

■ What is SPIRIT?

SPIRIT is a Java-based software to handle complex life science research data. It was originally developed for internal use by Actelion Pharmaceuticals Ltd. (Switzerland).

SPIRIT is used by more than hundred researchers in Actelion's Drug Discovery Departments. It is also used by the Actelion Research Biobank to manage its preclinical and clinical samples and data.

SPIRIT's data concept is generic and sample-centric. It can be configured to handle any type of samples and their relationships, including animals or humans. Results can be linked to samples and have an unlimited number of input and output parameters. Physical storage locations are managed by a fully configurable inventory system. Finally, a graphical study editor allows to plan, display, and record the progress of experiments involving groups of samples and results over time.

■ Software Structure

SPIRIT presents **four perspectives** to the user. Each perspective has its own tab in the main program window, but they are all linked. In these tabs, the user can do the following:

- **Samples** Create samples, find and display them as well as all related samples, edit sample information, print labels
(Administration: Define sample types and their parameters)
- **Locations** Register the location of samples and containers, find and move them, display inventory lists, print container labels (Admin.: Create locations)
- **Results** Store results, find and display them in pivoted tables, export results in spreadsheet format, visualize them in the DataWarrior software
(Administration: Define tests)
- **Studies** Graphically design and monitor the evolution of a **study** (experiment).

Studies consist of the following elements:

- multiple **samples** (including animals or humans) that are
- arranged in **groups** and subgroups (such as treated vs. control)
- in different **phases** (or time points) at which they are planned to
- undergo **treatments**,
- **samplings** (generating new samples), and
- **measurements** (generating results)

■ Database

SPIRIT can be used with any relational database, such as Oracle or MySQL.

■ Configuration

Each implementation of SPIRIT requires the definition of **sample types** (such as animals, blood, organs, DNA, cells) with their parameters; **container types** and **storage locations**, and **tests** to store results.

SPIRIT also requires the registration of **users** with different rights. Users may be part of a **group** with specific rights. It is delivered with its own user database or it can be connected to an existing system.

■ Extensions

SPIRIT links directly with Actelion's **DataWarrior** software to filter and display complex, multidimensional data. DataWarrior is available for free from www.openmolecules.org.

The main SPIRIT software is accompanied by a suite of applications built to support specific users in dedicated tasks:

■ AnimalCare	Monitoring of animal studies (randomization, weighing, measuring, labeling)
■ StockCare	Sample Inventory for cells, antibodies, etc.
■ SlideCare	Generation of paraffin blocks and microscopy slides
■ BioViewer	Simple sample information viewer with basic functionality (scanning, aliquoting)

At Actelion, SPIRIT also integrates seamlessly with the company's "Niobe" Electronic Lab Notebook (ELN) software, the "ORBIT" raw data file management system, and the "ORBIT Image Analysis" software.

■ Collaboration

SPIRIT is designed to provide many users a unified environment to manage their data, to collaborate, and to share their results. This is achieved by maintaining a single, system-wide configuration. Although users and groups have restricted rights, SPIRIT was not designed to completely isolate users from each other.

The latter could, in principle, be achieved through independent SPIRIT implementations. This will inevitably lead to diverging configurations, at the expense of data interchangeability.

■ Audit trail, backup, data recovery

Every modification in the SPIRIT database is recorded (time stamp, user, change). For each sample, a history can be displayed. Roll-back to a previous state is possible.

The database that SPIRIT connects with must be backed up, but no further backups are required.

Although SPIRIT stores its data in a relational database, it is possible to export its complete content in a (potentially huge) flat spreadsheet file at once.

■ Hardware integration

SPIRIT specifically supports this peripheral hardware:

- Brother P-Touch label printers
- barcode readers
- Mettler-Toledo balances

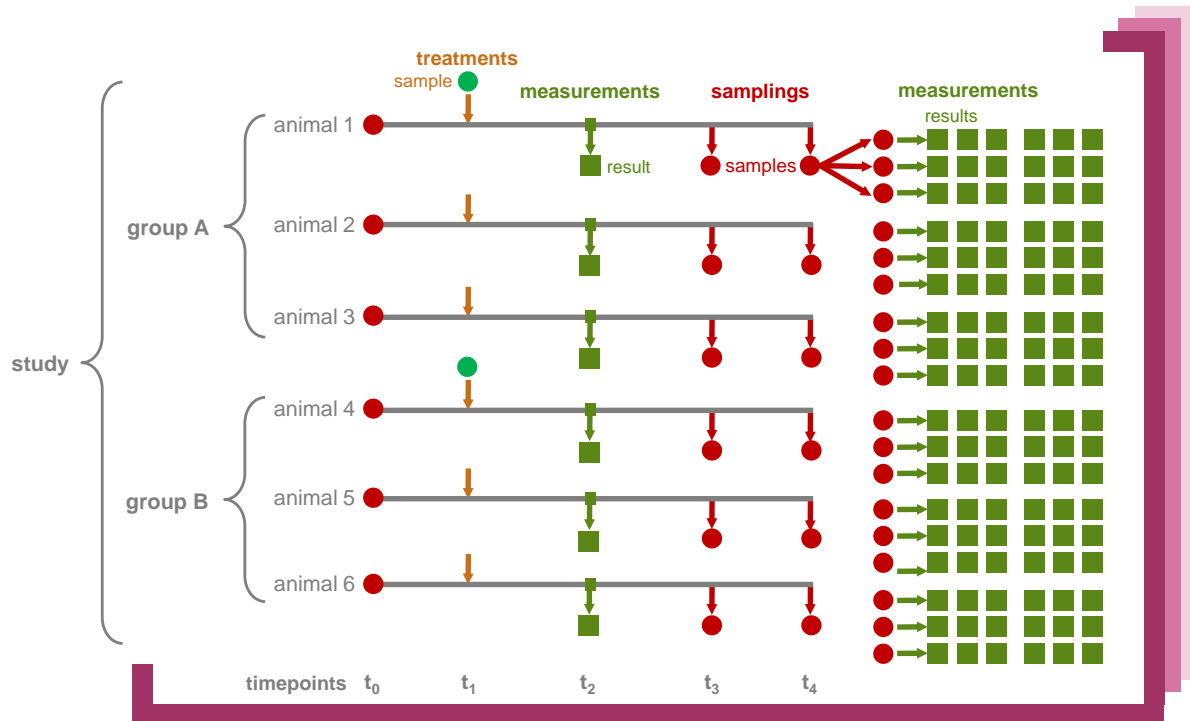
■ Implementations

- Actelion Pharmaceuticals Ltd., Allschwil, Switzerland
Drug Discovery Departments, including Actelion Research Biobank
- University Hospital Basel, Switzerland
Departement Biomedicine

■ Contact Information

- Software: [Joël Freyss](#)
- Applications: [Geoffroy Bourquin](#)
- Concept: [Oliver Peter](#)

Appendix 1: SPIRIT study concept



Appendix 2: SPIRIT Screenshots

Biosamples list:

The screenshot shows the SPIRIT software interface with the 'Biosamples' tab selected. The main window displays a table of biosamples with columns for #, StudyId, Group, Phase, Container/Location, SampleId, Metadata, Comments, Owner, and Cre.Date. The table contains 24 rows of data, including details for various studies (e.g., S-00077) and sample types (e.g., Vehicle, low dose). A left-hand sidebar provides filters for Study, BioType, Container, and TopParents, along with search options. The status bar at the bottom indicates '75 Biosamples / 75 Containers' and '109M of 518M'.

#	StudyId	Group	Phase	Container/Location	SampleId	Metadata	Comments	Owner	Cre.Date
1	S-00077	1. Vehicle		Cage	999050	1. Vehicle	Rat, RatWistar, M, 22.02.12	research/informatics/giraudi	03.09.12
2	S-00077	1. Vehicle	d00	FluidX_20ml	CELO01699	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
3	S-00077	1. Vehicle	d06	FluidX_20ml	CELO01714	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
4	S-00077	1. Vehicle	d24	FluidX_20ml	CELO01729	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
5	S-00077	1. Vehicle	d48	FluidX_20ml	CELO01744	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
6	S-00077	1. Vehicle		Cage	999051	1. Vehicle	Rat, RatWistar, M	research/informatics/giraudi	03.09.12
7	S-00077	1. Vehicle	d00	FluidX_20ml	CELO01700	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
8	S-00077	1. Vehicle	d06	FluidX_20ml	CELO01715	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
9	S-00077	1. Vehicle	d24	FluidX_20ml	CELO01730	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
10	S-00077	1. Vehicle	d48	FluidX_20ml	CELO01745	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
11	S-00077	1. Vehicle		Cage	999052	1. Vehicle	Rat, RatWistar, M	research/informatics/giraudi	03.09.12
12	S-00077	1. Vehicle	d00	FluidX_20ml	CELO01701	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
13	S-00077	1. Vehicle	d06	FluidX_20ml	CELO01716	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
14	S-00077	1. Vehicle	d24	FluidX_20ml	CELO01731	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
15	S-00077	1. Vehicle	d48	FluidX_20ml	CELO01746	1. Vehicle	Blood/Lymphocytes	blabla	04.09.12
16	S-00077	2. low dose		Cage	999053	2. low do	Rat, RatWistar, M	research/informatics/giraudi	03.09.12
17	S-00077	2. low dose	d00	FluidX_20ml	CELO01702	2. low do	Blood/Lymphocytes	blabla	04.09.12
18	S-00077	2. low dose	d06	FluidX_20ml	CELO01717	2. low do	Blood/Lymphocytes	blabla	04.09.12
19	S-00077	2. low dose	d24	FluidX_20ml	CELO01732	2. low do	Blood/Lymphocytes	blabla	04.09.12
20	S-00077	2. low dose	d48	FluidX_20ml	CELO01747	2. low do	Blood/Lymphocytes	blabla	04.09.12
21	S-00077	2. low dose		Cage	999054	2. low do	Rat, RatWistar, M	research/informatics/giraudi	03.09.12
22	S-00077	2. low dose	d00	FluidX_20ml	CELO01703	2. low do	Blood/Lymphocytes	blabla	04.09.12
23	S-00077	2. low dose	d06	FluidX_20ml	CELO01718	2. low do	Blood/Lymphocytes	blabla	04.09.12
24	S-00077	2. low dose	d24	FluidX_20ml	CELO01733	2. low do	Blood/Lymphocytes	blabla	04.09.12

Planning a sampling:

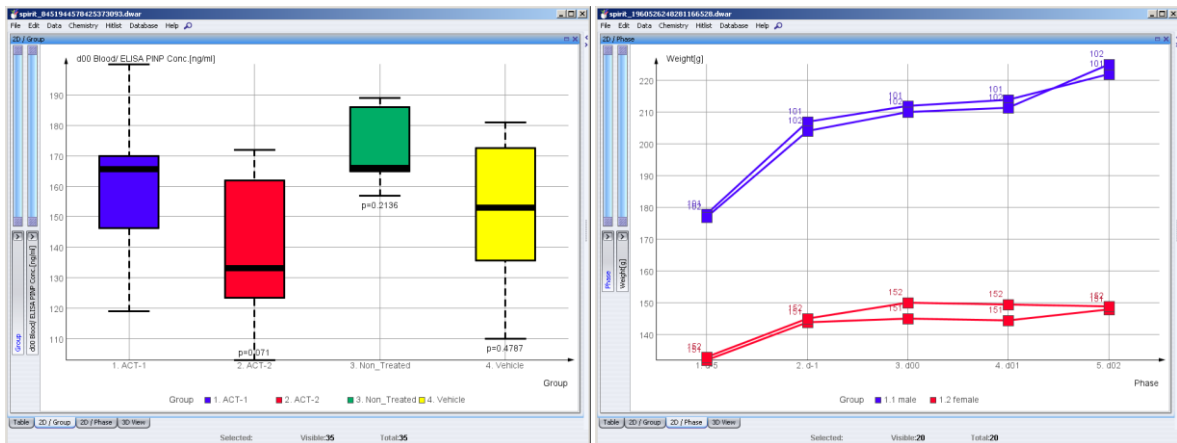
The screenshot shows the Label Printer software interface. On the left, there are options for different label types: Eppendorf 0.5ml (9 labels), FluidX 20ml (58 labels), Falcon 15ml (174 labels), Bottle (116 labels), and Slide (16 labels). The main window displays a table of biosamples with columns for #, Study, Group, Location, ContainerId, Infos, and Biosamples. The table contains 10 rows of data, including details for various studies (e.g., S-00063) and sample types (e.g., Healthy). A right-hand sidebar shows the 'Printer Config' section, including the printer name, media type (1.4PP Micronics), padding settings, and a preview of a label. The label preview shows the following text: BLOOD2673 | W-XXX, 3. Healthy, 01.07.12 - d00, ANL000899 [63], EDTA 1.0ml Test Group 1.

#	Study	Group	Location	ContainerId	Infos	Biosamples
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2673	S-00063 - IVA-XXX ANL000899 [63] 01.07.12 - d00	BLOOD2673:E
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2674	EDTA 1.0ml Test Group 1 S-00063 - IVA-XXX ANL000899 [63] 01.07.12 - d00 Hep. Li 1.0ml	BLOOD2674:H
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2675	S-00063 - IVA-XXX ANL000899 [63] 01.07.12 - d00 1.0ml	BLOOD2675:
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2693	S-00063 - IVA-XXX ANL000899 [63] 02.07.12 - d01	BLOOD2693:E
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2694	S-00063 - IVA-XXX ANL000899 [63] 02.07.12 - d01 Hep. Li 1.0ml	BLOOD2694:H
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2695	S-00063 - IVA-XXX ANL000899 [63] 02.07.12 - d01 1.0ml	BLOOD2695:
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2713	S-00063 - IVA-XXX ANL000899 [63] 06.07.12 - d05 EDTA 1.0ml Test Group 1	BLOOD2713:E
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2714	S-00063 - IVA-XXX ANL000899 [63] 06.07.12 - d05 Hep. Li 1.0ml	BLOOD2714:H
0	S-00063	3. Healthy		Eppendorf 0.5ml BLOOD2715	S-00063 - IVA-XXX ANL000899 [63] 06.07.12 - d05 1.0ml	BLOOD2715:

Results list:

The screenshot shows the Spirit software interface with a results list table. The table has the following columns: Study, Group, Treatment, TopParentId, TopParentNo, d00 Blood/ELISA PNP Conc (ng/ml), d01 Blood/ELISA PNP Conc (ng/ml), d02 Blood/ELISA PNP Conc (ng/ml), d03 Blood/ELISA PNP Conc (ng/ml), d04 Blood/ELISA PNP Conc (ng/ml), d05 Blood/ELISA PNP Conc (ng/ml), d06 Blood/ELISA PNP Conc (ng/ml), d07 Blood/ELISA PNP Conc (ng/ml), and d08 Blood/ELISA PNP Conc (ng/ml). The table contains 35 rows of data, with the 14th row highlighted in blue. The status bar at the bottom indicates '1013 Results - 35 rows, 29 columns'.

One-click export to DataWarrior:



Pivoting result tables:

The screenshot shows the 'Edit Pivot Table - BOX PLOT' dialog box. It has a 'Pivot Table' section with 'Row titles' and 'Column titles' fields. The 'Row titles' field contains: Study (Study), Group (Group), Treatment (Treatment), Phase (Phase Label), Compound (ActNo (ELN)), Biosample (TopParentId (Biotype)), Assay (ELISA). The 'Column titles' field contains: Result (Input/Analyte / Output/Value). There are also 'Display', 'Processing', and 'Deviation' options, and a 'DataWarrior Template' section with a 'DWTAT' field set to 'BoxPlot_Template.dwtat'.

Inventory management:

Spirit
Edit Export Tools Config Admin Help

Studies Biosamples Locations Results

Study: H91 - 04.K17 - Freezer -80°C - Tower A - A2 - 1: Human Brain RNA (Clontech Back-up @ 50 ng/ul)
Protected by CNS Biology
Updated by mawebj the 24.04.12

Name:
Reset Filter

Name	Type
H91	Bui
04.K17	Lac
Freezer -80°C	Fre
Tower A	Tow
A1	Sh
1: Human Brain RNA samples (Clontech)	Boi
2: Human Heart RNA samples (Clontech)	Boi
3: SynAging RNA samples	Boi
4: C57/Blk hAPP Tg mouse RNA samples	Boi
5: Rat Brain region RNA	Boi
6: Mouse Brain region RNA	Boi
A2	Sh
1: Human Brain RNA (Clontech Back-up @ 50 ng/ul)	Boi

	Testis	Amount: 40.0ul
1013770500		

Container:
 Location: H91 - 04.K17 - Freezer -80°C - Tower A - A2
 1: Human Brain RNA (Clontech Back-up @ 50 ng/ul):B/02
 ELB: ELB0029.0468

BioType: RNA
 Type: RNA
 Tissue Origin: Testis
 Species: Human
 Yield [ng/ul]: 50
 RIN:
 Treatment:
 Dose Tested/Final C.:

Metadata History Hierarchy Location Results Orbit
Graphical Table

H91 - 04.K17 - Freezer -80°C - Tower A - A2 - 1: Human Brain RNA (Clontech Back-up @ 50 ng/ul)												
A/01 1013770500	A/02 1013770500	A/03 1013770500	A/04 1013770500	A/05 1013770500	A/06 1013770500	A/07 1013770500	A/08 1013770500	A/09 1013770500	A/10 1013770500	A/11 1013770500	A/12 1013770500	
Brain, Cerebellum, Human, 50	Brain, whole, Human, 50	Brain, Fetal, Fetal, Human, 50	Fetal liver, Fetal liver, Human, 50	Heart, Human, 50	Kidney, Human, 50	Liver, Human, 50	Lung, Human, 50	Placenta, Human, 50	Prostate, Human, 50	Salivary gland, Human, 50	Skeletal muscle, Human, 50	
B/01 1013770500	B/02 1013770500	B/03 1013770500	B/04 1013770500	B/05 1013770500	B/06 1013770500	B/07 1013770500	B/08 1013770500	B/09 1013770500	B/10 1013770500	B/11 1013770500	B/12 1013770500	
Spleen	Testis	Thymus	Thyroid glan	Trachea	Uterus	Colon w/m	Small intes	Human Bow	Human Stor	Human Uter	Human Tons	
C/01 1013770500	C/02 1013770500	C/03 1013770500	C/04 1013770500	C/05 1013770500	C/06 1013770500	C/07 1013770500	C/08 1013770500	C/09 1013770500	C/10 1013770500	C/11 1013770500	C/12 1013770500	
Human Smc	Human Smc	Human Liver	Human Cok	Human Adip	Human Bloo	Human Pan	Human Lun	Human Bres	Human Saliv	Human Ovar	Human Man	
D/01 1013770500	D/02 1013770500	D/03 1013770500	D/04 1013770500	D/05 1013770500	D/06 1013770500	D/07 1013770500	D/08 1013770500	D/09 1013770500	D/10 1013770500	D/11 1013770500	D/12 1013770500	
Human Reti	Human brain	Human brain	Human Adr	Human brain	Human brain	Human brain	Human brain	Human brain	Human brain	Human brain	Human brain	
E/01 1013770500	E/02 1013770500	E/03 1013770500	E/04 1013770500	E/05 1013770500	E/06 1013770500	E/07 1013770500	E/08 1013770500	E/09 1013770500	E/10 1013770500	E/11 1013770500	E/12 1013770500	
Human brain	Human brain	Human brain	Human Dor	Human brain	Human brain	Human brain	Human brain	Human brain	Human brain	Human brain	Human brain	
F/01 1013770500	F/02 1013770500	F/03 1013770500	F/04 1013770500	F/05	F/06	F/07	F/08	F/09	F/10	F/11	F/12	
Human Spin	Human brain	Human brain	Human brain									
G/01	G/02	G/03	G/04	G/05	G/06	G/07	G/08	G/09	G/10	G/11	G/12	
H/01	H/02	H/03	H/04	H/05	H/06	H/07	H/08	H/09	H/10	H/11	H/12	

Study screenshot:

S-00063 IVV-XXX: Bug searching

Responsibles: bourqug
 Created the 02.08.12 08:15 by bourqug
 Updated the 14.09.12 10:25 by bourqug

#	Group	Container/ Location	Sarrnpleid	Metadata
1.	WillBeSick	Case 4	ANL000837 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
2.	WillBeSick	Case 3	ANL000838 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
3.	WillBeSick	Case 1	ANL000839 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
4.	WillBeSick	Case 2	ANL000843 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
5.	WillBeSick	Case 5	ANL000849 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
6.	WillBeSick	Case 3	ANL000850 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
7.	WillBeSick	Case 2	ANL000852 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
8.	WillBeSick	Case 6	ANL000856 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
9.	WillBeSick	Case 1	ANL000863 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24
10.	WillBeSick	Case 1	ANL000870 1. WillBeSick	Rat, RatWistar, M, 25.06.12, 24

Timeline events (approximate dates):

- 01.07.12: WillBeSick (20 Animals), WillBeVerySick (20 Animals), Healthy (20 Animals)
- 02.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 06.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 09.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 13.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 16.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 20.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 23.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 27.07.12: Cmpd1 (all groups), Blood Aliquot (all groups)
- 30.07.12: Cmpd1 (all groups), Blood Aliquot (all groups), Blood Aliquot Test Sampling (all groups)

Metadata table tabs: Metadata | History | Study | Hierarchy | Location | Results | Orbit

SlideCare

SlideCare is used by the histopathology technician to

- 1) Define the sample arrangement on microscopy slides
- 2) Print the slide labels
- 3) Manage the slide inventory

The screenshot displays the SlideCare software interface for slide creation. It is divided into two main sections: the Slide Designer and the Slide Creation table.

Slide Designer:

- Animal to be used as model:** ANL000009 (Treated)
- Container:** Cassette
- Organ options:** Brain, Bouin, CD19; Left ventricle, Davidson, CD31; Right ventricle, Davidson, CD31; Right Lobe, Formalin 4%, HSP90; Left Lobe, Formalin 4%, HSP90.
- Slide Templates:** Slide1 (Brain, Bouin, CD19), Slide2 (Left ventricle, Davidson, CD31), Slide3 (Left Lobe, Formalin 4%, HSP90; Right Lobe, Formalin 4%, HSP90).
- Staining:** CD19, CD31, and an empty field.
- Copies:** 1 for each slide template.
- Buttons:** Load Template, Save Template.

Slide Creation Table:

#	Group	Container/Location	Sampleid	Metadata	Biosamples	Cre.User	Cre.Date	Cre.Date
1	1. Treated	Slide 2	ANL000009 1. Treated	Rat, RatDTOR, M, 09.08.12, POTES				
2	1. Treated	Slide 2	ANL000010 1. Treated	Rat, RatDTOR, M, 09.08.12, POTES				
3	1. Treated	Slide 1	ANL000012 1. Treated	Rat, RatDTOR, F, 09.08.12, POTES1				
4	1. Treated	Slide 1	ANL000014 1. Treated	Rat, RatDTOR, F, 09.08.12, POTES1				
5	1. Treated	Slide 1	ANL000015 1. Treated	Rat, RatDTOR, F, 09.08.12, POTES1				
6	2. Vehicle	Slide 2	ANL000007 2. Vehicle	Rat, RatDTOR, M, 09.08.12, POTES				
7	2. Vehicle	Slide 3	ANL000008 2. Vehicle	Rat, RatDTOR, M, 09.08.12, POTES				
8	2. Vehicle	Slide 2	ANL000011 2. Vehicle	Rat, RatDTOR, M, 09.08.12, POTES				
9	2. Vehicle	Slide 4	ANL000013 2. Vehicle	Rat, RatDTOR, F, 09.08.12, POTES1				

Table Summary:

#	Location	Containerid	Label	TopParentid	Metadata	Biosamples	Cre.User	Cre.Date	Cre.Date
1.	Slide	ANL000009 07	SL001348	ANL000000 1.	Brain Bouin CD19	-- 1 Slide --	birkood1	05.09.12	05.09.12
2.	Slide	ANL000009 07	SL001950	ANL000000 1.	Heart/ Davidson CD31	-- 1 Slide / 2 samples --	birkood1	05.09.12	05.09.12
3.	Slide	ANL000009 07	SL001951	ANL000000 1.	Lung/ Formalin 4%	-- 1 Slide / 2 samples --	birkood1	05.09.12	05.09.12
4.	Slide	ANL000010 16	SL001349	ANL000010 1.	Brain Bouin CD19	-- 1 Slide --	birkood1	05.09.12	05.09.12
5.	Slide	ANL000010 16	SL001953	ANL000010 1.	Heart/ Davidson CD31	-- 1 Slide / 2 samples --	birkood1	05.09.12	05.09.12
6.	Slide	ANL000010 16	SL001954	ANL000010 1.	Lung/ Formalin 4%	-- 1 Slide / 2 samples --	birkood1	05.09.12	05.09.12

Slide Summary:

- Slide 1 -> 1 slide
- Slide 2 -> 1 slide
- Slide 3 -> 1 slide
- Slide 4 -> 1 slide
- Slide 5 -> 1 slide
- Slide 6 -> 1 slide
- Slide 7 -> 1 slide
- Slide 8 -> 1 slide
- Slide 9 -> 1 slide
- Total of 15 slides**

Buttons: Generate Slides, Save Slides & Print Labels.