkbox"/> SampleLogin	<input type="checkbox"/> SampleReview	<input type="checkbox"/> Study Manager
<input type="checkbox"/> SupervisorApproval	<input type="checkbox"/> Virtual	

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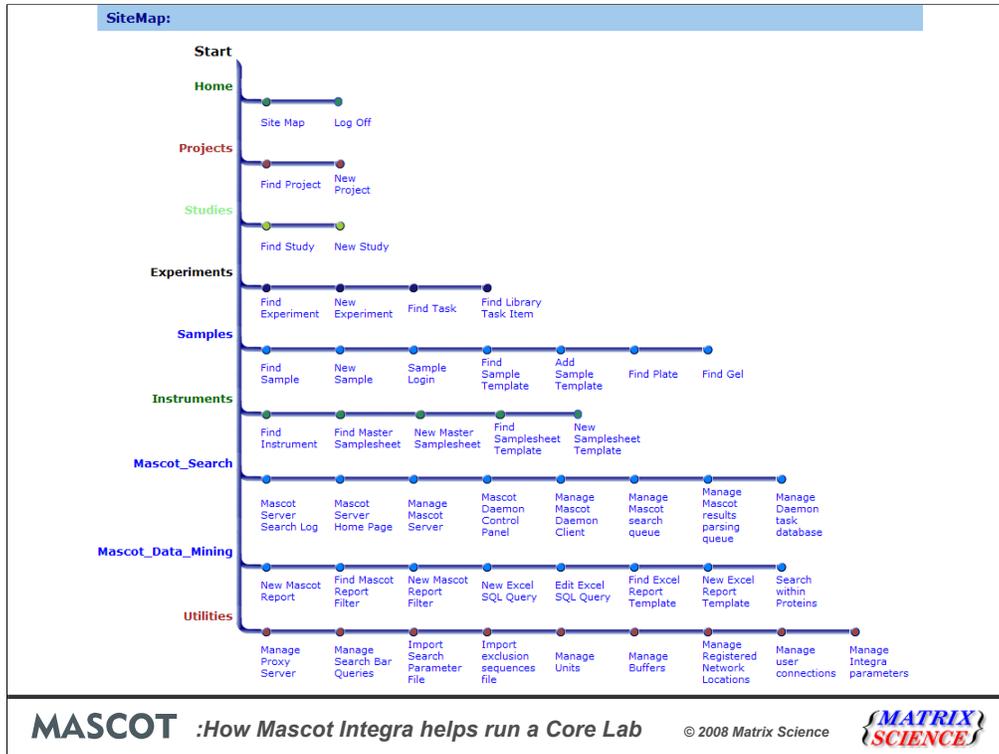
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If you wish, you can control access to the system using the built in role based security. For a large lab you might have an administrator that handles all the project paperwork, while technicians carry out the sample analysis.



In this example, tech plays a rather restricted role and can only process the samples. The role based security limits his options in Integra.



Compared to that of a unrestricted user.

Instrument Integration 1

- Handled by sample sheet exchange
- User extensible - you can add your own sample sheet types to the system
- Supports excel, tab delimited and comma separated values (csv) sheet for any instrument
- Allows support of nearly all instrument data systems
 - e.g. Mass-spec, plating robots etc

Now a change of track, lets look to see how Integra communicates with Instruments in the lab. Rather than direct control of the mass spectrometers Integra communicates via sample sheet exchange.

Integra ships with sample sheet templates already configured for the common mass specs and you can add your own. You can do this, even if you have a one of a kind robot system, as long as it accepts Excel sheets, tab or comma separated values files. This allows for support of nearly all instrument data systems.

On-line MS (EXP-080500432-1973) - Xcalibur run - Microsoft Internet Explorer

File Edit View Favorites Tools Help

MATRIX SCIENCE MASCOTIntegra LabVantage

Help: SiteMap LogOff Database: Integrademio User: Patrickc

Home Projects Studies Experiments Samples Instruments Mascot_Search Mascot_Data_Mining Utilities

On-line MS (EXP-080500432-1973)

Task: On-line MS

Select

Select All Collapse All

Group by Columns: None OK

Search by a Query:

- [4Plex_Samples](#)
- [8Plex_Samples](#)
- [AllSamples](#)
- [AvailableSamples](#)
- [By Project](#)
- [MySamples](#)
- [Quantitated Samples](#)
- [Samples By Task](#)
- [TodaysSamples](#)

Scan in Ids:

Add Clear OK

ID	External ID	Description	Sample Type
<input checked="" type="checkbox"/> S-080515-00002		fraction 1	Fraction
<input checked="" type="checkbox"/> S-080515-00003		fraction 2	Fraction
<input checked="" type="checkbox"/> S-080515-00004		fraction 3	Fraction
<input checked="" type="checkbox"/> S-080515-00005		fraction 4	Fraction
<input checked="" type="checkbox"/> S-080515-00006		fraction 5	Fraction
<input checked="" type="checkbox"/> S-080515-00007		fraction 6	Fraction
<input checked="" type="checkbox"/> S-080515-00008		fraction 7	Fraction
<input checked="" type="checkbox"/> S-080515-00009		fraction 8	Fraction
<input checked="" type="checkbox"/> S-080515-00010		fraction 9	Fraction
<input checked="" type="checkbox"/> S-080515-00011		fraction 10	Fraction
<input checked="" type="checkbox"/> S-080515-00012		fraction 11	Fraction
<input checked="" type="checkbox"/> S-080515-00013		fraction 12	Fraction
<input checked="" type="checkbox"/> S-080515-00014		fraction 13	Fraction
<input checked="" type="checkbox"/> S-080515-00015		fraction 14	Fraction
<input checked="" type="checkbox"/> S-080515-00016		fraction 15	Fraction
<input checked="" type="checkbox"/> S-080515-00017		fraction 16	Fraction
<input checked="" type="checkbox"/> S-080515-00018		fraction 17	Fraction
<input checked="" type="checkbox"/> S-080515-00019		fraction 18	Fraction
<input checked="" type="checkbox"/> S-080515-00020		fraction 19	Fraction
<input checked="" type="checkbox"/> S-080515-00021		fraction 20	Fraction

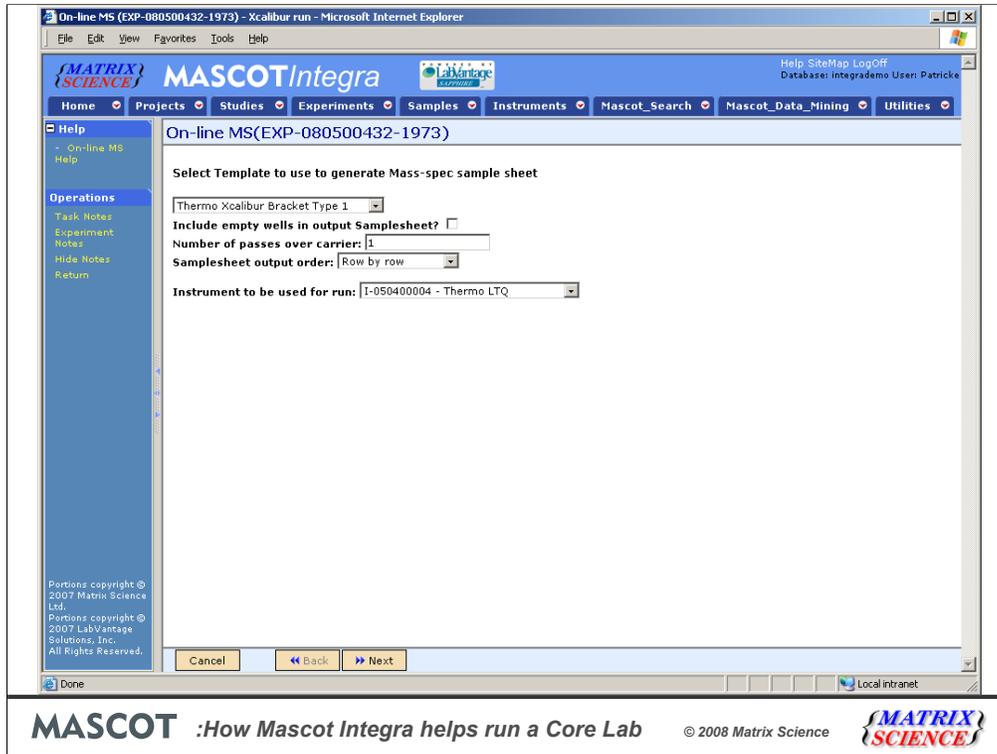
Cancel Back Next

Local intranet

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Here we have an example of exporting a sample sheet from Integra to the Thermo Xcalibur datasystem. During the experiment run we first select the samples (fractions) which will be injected into the MS.



Now we select the sample sheet template to use and record which instrument we intend to carry out the run on.

On-line MS (EXP-080500432-1973) - Xcalibur run - Microsoft Internet Explorer

File Edit View Favorites Tools Help

MATRIX SCIENCE Mascot Integra LabVantage

Help: SiteMap LogOff Database: Integrademio User: Patrick

Home Projects Studies Experiments Samples Instruments Mascot_Search Mascot_Data_Mining Utilities

On-line MS (EXP-080500432-1973)

Enter raw data output path (for Sapphire). This should be a UNC path (of the form \\Host name\Drive share\.....)
 [(Path)\(File Name)]

Enter raw data file or directory extension

Output hidden columns

Export column headings Bruker Headings

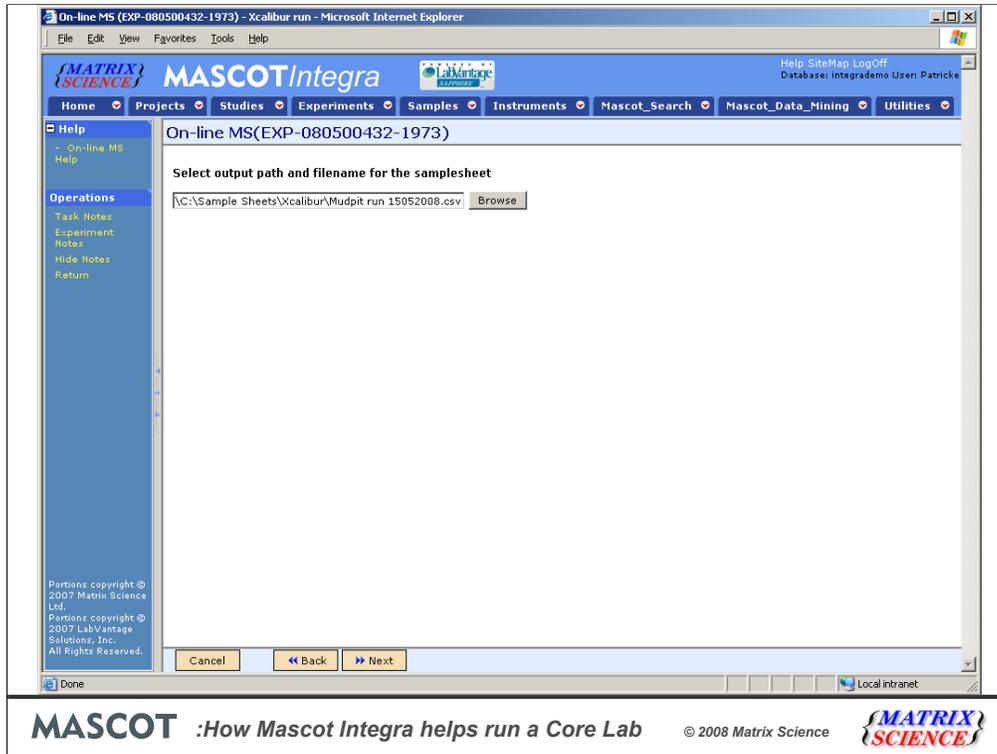
Cell No.	Sample Type	File Name	Sample Id	Path	Instrument Method	Process Met
-	Unknown	S-080515-00002	1	\\koala\Mudpit fractions		
-	Unknown	S-080515-00003	2	\\koala\Mudpit fraction		
-	Unknown	S-080515-00004	3	\\koala\Mudpit fraction		
-	Unknown	S-080515-00005	4	\\koala\Mudpit fraction		
-	Unknown	S-080515-00006	5	\\koala\Mudpit fraction		
-	Unknown	S-080515-00007	6	\\koala\Mudpit fraction		
-	Unknown	S-080515-00008	7	\\koala\Mudpit fraction		
-	Unknown	S-080515-00009	8	\\koala\Mudpit fractions		
-	Unknown	S-080515-00010	9	\\koala\Mudpit fraction		
-	Unknown	S-080515-00011	10	\\koala\Mudpit fraction		
-	Unknown	S-080515-00012	11	\\koala\Mudpit fraction		

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Local intranet

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We can fill in some of the values into the sample sheet. The sample sheet template we selected is a (user definable) view of the underlying sample sheet with some or all of the columns selected for viewing. Some columns are defined with default values (which can include tags to substitute in values related to the sample being run). We can fill in as much or as little as we choose at this point, but the critical columns to fill in are the Path and the File Name columns. In the case of the Xcalibur sample sheet, these will define where the raw data files generated by the instrument run will be created, so by entering this information, we're also telling Mascot Integra where to look for the raw files for the MS/MS experiment. Using this, the system can tell Mascot Daemon where to pick up the raw data from, use Mascot Distiller to automatically do peak detection, submit the search to Mascot and then import the results into Mascot Integra when the search has completed.



Now we simply have to tell the system where to save the exported csv file.

[Overlapped] - Sequence Setup - Home Page

File Edit Change Actions View GoTo Help

Run Manager
 No Devices
 Sequence
 Sample Name
 Working On
 Position
 Raw File
 Inst. Method

	File Name	Sample ID	Sample Type	Path	Inst Meth	Pe
1	S:080515-00002	1	Unknown	\\Koaala\Mudpit\fractoni	1	
2	S:080515-00003	2	Unknown	\\Koaala\Mudpit\fractoni	1	
3	S:080515-00004	3	Unknown	\\Koaala\Mudpit\fractoni	1	
4	S:080515-00005	4	Unknown	\\Koaala\Mudpit\fractoni	1	
5	S:080515-00006	5	Unknown	\\Koaala\Mudpit\fractoni	1	
6	S:080515-00007	6	Unknown	\\Koaala\Mudpit\fractoni	1	
7	S:080515-00008	7	Unknown	\\Koaala\Mudpit\fractoni	1	
8	S:080515-00009	8	Unknown	\\Koaala\Mudpit\fractoni	1	
9	S:080515-00010	9	Unknown	\\Koaala\Mudpit\fractoni	1	
10	S:080515-00011	10	Unknown	\\Koaala\Mudpit\fractoni	1	
11	S:080515-00012	11	Unknown	\\Koaala\Mudpit\fractoni	1	
12	S:080515-00013	12	Unknown	\\Koaala\Mudpit\fractoni	1	
13	S:080515-00014	13	Unknown	\\Koaala\Mudpit\fractoni	1	
14	S:080515-00015	14	Unknown	\\Koaala\Mudpit\fractoni	1	
15	S:080515-00016	15	Unknown	\\Koaala\Mudpit\fractoni	1	
16	S:080515-00017	16	Unknown	\\Koaala\Mudpit\fractoni	1	
17	S:080515-00018	17	Unknown	\\Koaala\Mudpit\fractoni	1	
18	S:080515-00019	18	Unknown	\\Koaala\Mudpit\fractoni	1	
19	S:080515-00020	19	Unknown	\\Koaala\Mudpit\fractoni	1	
20	S:080515-00021	20	Unknown	\\Koaala\Mudpit\fractoni	1	
*						

For Help, press F1

NLM | 15/05/2008 10:55 NOT SAVED

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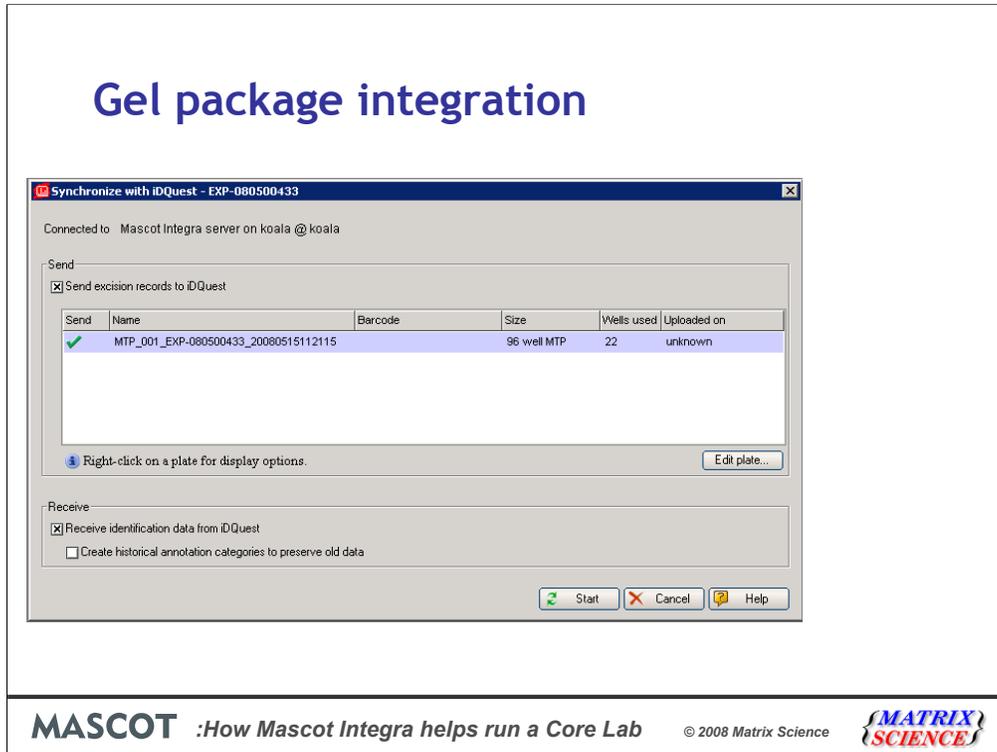
And import the file into Xcalibur.

Gel package integration

- **By XML file exchange:**
 - GE Healthcare DeCyder
 - NonLinear Dynamic Progenesis
- **By Web Service interface:**
 - Bio-Rad PDQuest
- **Two way**
 - Import spot details into Mascot Integra
 - Export protein hit information into gel package

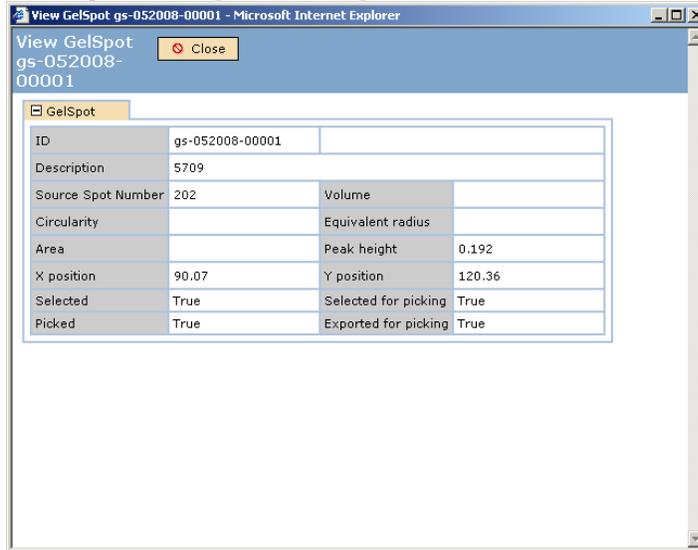
2D gel image analysis is a complicated task and I cannot pretend that we are experts at it. Rather than trying to perform the image analysis ourselves we interface with a number of popular packages. Because we are interfacing with another software package we can pass more information between the two systems and perform two way communication. This allows us to pick up the list of spots to identify by MS and pass back the final protein ID's.

Gel package integration



Here we have an example of data exchange between Mascot Integra and Bio-Rad PDQuest. Using the Synchronization method available in PDQuest, excised spot information is sent back to Mascot Integra where a matching experiment exists and is running.

Gel package integration



View GelSpot gs-052008-00001			
GelSpot			
ID	gs-052008-00001		
Description	5709		
Source Spot Number	202	Volume	
Circularity		Equivalent radius	
Area		Peak height	0.192
X position	90.07	Y position	120.36
Selected	True	Selected for picking	True
Picked	True	Exported for picking	True

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Here we can see some of the spot information that is stored in Mascot Integra when the systems are synchronised. Once the spot information is sent back, we can continue tracking the experiment in Mascot Integra, carry out Mascot searches, and approve and annotate these search results within Mascot Integra.

Gel package integration

The screenshot displays the PDQuest Advanced - B.B.3 interface. The main window shows a 2x4 grid of gel images with spot annotations. A 'PDQuest Synchronization Log' dialog box is open, showing synchronization events and details.

Synchronization date	Wells sent	Spots received	Status
14 May 2008 11:35	33	35	OK
15 May 2008 12:13	0	32	OK

PDQuest status	Local status	
0001	Awaiting search	No change
1006	Awaiting curation	No change
4003	Awaiting curation	No change
6102	Awaiting search	No change
6706	Curated	New
8007	Curated	New
8705	Awaiting curation	No change
4001	Awaiting curation	No change
8001	Curated	New
7904	Digestion	No change
8701	Awaiting curation	No change
8003	Digestion	No change
8805	Digestion	No change
8001	Curated	New
8604	Awaiting curation	No change

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Once this is done, we can resynchronise PDQuest and Mascot Integra. Integra sends the spot annotation information back to PDQuest – as we can see in the example here (all the spot identification information is being taken from Mascot Integra).

Integra can do similar annotation exchange with GEHealthcare Decyder and NonLinear Dynamics Progenesis software via XML file exchange.

Mascot search result filtering, approval and annotation

[COS_HUMAN](#) [COS_HUMAN](#) Complement C5 precursor (Contains: Complement C5 beta chain)
[TETH_HUMAN](#) [TETH_HUMAN](#) Tetrasolisin precursor (TH) (C-type lectin domain family 3 member B) (Plasminogen)
[CVC_MACOT](#) [CVC_MACOT](#) Cytochrome c - Macropus giganteus (Eastern gray kangaroo)
[CVC_TRAUC](#) [CVC_TRAUC](#) Cytochrome c - Trachypithecus cristatus (Silvered leaf monkey)
[BIMG_CERAF](#) [BIMG_CERAF](#) Beta-2-microglobulin precursor - Ceropithecus aethiops (Green monkey) (Grives)
[BIMG_GORGO](#) [BIMG_GORGO](#) Beta-2-microglobulin precursor - Gorilla gorilla gorilla (Lowland gorilla)
[CVC_GORGO](#) [CVC_GORGO](#) Cytochrome c - Gorilla gorilla gorilla (Lowland gorilla)

Original result file: [../GSM/20071015/029466.dat](#)

Approval status: Approval in progress

Notes:

Spot: [Display](#) [False discovery rate](#)
 Peptide matches above identity threshold: 5/0 6 1.11%
 Peptide matches above homology or identity threshold: 78/27 27 3.43%

Display options:

View results from hit: 1 to hit: 55 / 55

Show unassigned hit?

Format as Select summary?

Highlight significant peptides?

Show subset hits?

Display approved protein/peptide hits only:

Significance threshold p < 0.05

Show pep-up?

Show match summary images?

Display filter options:

Do not filter results

Selected hit only

Sign peptide

Carb TP

2 sig peptides

1 sig peptides

With Modifications

With Oxidation (M)

C-term matches

N-term matches

Exig at Y threshold

Pept must contain X

Mass >= X

Minimum mass X

Minimum % coverage

Protein score gles X

High Phospho

Primary hits

Click [here](#) for a printer friendly version

Peptide Select summary report

1: [ALBU_HUMAN](#) Mass: 71317 Total S: 121 emPAI: 10.91

Albumin precursor - Homo sa

[ALBU_HUMAN](#) has previously been identified in:

1: Richard et al. Apr 8, 2008 3:17:45

Query	Observed	Mr(exp)	Mr(Cal)	Mass	Delta	Score	Rank	Peptide
87	706.2956	705.2883	705.34			1.000	1	KCASLQK.F 58
121	386.6978	771.3810	771.43			0.999	1	KAAKLPK.I 58
223	438.2795	874.4372	874.5005			0.998	1	RLSQGPK.A 223 224 225
143	395.2110	708.4090	708.4644	-70	0	0.0261	2	KLVYDIK.V 58
264	464.2065	926.3908	926.4061	-95	0	1.804	2	KLYEIAK.R 367
282	440.6891	879.3436	879.4238	-80	0	0.6053	1	KAEFAVVK.L 288 289

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Now that we have covered instrument integration, let's look at how we handle all those search results. We can take advantage of the database backend when viewing and analyzing search results and filter the results as we wish.

Mascot search result filtering, approval and annotation

48: [UBIQ_BOVIN](#) Mass: 8559 Total Score: 70 Queries Matched: 4 emPAI: 1.80
Ubiquitin - Bos taurus (Bovine)



Query	Observed	Mr(exp)	Mr(Calc)	ppm	Miss	Score	Expect	Rank	Peptide
233	534.2730	1066.5314	1066.6135	-77	0	41	0.027	1	K.ESTLHLVLR.L
231	541.2346	1080.4546	1080.5451	-84	0	35	0.0695	1	R.TLSDYNIQK.E
1672	894.3764	1786.7422	1786.9200	-99	0	45	0.0067	1	K.TITLEVPSDTIENVK.A 1672

Proteins matching the same set of peptides:

[UBIQ_CAMEL](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Camelus dromedarius (Dromedary) (Arabian camel)

[UBIQ_CANFA](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Canis familiaris (Dog)

[UBIQ_CAVPO](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Cavia porcellus (Guinea pig)

[UBIQ_CERCA](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Ceratitis capitata (Mediterranean fruit fly)

[UBIQ_CHICK](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Gallus gallus (Chicken)

[UBIQ_CHING](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Cricetus griseus (Chinese hamster)

[UBIQ_DROME](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Drosophila melanogaster (Fruit fly)

[UBIQ_FELCA](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Felis silvestris catus (Cat)

[UBIQ_GORGO](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Gorilla gorilla gorilla (Lowland gorilla)

[UBIQ_HORSE](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Equus caballus (Horse)

[UBIQ_HUMAN](#) Mass: 8559 Score: 70 Queries Matched: 4
Ubiquitin - Homo sapiens (Human)

[UBIQ_HUMAN](#) has previously been selected by:
S. richardj on Apr 8, 2008 3:54:01 PM.

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Annotations about the selection can be recoded during the approval process. Proteins that have been approved can then be used for MCP conforming reports.

Custom results formatting

	A	B	C
1	Experiment ID	EXP-070700322	Mascot Search URL
2			http://shark/mascot/cgi/master_results.pl?file=../data/20071014/F029462.dat
3			http://shark/mascot/cgi/master_results.pl?file=../data/20071015/F029464.dat
4			http://shark/mascot/cgi/master_results.pl?file=../data/20071015/F029466.dat
5			http://shark/mascot/cgi/master_results.pl?file=../data/20071015/F029467.dat
6			http://shark/mascot/cgi/master_results.pl?file=../data/20071015/F029468.dat
7			http://shark/mascot/cgi/master_results.pl?file=../data/20071015/F029469.dat
8			
9			
10			
11			
12			

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Depending on a customer's experience and the type of experiment, different types of reports may be required. A very simple report might just consist of links to the Mascot search results or a list of protein accession numbers per a sample.

Custom results formatting

	A	B	C	D	E	G	H	I
1	Date	5/25/2008						
2	Project	P-070700045	Id proteins that complex DEADbox helicase Dhh1p					
3	Study	S-070700052	DEADbox Co IP					
4	Experiment	Exp-070700322	DEADbox Co IP					
5	Sample	S-070925-00026	DEADBox 1					
6	Search ID	mss-15102007-00001						
7								
8								
9	Accession Number	Description	Score	No. Pep	Length	Mass	pI	Seq. cov. (%)
10	TRFE_HUMAN	Serotransferrin precursor (Transferrin) (S	941	42	698	79280.47	6.81	50
11	ALBU_HUMAN	Serum albumin precursor - Homo sapien	846	58	609	71317.25	5.92	66
12	KCRM_HUMAN	Creatine kinase M-type (EC 2.7.3.2) (Cre	515	36	381	43301.98	6.77	71
13	GELS_HUMAN	Gelsolin precursor (Actin-depolymerizing	476	31	782	86043.34	5.9	40
14	TAU_HYLLA	Microtubule-associated protein tau - Hyl	443	28	776	81190.89	6.5	27
15	CATA_HUMAN	Catalase (EC 1.11.1.6) - Homo sapiens	380	26	527	59946.84	6.9	43
16	MYG_HUMAN	Myoglobin - Homo sapiens (Human)	356	20	154	17229.98	7.14	75
17	ANT3_HUMAN	Antithrombin-III precursor (ATIII) - Homo	311	23	464	53025.04	6.32	38

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A more advanced report would include Protein names, accession numbers, Mascot Score and coverage in one worksheet with the Peptide information and modification localization in the second work sheet.

Custom results formatting



Proteomics core service lab

Barnett College

Date	5/25/2008	
Project	P-070700045	Id proteins that complex DEADbox helicase Dhhl1p
Study	S-070700052	DEADbox Co IP
Experiment	Exp-070700322	DEADbox Co IP
Sample	S-070925-00026	DEADBox 1
Search ID	mss-15102007-00001	

Accession Number	Description	Score	No. Pep	Length	Mass	pl	Seq. cov. (%)
TRFE_HUMAN	Serotransferrin precursor (Transferrin) (S	941.5	42	698	79280.47	6.81	50
ALBU_HUMAN	Serum albumin precursor - Homo sapiens	846.2	58	609	71317.25	5.92	66
KCRM_HUMAN	Creatine kinase M-type (EC 2.7.3.2) (Cre	515.4	36	381	43301.98	6.77	71
GELS_HUMAN	Gelsolin precursor (Actin-depolymerizing	475.7	31	782	86043.34	5.9	40
TAU_HYLLA	Microtubule-associated protein tau - Hylot	443.5	28	776	81190.89	6.5	27
CATA_HUMAN	Catalase (EC 1.11.1.6) - Homo sapiens (t	380.2	26	527	59946.84	6.9	43
MYG_HUMAN	Myoglobin - Homo sapiens (Human)	356.3	20	154	17229.98	7.14	75
ANT3_HUMAN	Antithrombin-III precursor (ATIII) - Homo	310.8	23	464	53025.04	6.32	38

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Report formats that are already in use can be imported into Integra and with a little initial configuration can be produced automatically for each sample analyzed. Custom reports can also draw in information for outside data sources as long as Excel can interface to them. Data from another database in the lab for example. We've exposed the externalid column on the Experiment table so you can use this as a foreign key to the information.

Reporting to publication standards (MCP guidelines)

1. Supporting information
2. Information for each protein sequence identified
3. Additional potentially valuable information
4. Quantitative proteomic results supporting information
5. Posttranslational modification reporting
6. Peptide Mass Fingerprinting
7. Minimum set of protein sequences
 - Include MS/MS data as supplemental material

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Mascot Integra can produce reports that conform to the MCP reporting guidelines. This makes it a snap to generate the supporting information required by journals when the results are ready to be published.

Example MCP report

Export publication report

MCP PMF report parameters

Protein e-value threshold*

Calibration method*

Exclusion of contaminant ions*

Resolution*

Mascot Distiller version*

Sequence database release*

Export sample preparation details:

Export Mascot Distiller parameters:

Export peptide matches:

Export table of m/z values:

Annotate pmf spectrum with

Add link to report to experiment notes field?

*Required field

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As some of you will remember last year we covered Integra and the MCP guidelines. The report takes information captured while running the experiment and along with a small amount of additional information that may be missing depending on the peaklist format that was used. The core lab can optionally chose to make a link to the final report available to the customer.

Example MCP report

	A	B	C	D	E	F	G	H	I	J	K
1	EXP:07100056	Gel 1 Sec16p binding proteins									
2											
3	Sample preparation conditions										
4	Proteolytic digestion conditions: 10 mg of each sample were diluted using 10 ul of 25mM AmBic and subjected to proteolytic digestion using 50 mg of Trypsin at 37 degrees celcius for 16 hours.										
5											
6	Chemical demitisation step 1: 10 mg of each sample were diluted using 25 ul of 10 mM DTT in 25mM AmBic and incubated at 98 degrees celcius for 1 hours.										
7											
8	Chemical demitisation step 2: 10 mg of each sample were diluted using 25 ul of Iodacetamide and incubated at 21 degrees celcius for 45 minutes.										
9											
10	Purification step 1: Samples were purified by Blotting. Samples were diluted using 0.1%TFA/80% ACN. Samples were applied to C18 columns. The purified samples were then washed in 50 ul of 0.1%TFA/H ₂ O.										
11											
12											
13											
14											
15	Peak picking parameters										
16	Peak picking program: MDRO (Mascot Distiller engine) 2.1.1										
17											
18	Database search parameters										
19	Database search conditions set 1										
20	Search engine: Mascot 2.2.03										
21	Database: Sprot Sprot_62.1.fasta										
22	Database Size: 261513										
23	Taxonomy: All entries										
24	Database Size after Taxonomy: 261513										
25	Peptide Mass Accuracy: 100 ppm										
26	Maximum missed cleavages: 1										
27	Fixed modifications: Carbamidomethyl (C)										
28	Variable modifications: Acetyl (Protein N-term), Gln->pyro-Glu (N-term C), Oxidation (M)										
29	Enzyme: Trypsin										
30	Resolution: 10,000										
31	Calibration: Internal trypsin										
32	Exclusion of contaminant ions: None										
33											
34	Protein hit assignment criteria : FMP protein identifications were accepted if the expectation value (e-value) calculated by Mascot for the protein hit was below the 0.05 threshold. The most best non-homologous protein hit was determined by using NCBI BLASTCycler with the following conditions: 40% identical residues; 50% minimum length coverage on one of the pr										
35											
36											
37	SearchID	Search title	Source file	Protein Access	Protein Description	Mascot Score	Mascot e-value	Next best hit	Next best hit Mascot Score	Next best hit Mascot e-value	Number matched peaks
38	mss-19102007-00002	Id Gel 1 Sec16p binding proteins E:VMSDdata2RUJRECO_NEIMA	E:VMSDdata2RUJRECO_NEIMA	DNA repair protein recO	DNA repair protein recO	72	0.02	VG15_BPMU	56	0.70	10
39	mss-19102007-00003	Id Gel 1 Sec16p binding proteins E:VMSDdata2RUJRMixture 1	E:VMSDdata2RUJRMixture 1	Mixture from proteom: "S	Mixture from proteom: "S	118	4.11E-07	NA	NA	NA	37
40				SVY (GSEDSL							
41				RDQ2_RAT							
42	mss-19102007-00005	Id Gel 1 Sec16p binding proteins E:VMSDdata2RUJRMixture 1	E:VMSDdata2RUJRMixture 1	Mixture from proteom: "H	Mixture from proteom: "H	126	6.57E-11	SYO_DEIRA	50	0.40	36
43				K1C9_HUMAN	Keratin, type I cytoskeletal 9 (Cytokeratin-9) (CK-9) (Keratin-9) - Homo sapiens (Human)						
44				KCCT_HUMAN	Keratin, type II cytoskeletal 1 (Cytokeratin 1) (CK-1) (Keratin-1) (K1) (K1a cytokeratin) (Pilar alpha protein) - Homo sapiens (Human)						
45	mss-19102007-00006	Id Gel 1 Sec16p binding proteins E:VMSDdata2RUJRTSE_HUMAN	E:VMSDdata2RUJRTSE_HUMAN	Keratin, type I cytoskeletal	Keratin, type I cytoskeletal	117	5.22E-07	KCCT_HUMAN	86	0.08	23
46	mss-19102007-00007	Id Gel 1 Sec16p binding proteins E:VMSDdata2RUJRMixture 1	E:VMSDdata2RUJRMixture 1	Mixture from proteom: "H	Mixture from proteom: "H	209	1.26E-16	NDH1_PPICP	61	0.21	36
47				VATB_YEAST	Vacuolar ATP synthase subunit B (EC 3.6.3.14) (V-ATPase B subunit) (Vacuolar proton pump B subunit) (V-ATPase 57 kDa)						
48				ACT_HYDAT	Actin, non-muscle 6.2 - Hydra attenuata (Hydra) (Hydra vulgaris)						
49	mss-19102007-00008	Id Gel 1 Sec16p binding proteins E:VMSDdata2RUJRMixture 1	E:VMSDdata2RUJRMixture 1	Mixture from proteom: "Y	Mixture from proteom: "Y	147	1.60E-09	SYA_GLIUK06	59	0.36	26
50				Y218_AC1AD	UPF0246 protein AC1AD0218 - Acetabacter sp. (strain ADP1)						
51											
52	MCP Report Peptides: / MCP Report Peptides: / Peak detection parameters: / Peak detection parameters: / Fake discovery rate: / mss-19102007-00010										

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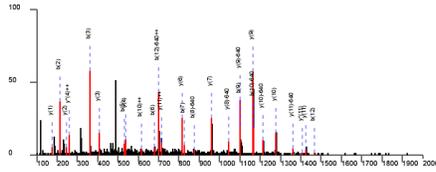
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The report is in the format of an excel sheet.

Example MCP report

MS/MS fragmentation of **DVFLGMLYEYAR**
 Match to query 1530 from mascot search mss-15102007-00005 (M05y1206.pkl 98166 (task EXP-070700322-1302) ABRF2006 ESI QTOF
 From datafile E:\MSData2\ABRF-s\PRG2006\98166\M05y1206.pkl



Monoisotopic mass of neutral peptide M_r(calc): 1638.7752
Fixed modifications: Carbamidomethyl (C)
Variable modifications:
M(6): Oxidation (M), with neutral losses 63.9983 (shown in table), 0
Ions Score: 45 **Expect:** 0.00331764
Matches (Bold Red): 28/172 fragment ions using 130 most intense peaks

#	b	b ⁺⁺	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y ⁻	y ⁺⁺	y ⁰	y ⁰⁺⁺	#
1	116.0342	58.5207	98.0237	49.5155	D							13
2	215.1026	108.055	197.0921	99.0497	V	1460.7573	730.8823	1443.7307	722.369	1442.7467	721.877	12
3	362.171	181.5892	344.1605	172.5839	F	1361.6889	681.3481	1344.6623	672.8348	1343.6783	672.3428	11
4	475.2551	238.1312	457.2445	229.1259	L	1214.6204	607.8139	1197.5939	599.3006	1196.6099	598.8086	10
5	532.2766	266.6419	514.266	257.6366	G	1101.5364	551.2718	1084.5098	542.7586			

Accounting and Billing

- **A list of accounts to be billed can be run:**
 - Monthly
 - Quarterly
 - or whenever you like.
- **Integra supplies the breakdown of samples analyzed by method for an experiment to an Excel template that can be used for billing**
- **The template holds the billing information and queries to integrate with an existing customer contact information databases**

Now that all the work has been done and the results distributed to the customer we need to bill them for work done. We can generate a list of experiments that are ready for billing in a chosen time period. All the information about the number of samples processed by different tasks during an experiment can be reported. Just as existing results reporting templates can be reused, existing accounting forms can also be used. The business logic for the accounting resides in the Excel template rather than Integra, allowing for the support of a wide range of accounting methods. The Excel sheet can also interface with existing databases that contains the customers contact information. Those databases can vary from a simple text file or Excel sheet to Microsoft Access or a SQL server.

Example billing method

Contacts.xls									
	A	B	C	D	E	F	G	H	I
1	BudgetID	FirstName	LastName	Address	Title	WorkPhon	Email		
2	1000	Bram	Stoker	101 Learning Way, Barnett College, NY	Dr	683-797-23	Stoker@barnett.edu		
3	2000	H.P.	Lovecraft	101 Learning Way, Barnett College, NY	Dr	683-967-63	Lovecraft@barnett.edu		
4	3000	Shirley	Jackson	101 Learning Way, Barnett College, NY	Dr	683-276-87	Jackson@barnett.edu		
5	4000	Franz	Kafka	101 Learning Way, Barnett College, NY	Dr	683-774-87	Kafka@barnett.edu		
6	4500	Kathe	Koja	101 Learning Way, Barnett College, NY	Dr	683-746-62	Koja@barnett.edu		
7	5000	Robert Louis	Stevensor	101 Learning Way, Barnett College, NY	Dr	683-259-11	Stevensor@barnett.edu		
8	6000	Arthur	Machen	101 Learning Way, Barnett College, NY	Dr	683-566-50	Machen@barnett.edu		
9	7000	William Peter	Blatty	101 Learning Way, Barnett College, NY	Dr	683-576-00	Blatty@barnett.edu		
10	8000	Mary	Shelley	101 Learning Way, Barnett College, NY	Dr	683-566-50	Shelley@barnett.edu		
11	9000	Stephen	King	101 Learning Way, Barnett College, NY	Dr	683-510-48	King@barnett.edu		
12									
13									
14									
15									
16									
17									

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Here I have a very simple customers database. I am using the BudgetID field as a key value to connect the customer to the their contact information in an Excel sheet.

Example billing method

Pricing example 1.xls					
	A	B	C	D	E
1	2D Gel-Based Analyses	2D-DIGE (per gel, includes image analysis)	2-dye	300	
2		2D-DIGE (per gel, includes image analysis)	3-dye	330	
3		2D-gel spot excision/in-gel digest /zipit/MS/bioinformatics	per spot	50	
4		2D-gel stained and imaged with Sypro Ruby only (no CY dyes or image analysis)	Each	140	
5	MS Analyses (no prior sample)	ESI-MS/MS (infusion)	Hour	60	
6		LC-MS/MS	Hour	60	
7		MALDI-TOF and -TOF/TOF	Hour	50	
8	Multidimensional HPLC/tandem	Ion Exchange fractionation of peptide digest, LC-MS/MS (per 10 fractions: standard 1h reverse phase gradient)	Run	500	
9	Protein Identification	1D band excision/in-gel digest /1hr MS/bioinformatics	per band	100	
10		Additional MS instrument time	per hr	60	
11		In-solution sample preparation /digest/hr MS/bioinformatics	per sample	100	
12					
13					
14					
15	Dye	LCMSMS	MALDI		
16	2 CyDyes	per hour	MALDI-TOF		
17	3 CyDyes	per fraction MudPIT	MALDI -TOF/TOF		
18	Other		ESI-MS/MS (infusion)		
19					
20					

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My accounting report contains all the pricing information is a separate worksheet.

Example billing method

Pricing example 1.xls						
	A	B	C	D	E	F
1	Date	5/19/2008				
2	Project					
3	Study					
4	Experiment					
5						
6	Principle Investigator	#N/A				
7	Budget Code					
8	Address	#N/A				
9	Phone No	#N/A				
10	Email	#N/A				
11						
12						
13						
14						
15		Item		Count	Unit price	
16	2D Gel-Based Analyses	Number of gels	2 CyDyes	0	300	\$0
17		Number of Spots		0	50	\$0
18					Sub total	\$0
19	MS Analyses	LC-MS/MS	per hour	0	60	\$0
20		MALDI-TOF	per hour	0	50	\$0
21					Sub total	\$0
22	Protein Identification	From 1D Bands		0	100	\$0
23		Additional MS time	per hour	0	60	\$0
24		In-solution		0	100	\$0
25					Sub total	\$0
26					Total	\$0
27						
28						
29						
30						
31						

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Which I have used to create a report template.

Example billing method 1

1211168949185.xls-00034.xls							
	A	B	C	D	E	F	
1	Date	5/18/2008					
2	Project	P-070900055	Sec16p biding proteins				
3	Study	S-071000066	Sec16p biding proteins				
4	Experiment	EXP-071000356	Gel 1 Sec16p biding proteins				
5							
6	Principle Investigator	Dr William Peter Blatty					
7	Budget Code	7000					
8	Address	101 Learning Way, Barnett College, NY					
9	Phone No	683-576-0052					
10	Email	Blatty@barnett.edu					
11							
12							
13							
14							
15		Item	Count	Unit price			
16	2D Gel-Based Analyses	Number of gels	2 CyDyes	0	300	\$0	
17		Number of Spots		0	50	\$0	
18					Sub total	\$0	
19	MS Analyses	LC-MS/MS	per hour	0	60	\$0	
20		MALDI-TOF	per hour	0	50	\$0	
21					Sub total	\$0	
22	Protein Identification	From 1D Bands		38	100	\$3,800	
23		Additional MS time	per hour		60	\$0	
24		In-solution		0	100	\$0	
25					Sub total	\$3,800	
26					Total	\$3,800	
27							
28							
29							
30							
31							
32							
33							
34							

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Here is a bill for a 1D gel experiment. Integra filled out the project, study, and experiment information along with the number of bands analyzed. Excel looked up the contact information based on the budget code Integra supplied.

Example billing method 1

 Proteomics core service lab		Barnett College	
Date	5/19/2008		
Project	P-070900055	Sec16p biding proteins	
Study	S-071000066	Sec16p biding proteins	
Experiment	EXP-071000356	Gel 1_Sec16p biding proteins	
Principle Investigator	Dr William Peter Blatty		
Budget Code	7000		
Address	101 Learning Way, Barnett College, NY		
Phone No	683-676-0052		
Email	Blatty@barnett.edu		
	Item	Count	Unit price
2D Gel-Based Analyses	Number of gels	2 CyDyes	0 300 \$0
	Number of Spots		0 50 \$0
			Sub total \$0
MS Analyses	LC-MS/MS	per hour	0 60 \$0
	MALDI-TOF	per hour	0 50 \$0
			Sub total \$0
Protein Identification	From 1D Bands		38 100 \$3,800
	Additional MS time	per hour	60 \$0
	In-solution		0 100 \$0
			Sub total \$3,800
		Total	\$3,800

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Add a header to the sheet and print it out and you have the final bill. If the accounting department needs the information in a different format then you could create a different template.

Customer interface

Experiment Id	External Id	Experiment Description	Experiment Status	Last task completed
EXP-080500363		M-phase synchronised centrosome fraction	In-progress	Mascot
Task	Status	Processed	Notes	
Sample Mix	In-progress	 100		
Off-line LC	In-progress	 100		
Digest	In-progress	 100	Samples diluted 4 fold in 100mM Amm Bic. Processed fractions from Mixture 1 (source 0001 & 0002). Mixture 2 will be run on 15/05/2008	
Off-line LC	In-progress	 100		
Off-line LC	In-progress	 100		
Peak lists	In-progress	 100		
Mascot	In-progress	 100	Identifications to date	
Follower	Ready	 100		
Follower	Planned	 100		
Overall progress				

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Our customers are not going to be happy with just a bill so Integra provides a simple password protected webpage interface to the experiment status page.

Customers can use this interface to follow the progress of their samples hopefully reducing the number of inquiry calls. The interface gives an indication of where in the process the samples are and how complete is the experiment.

Customer interface

 **MASCOT**Integra 

Sample	Parent	Processed?
S-080515-00011 Mixture 1 1-2	S-080515-00001 PS-0001 S-080515-00002 PS-0002	✓
S-080515-00012 Mixture 2 3-4	S-080515-00003 PS-0003 S-080515-00004 PS-0004	✓
S-080515-00013 Mixture 3 5-6	S-080515-00005 PS-0005 S-080515-00006 PS-0006	✗

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Clicking on a progress bar for a task gives a more detailed view of which samples have been processed through the task, and which are currently waiting to be run.

Customer interface

External Users

 Return

 Add

 Delete

<input type="checkbox"/>	User Id	Description
<input type="checkbox"/>	Blatty	William Peter Blatty
<input type="checkbox"/>	Jackson	Shirley Jackson
<input type="checkbox"/>	Kafka	Franz Kafka
<input type="checkbox"/>	King	Stephen King
<input type="checkbox"/>	Koja	Kathe Koja
<input type="checkbox"/>	Lovecraft	H. P. Lovecraft
<input type="checkbox"/>	Machen	Arthur Machen
<input type="checkbox"/>	Scott	Everybody knows Scott
<input type="checkbox"/>	Shelly	Mary Shelly
<input type="checkbox"/>	Stevenson	Robert Louis Stevenson
<input type="checkbox"/>	Stoker	Bram Stoker

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Access to the customer interface is controlled by a simple username and password list that does not give access to the complete system. Integra can also email administrators on errors, users on experiment status change and on completion of Mascot searches/importing.

Instrument usage, success rates and other metrics

- **Reports generated per a month/year/rolling year/whenever**
- **Service usage statistics:**
 - No. Samples
 - No. Runs
 - No. Users
 - Sample success rates
 - Samples per a customer/project
 - No. runs by analysis type by project

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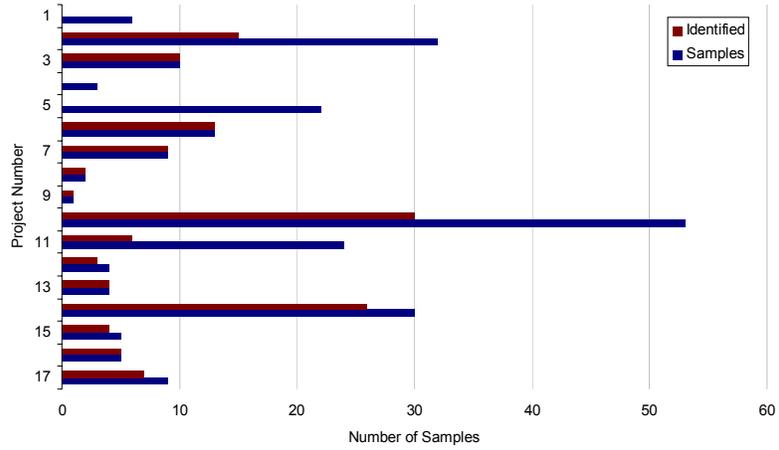
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Because Mascot Integra can record all the information about the experiments, it can be used to generate reports about instrument usage, analysis success rate, and other metrics useful to a core lab. These reports, like almost all reports in Integra, are stored as templates and can be generated every month, year or as necessary. The reports can range from the simple, e.g. the number of samples analyzed or the number samples run on an instrument to more complex, such as a breakdown of the number of runs by analysis type and project.

Instrument usage, success rates and other metrics

Analysis of samples by project



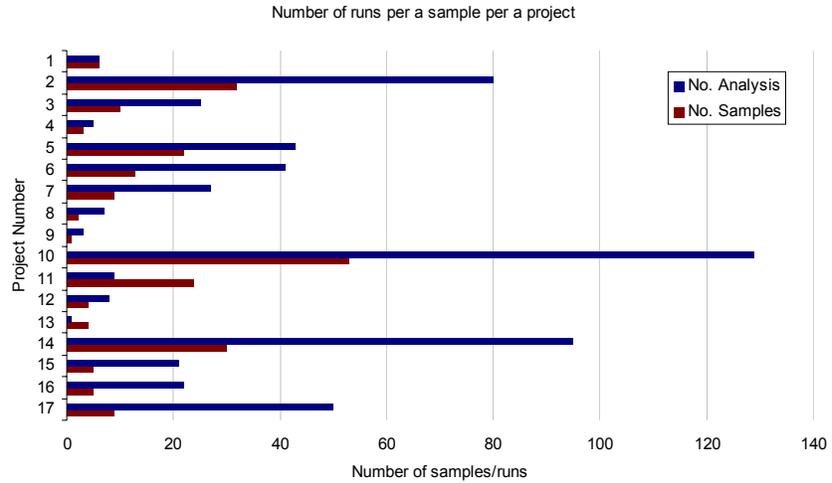
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Here are a few example reports I generated from data in my system. The number of successfully analyzed samples per project

Instrument usage, success rates and other metrics



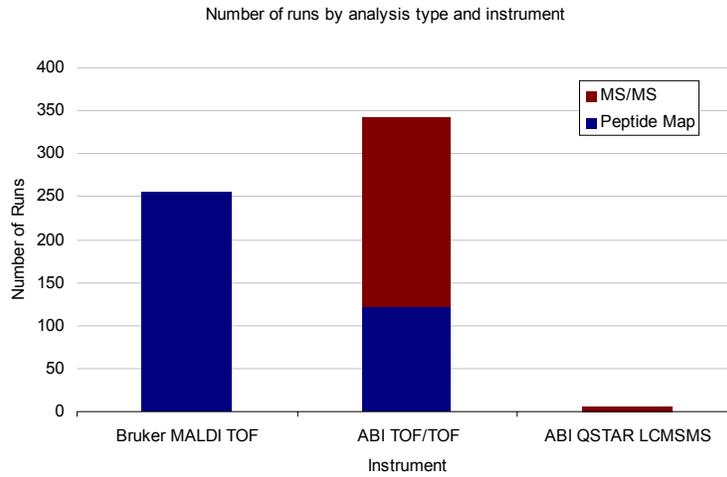
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The number of runs per a sample per a project.

Instrument usage, success rates and other metrics



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And the number of acquisitions per instrument. You can generate metrics based on pretty much any information stored in the system.

Mascot Integra provides:

- **Sample and project tracking.**
- **Flexible experiment design**
- **One or two way integration with instruments and software packages**
- **Powerful reporting system**
 - Search results
 - Accounting and billing reports
 - Core lab performance metrics
- **Easy to use interface for collaborators to**

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In this presentation I hope I have shown you how Mascot Integra can help run a core lab.

Integra provides the standard sample and project tracking that you would expect from any database suitable for a core lab. It also provides a flexible experiential design environment. Integra can integrate with all the common proteomics instruments and software with one or two-way communication which is combined with Mascot Daemon for automated data processing. The powerful reporting systems enables the design of standardised reports for everything from search results, to accounting and billing and performance metrics. Finally there is an easy to use interface for the labs customers to monitor a projects progress.