

16th EBF Open Symposium – Barcelona 2023

Case study on the implementation of a regulatory compliant data platform for planning and execution, collaboration, review and reporting of bioanalytical studies.

Norbert Bittner

15-Nov-2023

UP to data

or - Teaching Old Dogs New Tricks

„Take it from us - the only thing stopping our pets learning through life is our own prejudices.“

<https://www.walkervillevet.com.au/blog/myth-10-you-cant-teach-an-old-dog-new-tricks/>



- 01 — What does „Cloud Computing“ mean
- 02 — Cloud System vs. „in the Cloud“ System – what makes a difference
- 03 — Cloud System Case Studies on Small and Midsized Labs:
 - Capture data where created
 - Enable investigation of data
 - Enable data communication between sponsor and lab
 - Create a long-term archive

Is this „the cloud“?

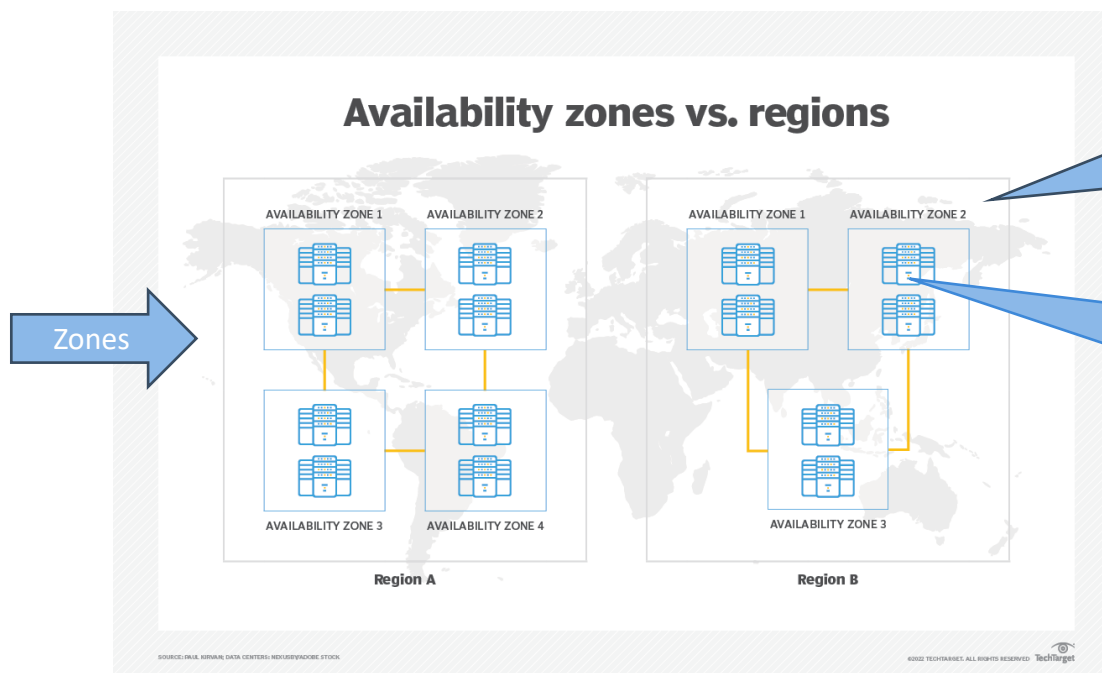
■ AWS Data Center Oregon



„The number of servers in each data centre can range from 50,000 to 80,000.“

Region – Availability Zone - Data Center

Region	Availability Zone
USA Ost (Nord-Virginia)	us-east-1
USA Ost (Ohio)	us-east-2
USA West (Nordkalifornien)	us-west-1
USA West (Oregon)	us-west-2
Asien-Pazifik (Mumbai)	ap-south-1
Asien-Pazifik (Osaka)	ap-northeast-3
Asien-Pazifik (Seoul)	ap-northeast-2
Asien-Pazifik (Singapur)	ap-southeast-1
Asien-Pazifik (Sydney)	ap-southeast-2
Asien-Pazifik (Tokio)	ap-northeast-1
Kanada (Central)	ca-central-1
Europa (Frankfurt)	eu-central-1
Europa (Irland)	eu-west-1
Europa (London)	eu-west-2
Europa (Paris)	eu-west-3
Europa (Stockholm)	eu-north-1
Südamerika (São Paulo)	sa-east-1
Es gibt 11 Regionen, die für dieses Konto nicht aktiviert sind	
Afrika (Kapstadt)	af-south-1
Asien-Pazifik (Hongkong)	ap-east-1
Asien-Pazifik (Hyderabad)	ap-south-2
Asien-Pazifik (Jakarta)	ap-southeast-3
Asien-Pazifik (Melbourne)	ap-southeast-4
Europa (Mailand)	eu-south-1
Europa (Spanien)	eu-south-2
Europa (Zürich)	eu-central-2
Näher Osten (Bahrain)	me-south-1
Näher Osten (VAE)	me-central-1
Israel (Tel Aviv)	il-central-1
Regionen verwalten	



The AWS Cloud spans 102 Availability Zones within 32 geographic regions around the world, with announced plans for 15 more Availability Zones and 5 more AWS Regions in Canada, Germany, Malaysia, New Zealand, and Thailand.

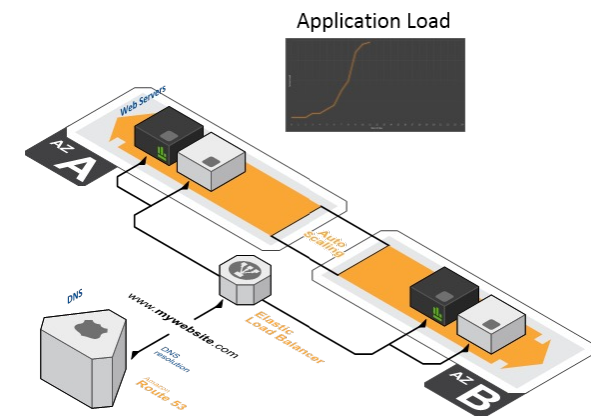
„A common misconception is that a single zone equals a single data center. In fact, each zone is backed by one or more physical data centers, with the largest backed by five.“

<https://docs.aws.amazon.com/whitepapers/latest/aws-overview/global-infrastructure.html>

Example services within and across zones and regions

- load balancing
- failover redundancy
- backups

<https://baxtel.com/data-center/aws-eu-frankfurt-region-eu-central-1>



Cloud computing is the **on-demand** delivery of **IT resources** over the **Internet** with **pay-as-you-go pricing**.

https://aws.amazon.com/what-is-cloud-computing/?nc1=h_ls

Cloud computing is the **on-demand** delivery of **IT resources** over the **Internet** with **pay-as-you-go pricing**.

https://aws.amazon.com/what-is-cloud-computing/?nc1=h_ls

Cloud computing is the **on-demand** delivery of **IT resources** over the **Internet** with **pay-as-you-go pricing**.

https://aws.amazon.com/what-is-cloud-computing/?nc1=h_ls

Cloud computing is the **on-demand** delivery of **IT resources** over the **Internet** with **pay-as-you-go pricing**.

https://aws.amazon.com/what-is-cloud-computing/?nc1=h_ls

Cloud computing is the **on-demand** delivery of **IT resources** over the **Internet** with **pay-as-you-go pricing**.

Instead of buying, owning, and maintaining physical data centers and servers, you can access technology services, such as computing power, storage, and databases, on an as-needed basis from a cloud provider like Amazon Web Services (AWS).

https://aws.amazon.com/what-is-cloud-computing/?nc1=h_ls

Cloud system vs. „in the Cloud“ system – what makes the difference

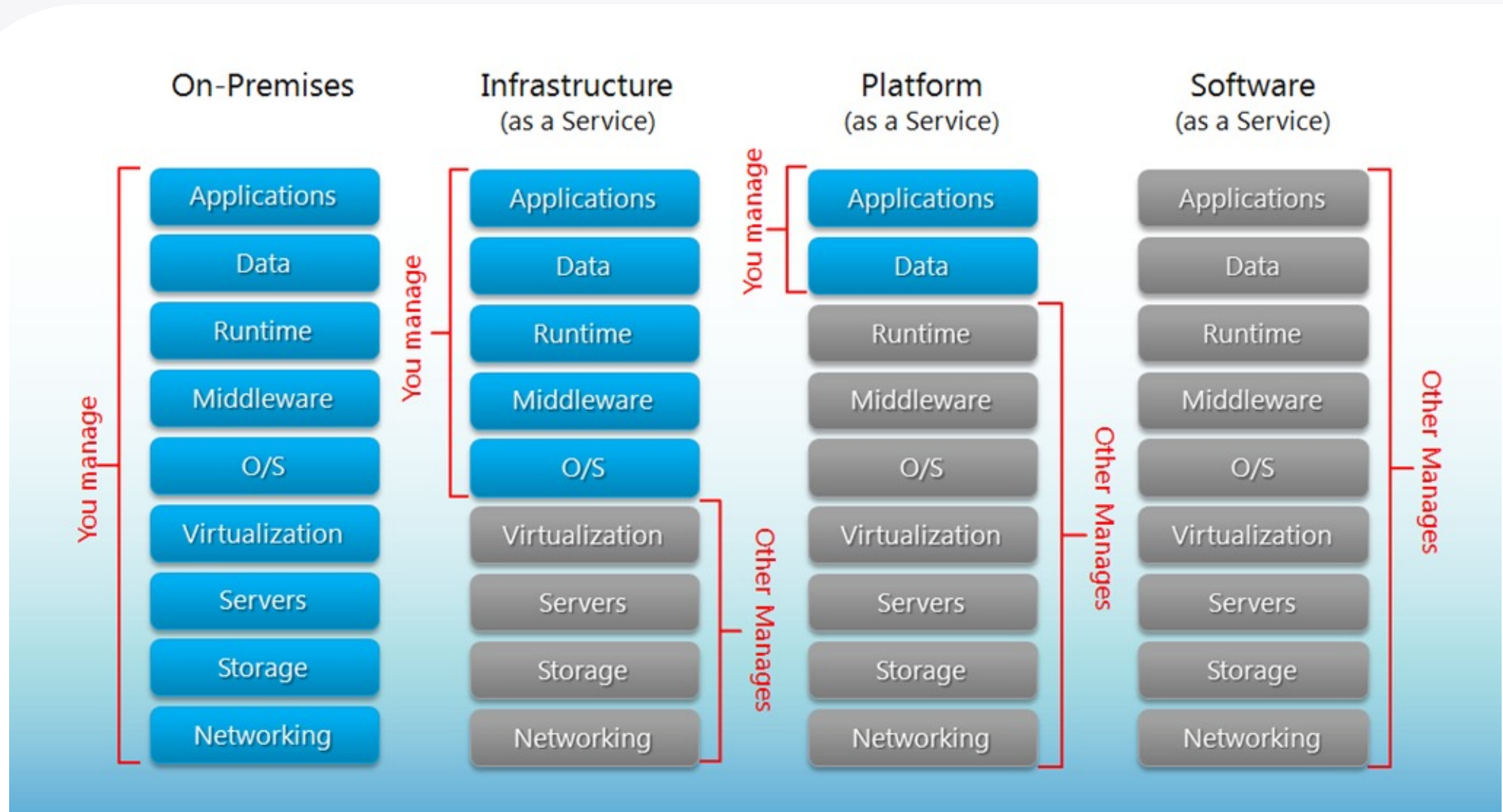
Move existing systems „in the cloud“:

Server virtualization

- „Run the Software on someone else’s hardware“
 - Benefits
 - Some services
 - Delegate responsibility
 - **IaaS (Infrastructure as a service)**
- or
- **PaaS (Platform as a service)**

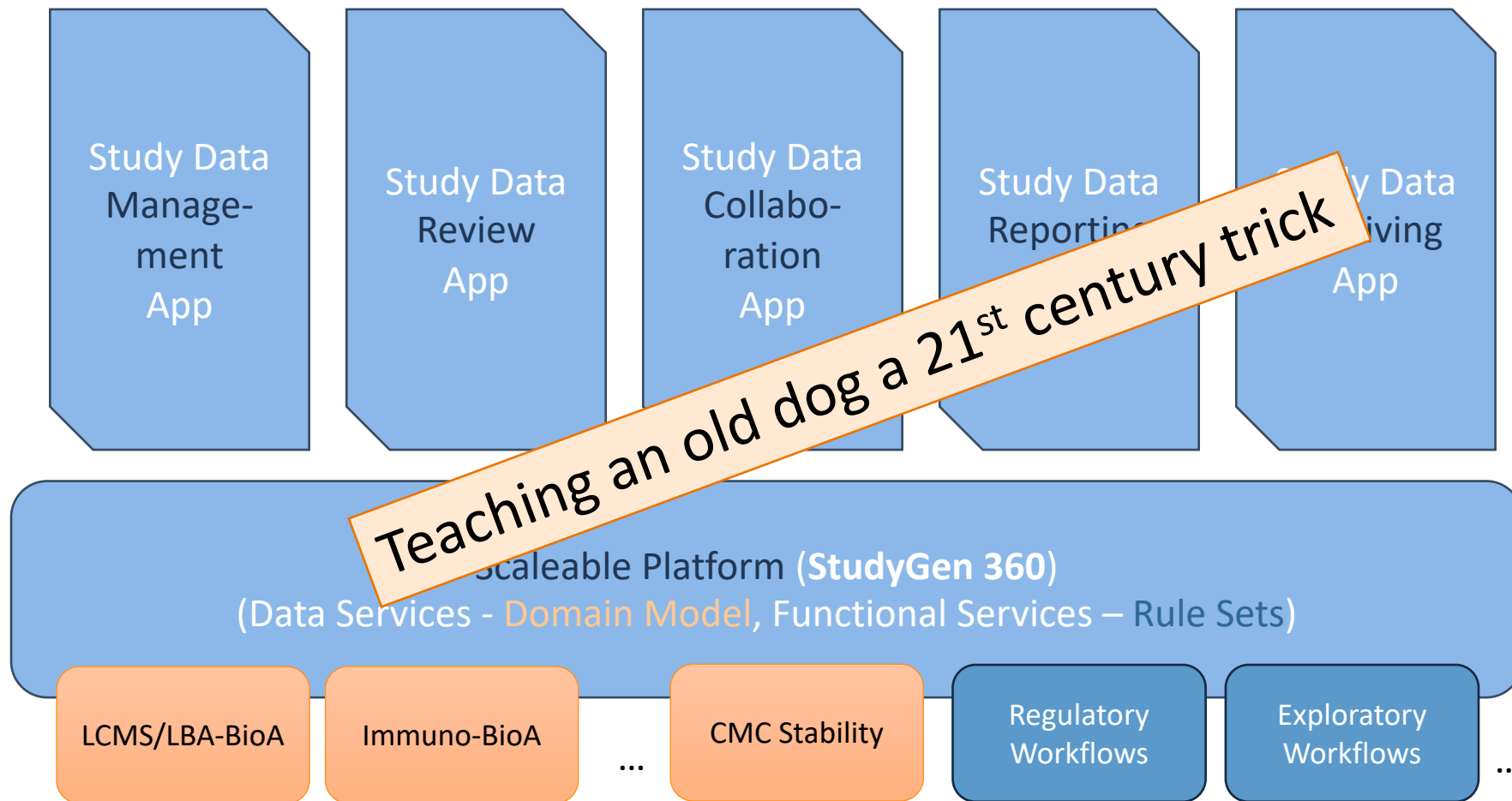


Cloud Systems - Shared Responsibility



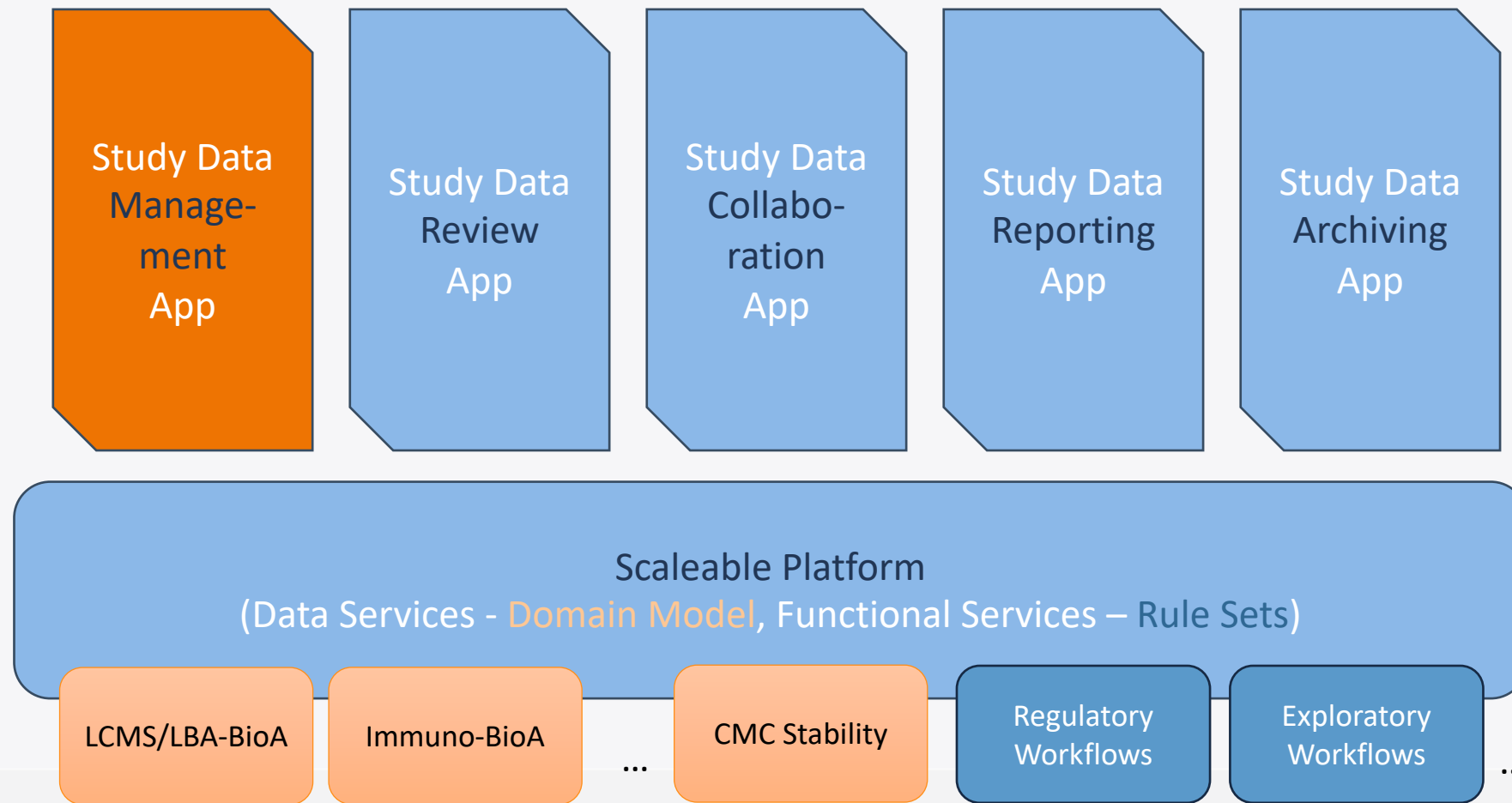
https://www.researchgate.net/figure/Shared-responsibility-model-of-cloud-computing-Source_fig1_352285658

Cloud System – Study Data Management Architecture



EU Funded





Study Data Management

Case Study: Capture data where created

Manual Workflow - without LIMS



Sample Demographic

BA number:	BA-17.053	Sample check under sodium light:	no
Study no.:	20135531	Samples checked by:	A. Steurer
Project:	CXCR3	from - to:	1 - 367
Matrix:	plasma and urine		
Species:	dog	Date and signature:	

* Labeling and general condition of each sample will be checked (see SOP-000312). Only, if conditions of the sample are non-standard or unexpected, these will be recorded in this column.

no manual entry in this column **Enter in these columns the exact sample identify as presented on the tubes**

original sample identification plus dose test facility / CRO	sample identification	group	sex	animal ID	occasion [day]	time point h	dose mg/kg	comments	sample inspection ²
group 1, M, 1, day 1, -0,33 h, 0,5 mg/kg	BA-17.053_001	1	M	1	1	-0,33	0,5	period 1	
group 1, M, 2, day 1, -0,33 h, 0,5 mg/kg	BA-17.053_002	1	M	2	1	-0,33	0,5	period 1	
group 1, M, 3, day 1, -0,33 h, 0,5 mg/kg	BA-17.053_003	1	M	3	1	-0,33	0,5	period 1	
group 1, M, 4, day 1, -0,33 h, 0,5 mg/kg	BA-17.053_004	1	M	4	1	-0,33	0,5	period 1	
group 1, M, 1, day 1, 0 h, 0,5 mg/kg	BA-17.053_005	1	M	1	1	0	0,5	period 1	
group 1, M, 2, day 1, 0 h, 0,5 mg/kg	BA-17.053_006	1	M	2	1	0	0,5	period 1	
group 1, M, 3, day 1, 0 h, 0,5 mg/kg	BA-17.053_007	1	M	3	1	0	0,5	period 1	
group 1, M, 4, day 1, 0 h, 0,5 mg/kg	BA-17.053_008	1	M	4	1	0	0,5	period 1	
group 1, M, 1, day 1, 0,033 h, 0,5 mg/kg	BA-17.053_009	1	M	1	1	0,033	0,5	period 1	
group 1, M, 2, day 1, 0,033 h, 0,5 mg/kg	BA-17.053_010	1	M	2	1	0,033	0,5	period 1	
group 1, M, 3, day 1, 0,033 h, 0,5 mg/kg	BA-17.053_011	1	M	3	1	0,033	0,5	period 1	
group 1, M, 4, day 1, 0,033 h, 0,5 mg/kg	BA-17.053_012	1	M	4	1	0,033	0,5	period 1	
group 1, M, 1, day 1, 0,167 h, 0,5 mg/kg	BA-17.053_013	1	M	1	1	0,167	0,5	period 1	
group 1, M, 2, day 1, 0,167 h, 0,5 mg/kg	BA-17.053_014	1	M	2	1	0,167	0,5	period 1	
group 1, M, 3, day 1, 0,167 h, 0,5 mg/kg	BA-17.053_015	1	M	3	1	0,167	0,5	period 1	
group 1, M, 4, day 1, 0,167 h, 0,5 mg/kg	BA-17.053_016	1	M	4	1	0,167	0,5	period 1	
group 1, M, 1, day 1, 0,5 h, 0,5 mg/kg	BA-17.053_017	1	M	1	1	0,5	0,5	period 1	
group 1, M, 2, day 1, 0,5 h, 0,5 mg/kg	BA-17.053_018	1	M	2	1	0,5	0,5	period 1	
group 1, M, 3, day 1, 0,5 h, 0,5 mg/kg	BA-17.053_019	1	M	3	1	0,5	0,5	period 1	
group 1, M, 4, day 1, 0,5 h, 0,5 mg/kg	BA-17.053_020	1	M	4	1	0,5	0,5	period 1	
group 1, M, 1, day 1, 1 h, 0,5 mg/kg	BA-17.053_021	1	M	1	1	1	0,5	period 1	
group 1, M, 2, day 1, 1 h, 0,5 mg/kg	BA-17.053_022	1	M	2	1	1	0,5	period 1	
group 1, M, 3, day 1, 1 h, 0,5 mg/kg	BA-17.053_023	1	M	3	1	1	0,5	period 1	

sample identification	group	sex	animal ID	occasion [day]	time point h	dose mg/kg
BA-17.053_001	1	M	1	1	-0,33	0,5
BA-17.053_002	1	M	2	1	-0,33	0,5

group 1, M, 3, day 1, 8 h, 0,5 mg/kg	BA-17.053_039	1	M	3	1	8	0,5	period 1	
group 1, M, 4, day 1, 8 h, 0,5 mg/kg	BA-17.053_040	1	M	4	1	8	0,5	period 1	
group 1, M, 1, day 1, 24 h, 0,5 mg/kg	BA-17.053_041	1	M	1	1	24	0,5	period 1	
group 1, M, 2, day 1, 24 h, 0,5 mg/kg	BA-17.053_042	1	M	2	1	24	0,5	period 1	
group 1, M, 3, day 1, 24 h, 0,5 mg/kg	BA-17.053_043	1	M	3	1	24	0,5	period 1	
group 1, M, 4, day 1, 24 h, 0,5 mg/kg	BA-17.053_044	1	M	4	1	24	0,5	period 1	
group 1, M, 1, day 1, 32 h, 0,5 mg/kg	BA-17.053_045	1	M	1	1	32	0,5	period 1	
group 1, M, 2, day 1, 32 h, 0,5 mg/kg	BA-17.053_046	1	M	2	1	32	0,5	period 1	
group 1, M, 3, day 1, 32 h, 0,5 mg/kg	BA-17.053_047	1	M	3	1	32	0,5	period 1	
group 1, M, 4, day 1, 32 h, 0,5 mg/kg	BA-17.053_048	1	M	4	1	32	0,5	period 1	
group 1, M, 1, day 1, 48 h, 0,5 mg/kg	BA-17.053_049	1	M	1	1	48	0,5	period 1	
group 1, M, 2, day 1, 48 h, 0,5 mg/kg	BA-17.053_050	1	M	2	1	48	0,5	period 1	
group 1, M, 3, day 1, 48 h, 0,5 mg/kg	BA-17.053_051	1	M	3	1	48	0,5	period 1	
group 1, M, 4, day 1, 48 h, 0,5 mg/kg	BA-17.053_052	1	M	4	1	48	0,5	period 1	
group 1, M, 1, day 1, -0,33 h, 2,5 mg/kg	BA-17.053_053	1	M	1	1	-0,33	2,5	period 2	
group 1, M, 2, day 1, -0,33 h, 2,5 mg/kg	BA-17.053_054	1	M	2	1	-0,33	2,5	period 2	
group 1, M, 3, day 1, -0,33 h, 2,5 mg/kg	BA-17.053_055	1	M	3	1	-0,33	2,5	period 2	
group 1, M, 4, day 1, -0,33 h, 2,5 mg/kg	BA-17.053_056	1	M	4	1	-0,33	2,5	period 2	

Seite 1

Either Uploading Data (Demographics) or ...

Usersampleid	Vialsampleid	Subject Group	Gender	Subject id	STARTDAY	STARTHOUR	Dosage	Period
BA-17-053_277	group 1, M, 1, day 1, 4 0.033, 2.5 0.5	1	M	1	4	2.5	period 6	
BA-17-053_185	group 1, M, 1, day 1, 6 0.033, 0.5 0.5	1	M	1	6	0.5	period 4	
BA-17-053_183	group 1, M, 3, day 1, 4 0.033, 0.5 0.5	1	M	3	4	0.5	period 4	
BA-17-053_067	group 1, M, 3, day 1, 0.167 0.033, 2.5 0.5	1	M	3	0.167	2.5	period 2	
BA-17-053_066	group 1, M, 2, day 1, 0.167 0.033, 2.5 0.5	1	M	2	0.167	2.5	period 2	
BA-17-053_065	group 1, M, 1, day 1, 0.167 0.033, 2.5 0.5	1	M	1	0.167	2.5	period 2	
BA-17-053_064	group 1, M, 4, day 1, 0.033 0.033, 2.5 0.5	1	M	4	0.033	2.5	period 2	
BA-17-053_063	group 1, M, 3, day 1, 0.033 0.033, 2.5 0.5	1	M	3	0.033	2.5	period 2	
BA-17-053_062	group 1, M, 2, day 1, 0.033 0.033, 2.5 0.5	1	M	2	0.033	2.5	period 2	
BA-17-053_061	group 1, M, 1, day 1, 0.033 0.033, 2.5 0.5	1	M	1	0.033	2.5	period 2	
BA-17-053_060	group 1, M, 4, day 1, 0 0.033, 2.5 0.5	1	M	4	0	2.5	period 2	
BA-17-053_059	group 1, M, 3, day 1, 0 0.033, 2.5 0.5	1	M	3	0	2.5	period 2	
BA-17-053_058	group 1, M, 2, day 1, 0 0.033, 2.5 0.5	1	M	2	0	2.5	period 2	
BA-17-053_057	group 1, M, 1, day 1, 0 0.033, 2.5 0.5	1	M	1	0	2.5	period 2	
BA-17-053_056	group 1, M, 4, day 1, -0.33 0.033, 2.5 0.5	1	M	4	-0.33	2.5	period 2	
BA-17-053_055	group 1, M, 3, day 1, -0.33 0.033, 2.5 0.5	1	M	3	-0.33	2.5	period 2	
BA-17-053_054	group 1, M, 2, day 1, -0.33 0.033, 2.5 0.5	1	M	2	-0.33	2.5	period 2	
BA-17-053_053	group 1, M, 1, day 1, -0.33 0.033, 2.5 0.5	1	M	1	-0.33	2.5	period 2	
BA-17-053_052	group 1, M, 4, day 1, 48 0.033, 0.5 0.5	1	M	4	48	0.5	period 1	
BA-17-053_051	group 1, M, 3, day 1, 48 0.033, 0.5 0.5	1	M	3	48	0.5	period 1	
BA-17-053_050	group 1, M, 2, day 1, 48 0.033, 0.5 0.5	1	M	2	48	0.5	period 1	
BA-17-053_049	group 1, M, 1, day 1, 48 0.033, 0.5 0.5	1	M	1	48	0.5	period 1	
BA-17-053_048	group 1, M, 4, day 1, 0.167 0.033, 2.5 0.5	1	M	4	0.167	2.5	period 2	
BA-17-053_047	group 1, M, 3, day 1, 32 0.033, 0.5 0.5	1	M	3	32	0.5	period 2	
BA-17-053_046	group 1, M, 2, day 1, 0.5 0.033, 2.5 0.5	1	M	2	0.5	2.5	period 2	
BA-17-053_045	group 1, M, 1, day 1, 0.5 0.033, 2.5 0.5	1	M	1	0.5	2.5	period 2	
BA-17-053_044	group 1, M, 2, day 1, 8 0.033, 2.5 0.5	1	M	2	8	2.5	period 2	
BA-17-053_043	group 1, M, 1, day 1, 8 0.033, 2.5 0.5	1	M	1	8	2.5	period 2	
BA-17-053_042	group 1, M, 4, day 1, 6 0.033, 2.5 0.5	1	M	4	6	2.5	period 2	
BA-17-053_041	group 1, M, 3, day 1, 6 0.033, 2.5 0.5	1	M	3	6	2.5	period 2	
BA-17-053_040	group 1, M, 2, day 1, 6 0.033, 2.5 0.5	1	M	2	6	2.5	period 2	
BA-17-053_039	group 1, M, 1, day 1, 6 0.033, 2.5 0.5	1	M	1	6	2.5	period 2	
BA-17-053_038	group 1, M, 4, day 1, 4 0.033, 2.5 0.5	1	M	4	4	2.5	period 2	
BA-17-053_037	group 1, M, 3, day 1, 4 0.033, 2.5 0.5	1	M	3	4	2.5	period 2	
BA-17-053_036	group 1, M, 2, day 1, 4 0.033, 2.5 0.5	1	M	2	4	2.5	period 2	
BA-17-053_035	group 1, M, 1, day 1, 4 0.033, 2.5 0.5	1	M	1	4	2.5	period 2	
BA-17-053_034	group 1, M, 4, day 1, 2 0.033, 2.5 0.5	1	M	4	2	2.5	period 2	
BA-17-053_033	group 1, M, 3, day 1, 2 0.033, 2.5 0.5	1	M	3	2	2.5	period 2	
BA-17-053_032	group 1, M, 2, day 1, 2 0.033, 2.5 0.5	1	M	2	2	2.5	period 2	
BA-17-053_031	group 1, M, 1, day 1, 2 0.033, 2.5 0.5	1	M	1	2	2.5	period 2	
BA-17-053_030	group 1, M, 4, day 1, 1 0.033, 2.5 0.5	1	M	4	1	2.5	period 2	
BA-17-053_029	group 1, M, 3, day 1, 1 0.033, 2.5 0.5	1	M	3	1	2.5	period 2	
BA-17-053_028	group 1, M, 2, day 1, 1 0.033, 2.5 0.5	1	M	2	1	2.5	period 2	
BA-17-053_027	group 1, M, 1, day 1, 1 0.033, 2.5 0.5	1	M	1	1	2.5	period 2	
BA-17-053_026	group 1, M, 4, day 1, 0.5 0.033, 2.5 0.5	1	M	4	0.5	2.5	period 2	
BA-17-053_025	group 1, M, 3, day 1, 0.5 0.033, 2.5 0.5	1	M	3	0.5	2.5	period 2	
BA-17-053_024	group 1, M, 2, day 1, 0.5 0.033, 2.5 0.5	1	M	2	0.5	2.5	period 2	
BA-17-053_023	group 1, M, 1, day 1, 0.5 0.033, 2.5 0.5	1	M	1	0.5	2.5	period 2	
BA-17-053_022	group 1, M, 4, day 1, 32 0.033, 0.5 0.5	1	M	4	32	0.5	period 1	
BA-17-053_021	group 1, M, 3, day 1, 32 0.033, 0.5 0.5	1	M	3	32	0.5	period 1	
BA-17-053_020	group 1, M, 2, day 1, 32 0.033, 0.5 0.5	1	M	2	32	0.5	period 1	
BA-17-053_019	group 1, M, 1, day 1, 1 0.033, 0.5 0.5	1	M	1	1	0.5	period 1	
BA-17-053_018	group 1, M, 4, day 1, 0.5 0.033, 0.5 0.5	1	M	4	0.5	0.5	period 1	
BA-17-053_017	group 1, M, 3, day 1, 0.5 0.033, 0.5 0.5	1	M	3	0.5	0.5	period 1	
BA-17-053_016	group 1, M, 2, day 1, 0.5 0.033, 0.5 0.5	1	M	2	0.5	0.5	period 1	
BA-17-053_015	group 1, M, 1, day 1, 0.5 0.033, 0.5 0.5	1	M	1	0.5	0.5	period 1	
BA-17-053_014	group 1, M, 4, day 1, 0.167 0.033, 0.5 0.5	1	M	4	0.167	0.5	period 1	
BA-17-053_013	group 1, M, 3, day 1, 0.167 0.033, 0.5 0.5	1	M	3	0.167	0.5	period 1	
BA-17-053_012	group 1, M, 2, day 1, 0.167 0.033, 0.5 0.5	1	M	2	0.167	0.5	period 1	
BA-17-053_011	group 1, M, 1, day 1, 0.167 0.033, 0.5 0.5	1	M	1	0.167	0.5	period 1	



Upload Files

Select file or Drop file here

Details.xlsx 27 kb
Uploaded

Note: You are experiencing this sample list auto selection because you have

Use Existing
 Create New Mapping

Created_By

Created_On

Dosage

Gender

Period

Sample_Name

Sample_Status

STARTDAY

Field	Value
ENDHOUR	
ENDMINUTE	
ENDSECOND	
FastOrFed	
Formation	
Gender	
GenderDecision	
INFECTIOUS	
IsPlacebo	
MATRIX	
MONTH	
Period	
Placebo	
PlannedNumber	
Race	
RELATIVEDAY	
Do Not Map	
Do Not Map	
Do Not Map	
Do Not Map	
Do Not Map	
Do Not Map	

StudyGen Selected Study DemoM10

- Samples
- Data
- Reference Material
- Stock Solutions
- Spike Solutions
- Blank Matrix
- Shipments
- Analysis Information
- Stability Information
- Samples Received
- Reports

Study Status

Modified

Samples

Drag a column header here to group by that column

Reset Grid +

USERSAMPLEID	Sample Status	Created On	Created By	Original sample id	Subject Group	Gen
BA-17-053_002	Created	2023-06-05T06:41:06.938573	mini@innidata.com	group 1, M, 2, day 1, -0.33 0.033, 0.5 0.5	1	M
BA-17-053_003	Created	2023-06-05T06:41:06.942033	mini@innidata.com	group 1, M, 3, day 1, -0.33 0.033, 0.5 0.5	1	M
BA-17-053_004	Created	2023-06-05T06:41:06.942508	mini@innidata.com	group 1, M, 4, day 1, -0.33 0.033, 0.5 0.5	1	M
BA-17-053_005	Created	2023-06-05T06:41:06.942601	mini@innidata.com	group 1, M, 1, day 1, 0 0.033, 0.5 0.5	1	M
BA-17-053_006	Created	2023-06-05T06:41:06.942639	mini@innidata.com	group 1, M, 2, day 1, 0 0.033, 0.5 0.5	1	M
BA-17-053_007	Created	2023-06-05T06:41:06.94267	mini@innidata.com	group 1, M, 3, day 1, 0 0.033, 0.5 0.5	1	M
BA-17-053_008	Created	2023-06-05T06:41:06.942695	mini@innidata.com	group 1, M, 4, day 1, 0 0.033, 0.5 0.5	1	M
BA-17-053_009	Created	2023-06-05T06:41:06.942738	mini@innidata.com	group 1, M, 1, day 1, 0.033 0.033, 0.5 0.5	1	M
BA-17-053_010	Created	2023-06-05T06:41:06.942768	mini@innidata.com	group 1, M, 2, day 1, 0.033 0.033, 0.5 0.5	1	M

Count: 366

Create Filter



Entering Data in Forms

StudyGen Selected Study DemoM10 Norbert Bittner

Stock Solution

Drag a column header here to group by that column

Reset Grid

Solution ID	Unique ID	Prep Date	Expiry Date	Storage Conditions
SS1-STD	SS1-1-EBF-220028-033/13	8/11/2022	8/21/2022	6°C

Solution ID: Unique ID: Prep Date:

Expiry Date: Storage Conditions:

Save

Count: 2

Create Filter

Sample Receipt and Storage

Shipments

Drag a column header here to group by that column

Reset Grid [Grid Icon] Search...

Arrival Date [Filter Icon] Shipment Date [Filter Icon]

Q [Calendar Icon] Q [Calendar Icon]

Arrival Date: *

10/17/2022, 3:53

Count: 1

Today

OK Cancel

Save Sample Modal

Drag a column header here to group by that column

Reset Grid [Grid Icon] Search...

<input type="checkbox"/>	TIMETEXT	Subject	Period	Time	USERSAMPLEID	Sample Name	Sample Status	Location ...	Subject Group
	Q		Q		Q		Q	(All)	Q
	12		7		S1523_GD_7_12HRPD		Created		S1523_GD_7_12HRPD
	24		7		S1523_GD_7_24HRPD		Created		S1523_GD_7_24HRPD
	36		7		S1523_GD_7_36HRPD		Created		S1523_GD_7_36HRPD
	48		7		S1523_GD_7_48HRPD		Created		S1523_GD_7_48HRPD
	0.25		9		S1523_GD_9_0.25HRPD		Created		S1523_GD_9_0.25HRPD
	0		11		S1523_GD_11_PREDOSE		Created		S1523_GD_11_PREDOSE
	0.25		11		S1523_GD_11_0.25HRPD		Created		S1523_GD_11_0.25HRPD
	0		13		S1523_GD_13_PREDOSE		Created		S1523_GD_13_PREDOSE
	0.25		13		S1523_GD_13_0.25HRPD		Created		S1523_GD_13_0.25HRPD
	0		15		S1523_GD_15_PREDOSE		Created		S1523_GD_15_PREDOSE
	0.25		15		S1523_GD_15_0.25HRPD		Created		S1523_GD_15_0.25HRPD
	0		17		S1523_GD_17_PREDOSE		Created		S1523_GD_17_PREDOSE
	0.25		17		S1523_GD_17_0.25HRPD		Created		S1523_GD_17_0.25HRPD

Count: 113

Select Sample Status [Dropdown]

Assign Location Save Samples Status

Move to Location

Files

Name	Modified	Created
B1	10/17/2022	
B2	10/17/2022	

Cancel Move Samples

Run/Batch-Planning and Plate-Layout design

Assay Design

Acknowledgement

Basic Information

Assay ID: Test-001
 Assay Type:
 Approval Date:
 Project ID:
 Biological Matrix:
 Species:
 Assay Description:
 Assay Comments:
 Instrument Type:
 Instrument Interface:
 Import Data Format:
 Peak Type:
 Regression Type:
 Do Residual Outlier Test:

Analyte Information

Drag a column header here to group by that column

Name	ISName	Conc Units	LSLQ	USLQ
Alt1	Alt1-IS	ng/ml	0.1	1000
Alt2	Alt2-IS	ng/ml	0.1	1000

Count: 2

Detail Calibration Standard Information

Drag a column header here to group by that column

Number Of Standards	Number Of Replicates	Flag Percent Diff	Alt 1 ng/ml	Alt 2 ng/ml
STD1	2	50	0	0
STD2	2	50	0	0

Count: 2

Detail QC Information

Drag a column header here to group by that column

Name	Number Of Replicates	Flag Percent Diff	Dilution Factor	Alt 1 ng/ml	Alt 2 ng/ml
QC1	2	20	.01	0	0
QC2	2	20	.01	0	0

Count: 2

Save

Assay to Plate-Template

Samples In Run

Reset Grid

Add Plate Plate# 1

Sample Name	vial	Drag
STD1-2	(All)	Drag
STD2-1		Drag
STD2-2		Drag
QC1-1		Drag
STD1-1		Drag
QC2-1		Drag
QC2-2		Drag
QC1-2		Drag
Blank		Drag

Count: 12

We will save this info for next step. Back Save Run Template

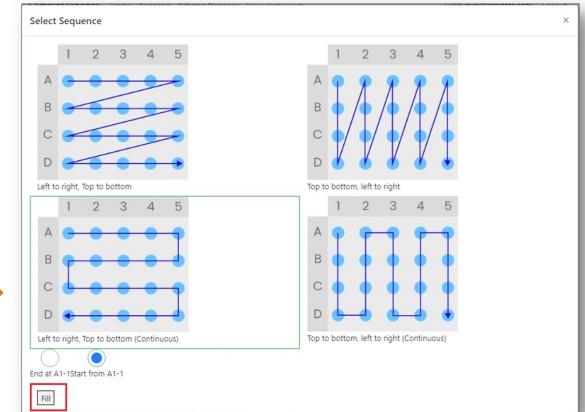


Plate-Template and Sample to create a Sequence

Selections: Selected Sponsor: Test Run - 001 Selected Study: Test 001

Print

Run Name: Run_1

Plate# 1

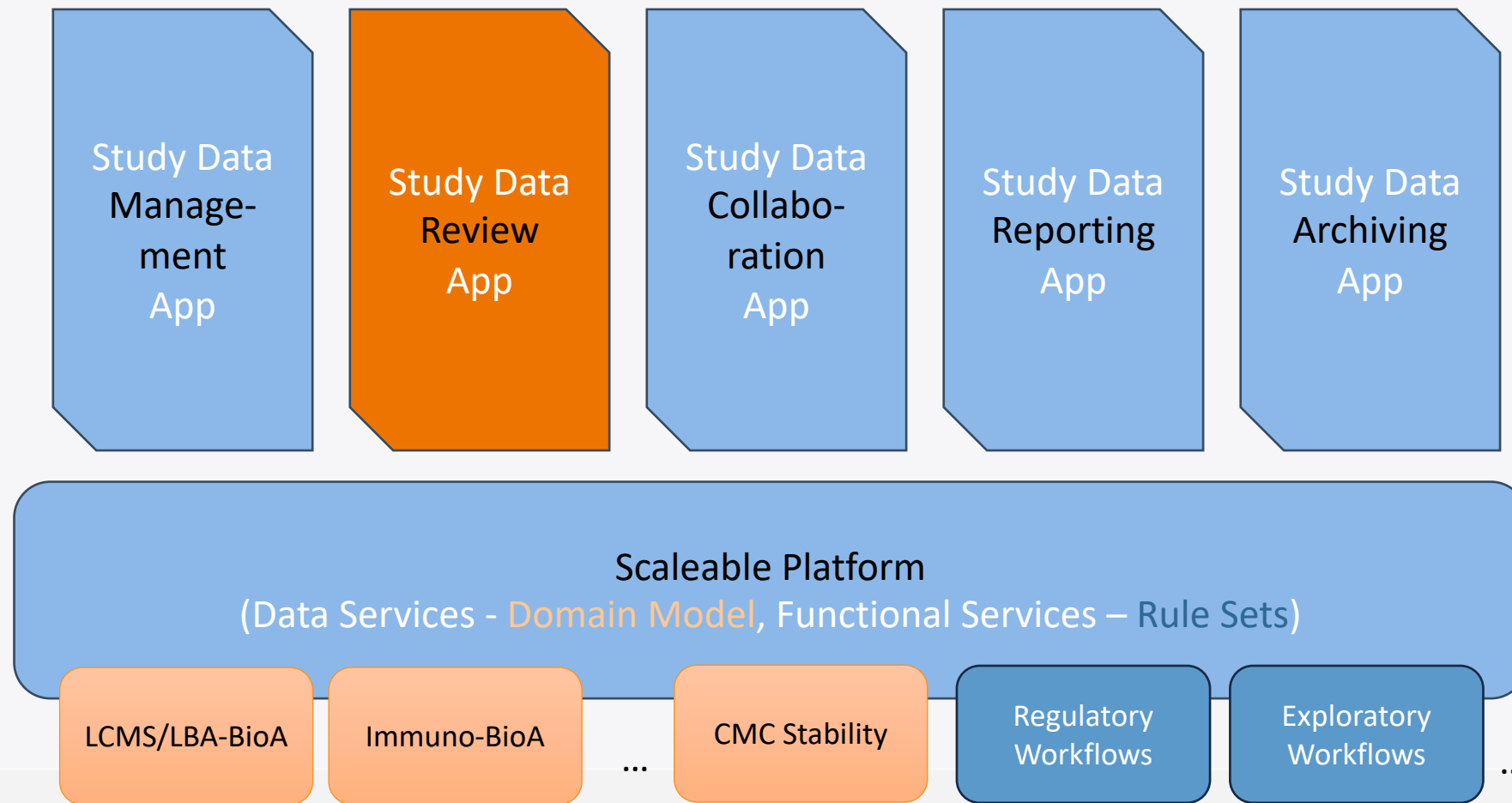
	1	2	3	4	5	6	7	8	9	10	11	12
A	A1	A2	A3	STD2-2	QC1-1	A6	A7	A8	A9	A10	A11	A12
B	B1	B2	B3	STD2-1	QC1-2	B6	B7	B8	B9	B10	B11	B12
C	C1	C2	C3	STD1-2	QC2-1	C6	C7	C8	C9	C10	C11	C12
D	D1	D2	D3	STD1-1	QC2-2	D6	D7	D8	D9	D10	D11	D12
E	E1	E2	E3	E4	Blank	E6	E7	E8	E9	E10	E11	E12
F	F1	F2	F3	F4	Blank	F6	F7	F8	F9	F10	F11	F12
G	G1	G2	G3	G4	SST	Blank	G7	G8	G9	G10	G11	G12
H	H1	H2	H3	H4	Double Blank	Double Blank	H7	H8	H9	H10	H11	H12

Show Plates Design Export Sequence File

Drag a column header here to group by that column

Sample Name	Vial Pos	Dilut Fact	Type	Plate Code	Rack Code	Sample ID
Q1	Q1	Q1	Q1	Q1	Q1	Q1
STD1-2	28	1	Standard	Deep Well MTP 96	Rack Order (Column)	2
STD2-1	16	1	Standard	Deep Well MTP 96	Rack Order (Column)	3
STD2-2	4	1	Standard	Deep Well MTP 96	Rack Order (Column)	4
QC1-1	5	1	Quality Control	Deep Well MTP 96	Rack Order (Column)	5
QC1-2	17	1	Quality Control	Deep Well MTP 96	Rack Order (Column)	6
QC2-1	29	1	Quality Control	Deep Well MTP 96	Rack Order (Column)	7
QC2-2	41	1	Quality Control	Deep Well MTP 96	Rack Order (Column)	8
S210-2525-15-0-25-52525_GROUP2_GD_15_0_25HRPD-null-Available	1		Unknown			9
S274-4523-17-0-25-S4523_GD_17_0_25HRPD-null-Available	1		Unknown			10
Blank	53	1	Blank	Deep Well MTP 96	Rack Order (Column)	11
Blank	65	1	Blank	Deep Well MTP 96	Rack Order (Column)	12
SST	77	1	SST	Deep Well MTP 96	Rack Order (Column)	13
Double Blank	89	1	Double Blank	Deep Well MTP 96	Rack Order (Column)	14
Double Blank	90	1	Double Blank	Deep Well MTP 96	Rack Order (Column)	15
Blank	78	1	Blank	Deep Well MTP 96	Rack Order (Column)	16
S211-4525-17-0-54525_GD_17_PREDOSE-null-Available	1		Unknown			17
S212-5523-17-0-55523_GD_17_PREDOSE-null-Available	1		Unknown			18
S213-5524-15-0-25-55524_GD_15_0_25HRPD-null-Available	1		Unknown			19

Count: 19



Study Data Review

Case Study: Enable Scientists to Investigate Data

Sponsors concerns

- Quality Parameter driven data review to meet **scientific quality objectives**
 - beyond “standard” reporting provided by CRO
- Individual definition of
 - Quality Parameters (e.g.)
 - Sequence of samples/injections consistent
 - Was there a stop/restart
 - Quality Attributes (e.g.)
 - Precision and Accuracy
 - Is there a cross well contamination
 - Matrix effect on STDs/QCs vs. Samples
 - Background and STDs/QC response drift and range changes (in/between runs)
 - S/N consistency
 - Specifics for LC/MS
 - Integration parameters, peak shape, IS variation, retention time variation, carryover, interference peak ...
- Templateable and reusable data analysis
- Trackable collaboration on data-review

Summary Consistency Check

Invalid Names

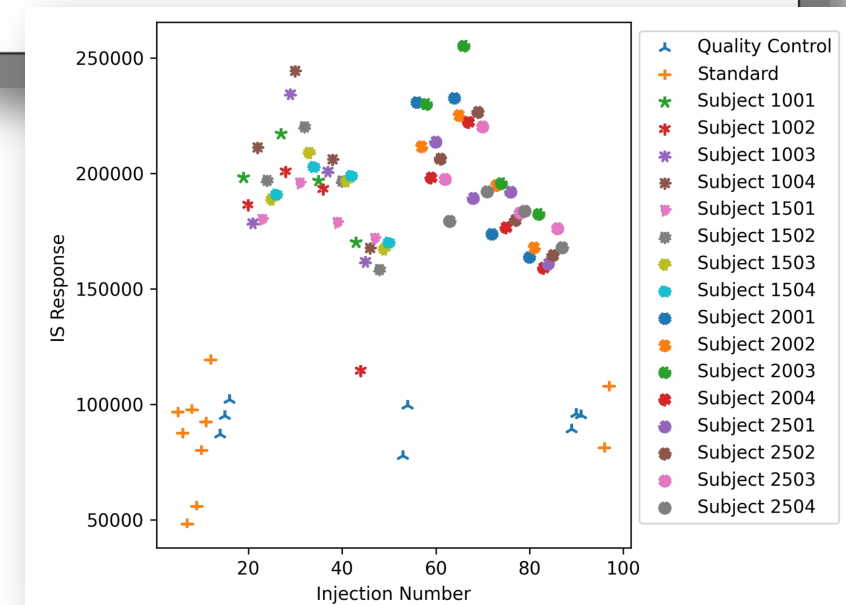
File Name	Seq Number	Sample Name
BA-17.053_Batch01\BA-17.053_Batch01.wiff	40	BB-17.053_132
BA-17.053_Batch01\BA-17.053_Batch01.wiff	43	BB-17.053_135

Duplicate Unknowns

File Name	Seq Number	Sample Name
BA-17.053_Batch01\BA-17.053_Batch01.wiff	50	BA-17.053_139
BA-17.053_Batch01\BA-17.053_Batch01.wiff	51	BA-17.053_139
BA-17.053_Batch01\BA-17.053_Batch01.wiff	92	BA-17.053_321
BA-17.053_Batch01\BA-17.053_Batch01.wiff	93	BA-17.053_321
BA-17.053_Batch01\BA-17.053_Batch01.wiff	94	BA-17.053_321
BA-17.053_Batch01\BA-17.053_Batch01.wiff	119	BA-17.053_344
BA-17.053_Batch01\BA-17.053_Batch01.wiff	120	BA-17.053_344
BA-17.053_Batch01\BA-17.053_Batch01.wiff	121	BA-17.053_344

Samples in sample list
366

Samples in selected data
87



Data-Review –Templates

- Interactive Scenario-Builder to create Review-Templates
 - GUI to support configuration

The screenshot displays the 'Data Review' application interface. At the top, the title bar reads 'Data Review' and includes navigation options: 'Selected Branch: Start', 'Generate Script', 'Save Template For Report', 'Save Review As Template', and 'Save Review'. Below the title bar, there are tabs for 'Starting Environment' and 'Current Environment'. A sidebar on the left lists various functions: 'Get From Env', 'Get From Store', 'Raw', 'kdePlot', 'Plot', 'AddCol', 'Group', 'Filter', 'Numeric', 'signum', 'sigfig', 'distinct', 'select', 'If', and 'Format'. The main workspace is titled 'Selected Table: data' and shows a 'Create Statement (Group)' dialog box. This dialog box contains the following fields and options:

- Source: data
- GroupOn: Sample_Type
- Name of the new column to be added: CountOfSamples
- Expression: (g): count(g)
- Options: Update Source, Create New Source
- New Source Name: data_with_sample_type_count
- Submit button

Below the dialog box, a table displays data rows:

18	BA-17.053_114	Unknown	0	1_HR_ACT-777991_do
19	BA-17.053_115	Unknown	0	1_HR_ACT-777991_do
20	BA-17.053_116	Unknown	0	1_HR_ACT-777991_do

On the right side of the interface, a flowchart illustrates the data processing pipeline:

- Start
- Get From Env
- data => select => samples
- samples => Filter => samples
- samples => Numeric => samples (displaying '123')
- samples => Numeric => samples (displaying '123')

Applying a preconfigured Review-Template

Starting Environment Current Environment

Functions Tables Variables Create Visualization

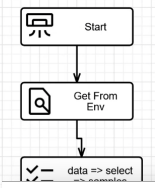
- data
- samples
- Charts

Selected Table: Charts

Drag a column header here to group by that column

Name	SVG
UnknownConcentration	

[Create Filter](#)



Copied!

Content copied to clipboard

OK

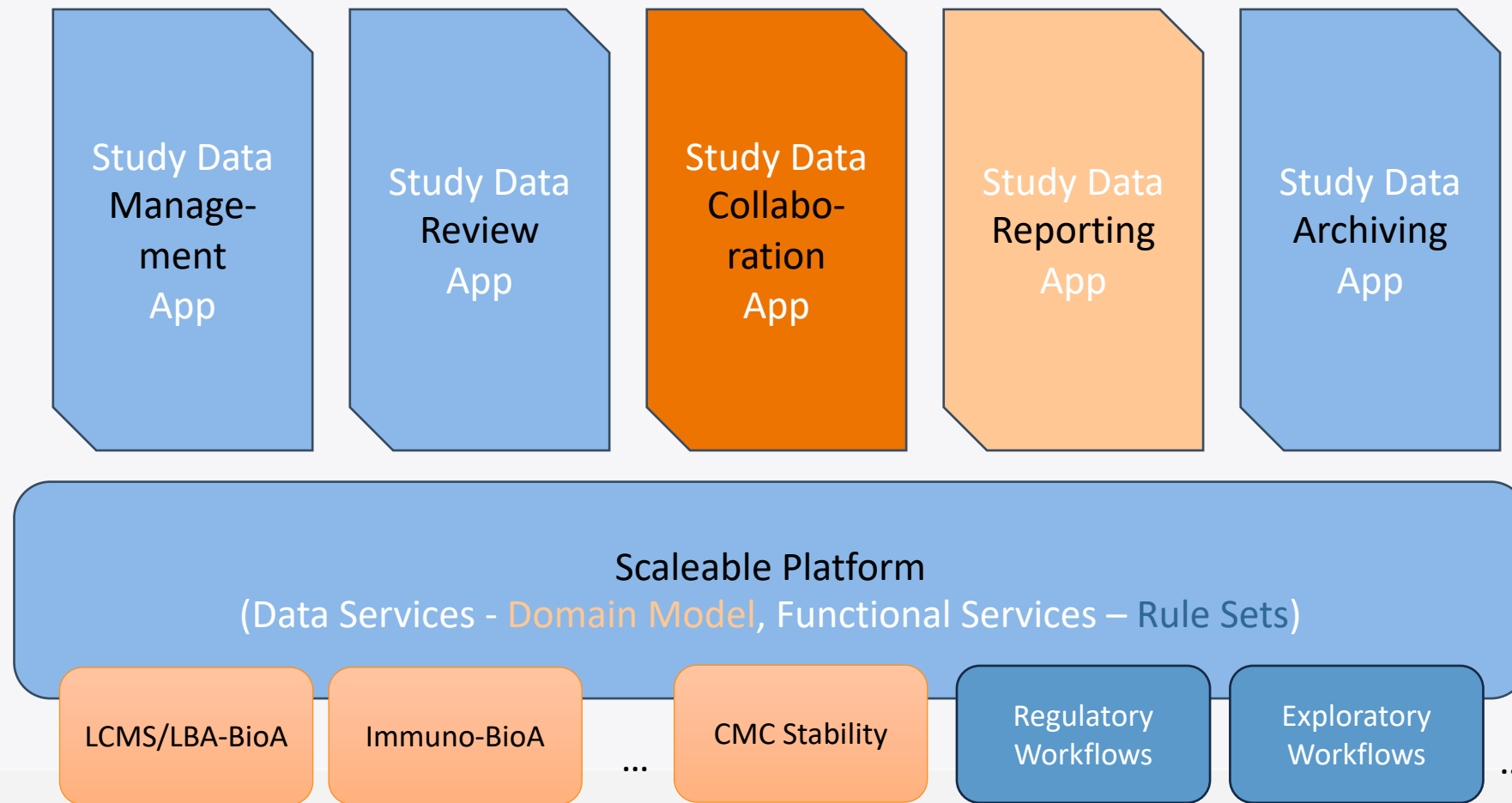
Confidential
Page 9 of 10

Standards S/N

File Name	Seq Number	Sample Name	S/N ratio
BA-17.053_Batch01BA-17.053_Batch01.wiff	2	Ca11	2790.
BA-17.053_Batch01BA-17.053_Batch01.wiff	3	Ca12	6370.
BA-17.053_Batch01BA-17.053_Batch01.wiff	4	Ca13	N/A
BA-17.053_Batch01BA-17.053_Batch01.wiff	5	Ca14	172000.
BA-17.053_Batch01BA-17.053_Batch01.wiff	6	Ca15	112000.
BA-17.053_Batch01BA-17.053_Batch01.wiff	7	Ca16	291000.
BA-17.053_Batch01BA-17.053_Batch01.wiff	8	Ca17	258000.
BA-17.053_Batch01BA-17.053_Batch01.wiff	9	Ca18	1130000.
BA-17.053_Batch05BA-17.053_Batch05.wiff	2	Ca11	112.
BA-17.053_Batch05BA-17.053_Batch05.wiff	3	Ca12	212.
BA-17.053_Batch05BA-17.053_Batch05.wiff	4	Ca13	456.
BA-17.053_Batch05BA-17.053_Batch05.wiff	5	Ca14	1950.
BA-17.053_Batch05BA-17.053_Batch05.wiff	6	Ca15	9680.
BA-17.053_Batch05BA-17.053_Batch05.wiff	7	Ca16	20400.
BA-17.053_Batch05BA-17.053_Batch05.wiff	8	Ca17	22900.
BA-17.053_Batch05BA-17.053_Batch05.wiff	9	Ca18	26300.
BA-17.053_Batch02BA-17.053_Batch02.wiff	2	Ca11	4130.
BA-17.053_Batch02BA-17.053_Batch02.wiff	3	Ca12	8150.
BA-17.053_Batch02BA-17.053_Batch02.wiff	4	Ca13	27200.
BA-17.053_Batch02BA-17.053_Batch02.wiff	5	Ca14	78300.
BA-17.053_Batch02BA-17.053_Batch02.wiff	6	Ca15	168000.
BA-17.053_Batch02BA-17.053_Batch02.wiff	7	Ca16	227000.
BA-17.053_Batch02BA-17.053_Batch02.wiff	8	Ca17	475000.
BA-17.053_Batch02BA-17.053_Batch02.wiff	9	Ca18	564000.
BA-17.053_Batch04BA-17.053_Batch04.wiff	2	Ca11	75.2
BA-17.053_Batch04BA-17.053_Batch04.wiff	3	Ca12	198.
BA-17.053_Batch04BA-17.053_Batch04.wiff	4	Ca13	452.
BA-17.053_Batch04BA-17.053_Batch04.wiff	5	Ca14	2460.
BA-17.053_Batch04BA-17.053_Batch04.wiff	6	Ca15	9030.
BA-17.053_Batch04BA-17.053_Batch04.wiff	7	Ca16	22200.
BA-17.053_Batch04BA-17.053_Batch04.wiff	8	Ca17	26500.
BA-17.053_Batch04BA-17.053_Batch04.wiff	9	Ca18	22200.
BA-17.053_Batch03BA-17.053_Batch03.wiff	2	Ca11	100.
BA-17.053_Batch03BA-17.053_Batch03.wiff	3	Ca12	232.
BA-17.053_Batch03BA-17.053_Batch03.wiff	4	Ca13	557.
BA-17.053_Batch03BA-17.053_Batch03.wiff	5	Ca14	2390.
BA-17.053_Batch03BA-17.053_Batch03.wiff	6	Ca15	7640.
BA-17.053_Batch03BA-17.053_Batch03.wiff	7	Ca16	9630.

Confidential
Page 10 of 10

File Name	Seq Number	Sample Name	S/N ratio
BA-17.053_Batch03BA-17.053_Batch03.wiff	8	Ca17	13400.
BA-17.053_Batch03BA-17.053_Batch03.wiff	9	Ca18	12900.

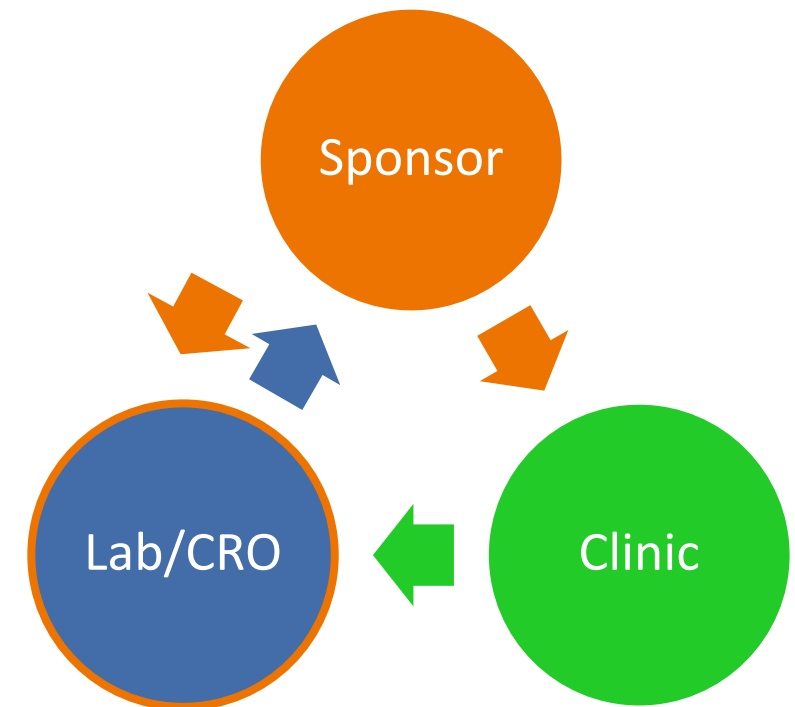


Study Data Collaboration & Reporting

Case Study: Enable Communication and Access

Who creates / is in need of what study data

- Study Data Management
 - Receive Multiple **Sample Shipment Manifest**
 - Sample **Receipt Data** Documentation
 - Handle **Demographics data** incl. „**Reconciliation**“
 - Sample Storage Documentation
 - Sample Preparation Documentation, incl. Materials
 - Run/Batch Data
 - Assay and Method Documentation
 - Run/Batch-Planning and Plate-Layout design
 - Interfacing with devices (Run-Sequence, Result-Files)
 - **Data Review and Evaluation**
 - Reassay-Handling
- Study Data Reporting
 - **Regulatory Reporting** (BioA-Report, Validation-Report)
 - **DTA Files**
 - **SEND PC-Domain Files**



DTA Files

- Configurable per Sponsor/DTA
- Consistent with any other reports

	A	B	C	D	E	F	G	H	I	J	K	L
4	Actual Sampling Date/Time	Analyte	Subject	Subject Group	Time Text	Nominal Time (Design)	Run Id	Biological Matrix Abbreviation	Concentration	Concentration (Rounded)	Concentration (Sig.Figs.)	Concentration Units
5												
6	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
7	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
8	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
9	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
10	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
11	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
12	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
13	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
14	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
15	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
16	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
17	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
18	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
19	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
20	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
21	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
22	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM				ng/mL
23	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
24	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
25	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
26	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
27	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
28	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
29	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
30	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
31	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
32	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
33	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
34	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
35	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
36	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
37	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
38	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
39	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
40	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
41	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
42	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
43	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL
44	25-Jan-2019	Analyte1	101-001	1	D2 24H	48	1	PLM	14,1752135556753	14,18	14	ng/mL

Regulatory Reporting (M10 Scope)

2.4. Standard and Quality Control Solutions Summary

Human plasma and whole blood treated with K₂EDTA was used to prepare calibration standards and quality control samples. Standards and QCs were prepared by spiking DRUG1-001 working solutions into human plasma or whole blood. Dried blood standards and QCs were prepared from the spiked human whole blood. Spiking volume was never greater than 5% of the total volume. For dried blood standard and QC preparation, spiked human whole blood was added to Tasso M20 devices at a volume of 90µL to simulate sample collection. The device was then dried overnight at room temperature before standard and QC qualification. Plasma and whole blood standards and QCs were aliquoted and stored at -20°C for future use.

Solution ID	Unique ID	Prep Date	Expiry Date	Storage Conditions
STDs	STD-DRUG1-220028-033/15	19-Aug-22	6-Sep-22	-20°C
QCs	QC-DRUG1-220028-033/15	19-Aug-22	6-Sep-22	-20°C
STDs	STD-DRUG1-220028-034/10	20-Aug-22	7-Sep-22	-20°C

Solution ID	Unique ID	Prep Date	Expiry Date	Storage Conditions
QCs	QC-DRUG1-220028-034/10	20-Aug-22	7-Sep-22	-20°C
STDs	STD-DRUG1-220028-035/9	20-Aug-22	30-Aug-22	RT
QCs	QC-DRUG1-220028-035/9	20-Aug-22	30-Aug-22	RT

2.5. Acceptance Criteria of Calibration Standards

For in Human Dried Blood, Human Plasma and Human Whole Blood, a <Regression> was used to determine the concentration/detector response relationship. A representative calibration curve is shown for in Human Dried Blood, Human Plasma and Human Whole Blood. The correlation coefficient (r value) must be ≥0.99 in order to demonstrate adequate linearity of the batch. One set of eight calibration standards was included in each quantitative batch. For the batch to be accepted, at least 75% of the calibration standards must have a back-calculated concentration of 100% ± 15.0% of nominal concentration (100% ± 20.0% for the LLOQ). Back-calculated calibration curve standard concentrations for Human Dried Blood, Human Plasma and Human Whole Blood are presented in Table 2- Table 4 respectively. Standard curve parameters for Human Dried Blood, Human Plasma and Human Whole Blood are presented in Table 5- Table 7 respectively.

Analyte	Matrix	Standards Accuracy Range (%)	Standards Precision Range (%)
DRUG1-001	Human Whole Blood	N/A	N/A
DRUG1-001	Human Plasma	95.2% - 103.0%	0.6% - 7.4%
DRUG1-001	Human Dried Blood	93.8% - 104.2%	1.0% - 8.5%

2.6. Acceptance Criteria of Quality Control Samples

Each batch contained at minimum 2 sets of quality control samples at each level (low, medium, and high). At least two-thirds of all QC samples (LQC, MQC, HQC) and at least half at each concentration level must have a back calculated concentration of 100% ± 15.0% of nominal. The concentration data from the QCs for plasma, whole blood, and dried blood are presented in Table 8- Table 10 respectively.

Analyte	Matrix	Nominal Concentration (ng/mL)	QC Inter-Batch Accuracy (%)	QC Inter-Batch Precision (%)
DRUG1-001	Human Whole Blood	3.00	99.0%	7.4%
DRUG1-001	Human Whole Blood	30.0	107.0%	1.2%
DRUG1-001	Human Whole Blood	375	108.0%	3.2%

Table 4 Calibration Standards Concentration for DRUG1-001 in Human Dried Blood

Batch	1.00 ng/mL		2.00 ng/mL		5.00 ng/mL		10.0 ng/mL		50.0 ng/mL		100 ng/mL		400 ng/mL		500 ng/mL	
	Conc	%RD	Conc	%RD	Conc	%RD	Conc	%RD	Conc	%RD	Conc	%RD	Conc	%RD	Conc	%RD
1	1.01	1.0	1.98	-1.0	5.11	2.2	9.37	-6.3	54.4	8.8	99.6	-0.4	410	2.5	469	-6.2
6	1.03	3.0	1.96	-2.0	4.32	-13.6	10.6	6.0	52.3	4.6	107	7.0	397	-0.8	478	-4.4
7	1.01	1.0	2.00	0.0	4.64	-7.2	10.4	4.0	49.7	-0.6	95.8	-4.2	417	4.3	515	3.0
N	3		3		3		3		3		3		3		3	
Mean	1.02		1.98		4.69		10.1		52.1		101		408		487	
SD	0.0115		0.0200		0.397		0.660		2.35		5.70		10.1		24.4	
%CV	1.1		1.0		8.5		6.5		4.5		5.6		2.5		5.0	
% Accuracy	102.0		99.0		93.8		101.0		104.2		101.0		102.0		97.4	

Table 5 Calibration Curve Parameters for DRUG1-001 in Human Whole Blood

Batch	Slope	Intercept	r-value
4	0.00743	0.00597	0.9973
8	0.00707	0.00132	0.9995

Table 6 Calibration Curve Parameters for DRUG1-001 in Human Plasma

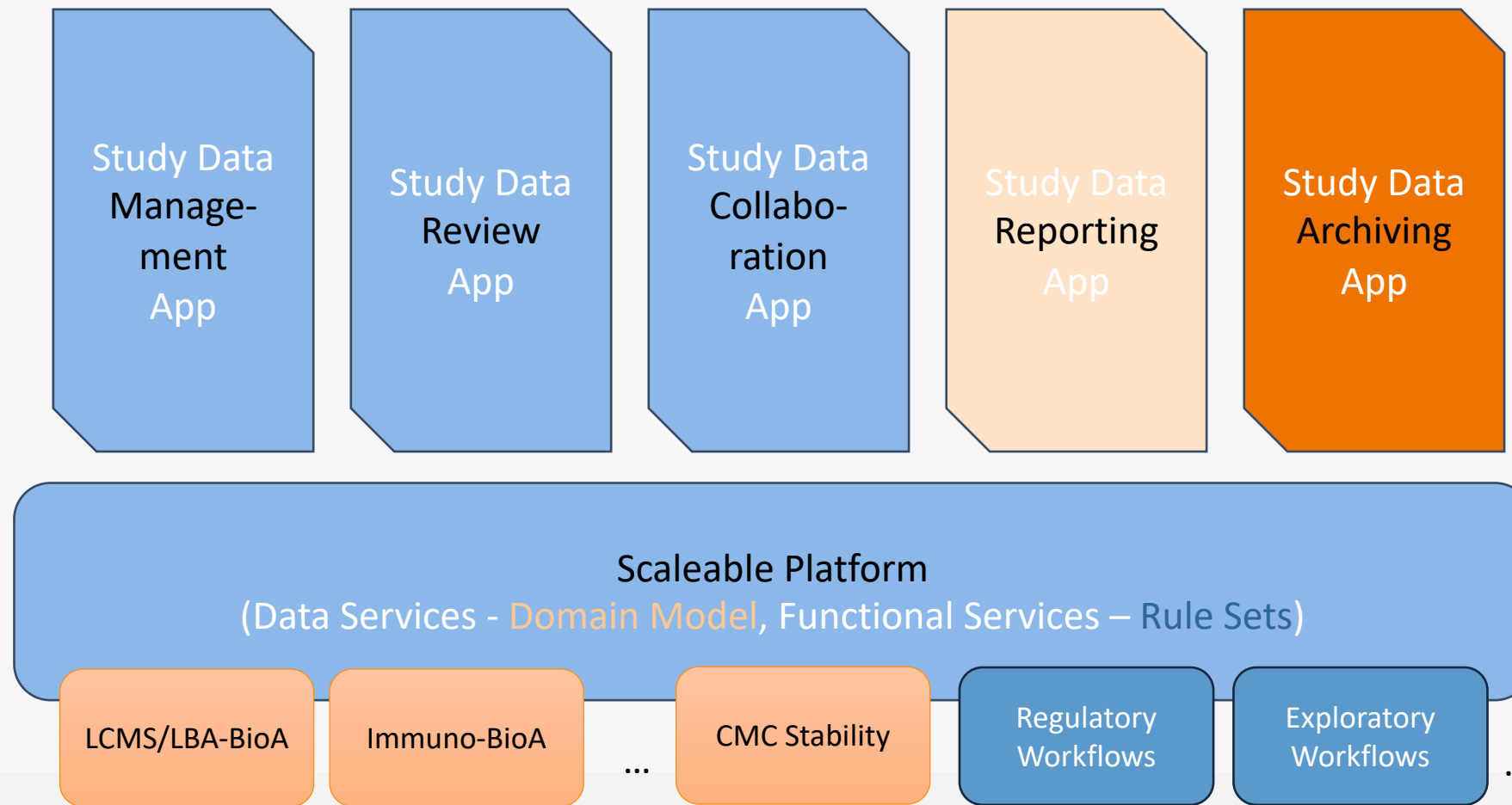
Batch	Slope	Intercept	r-value
2	0.0116	0.000727	0.9995
3	0.0118	0.000222	0.9994
9	0.00941	-0.00146	0.9975
10	0.0102	0.000612	0.9993

Table 7 Calibration Curve Parameters for DRUG1-001 in Human Dried Blood

Batch	Slope	Intercept	r-value
1	0.00974	0.00113	0.9985
6	0.0102	-0.000275	0.9970
7	0.00942	0.00136	0.9990

Table 8 Summary of DRUG1-001 QC samples in Human Whole Blood in the 3.00-375 ng/mL range

Batch	3.00 ng/mL		30.0 ng/mL		375 ng/mL	
	Conc	%RD	Conc	%RD	Conc	%RD
4	2.92	-2.7	31.9	6.3	417	11.2
4	2.71	-9.7	32.5	8.3	389	3.7
N	2		2		2	
Mean	2.82		32.2		403	
SD						
%CV	-		-		-	
%Accuracy	-		-		-	
8	3.24	8.0	31.6	5.3	400	6.7
8	3.01	0.3	32.2	7.3	414	10.4
N	2		2		2	
Mean	3.13		31.9		407	



Study Data Archiving

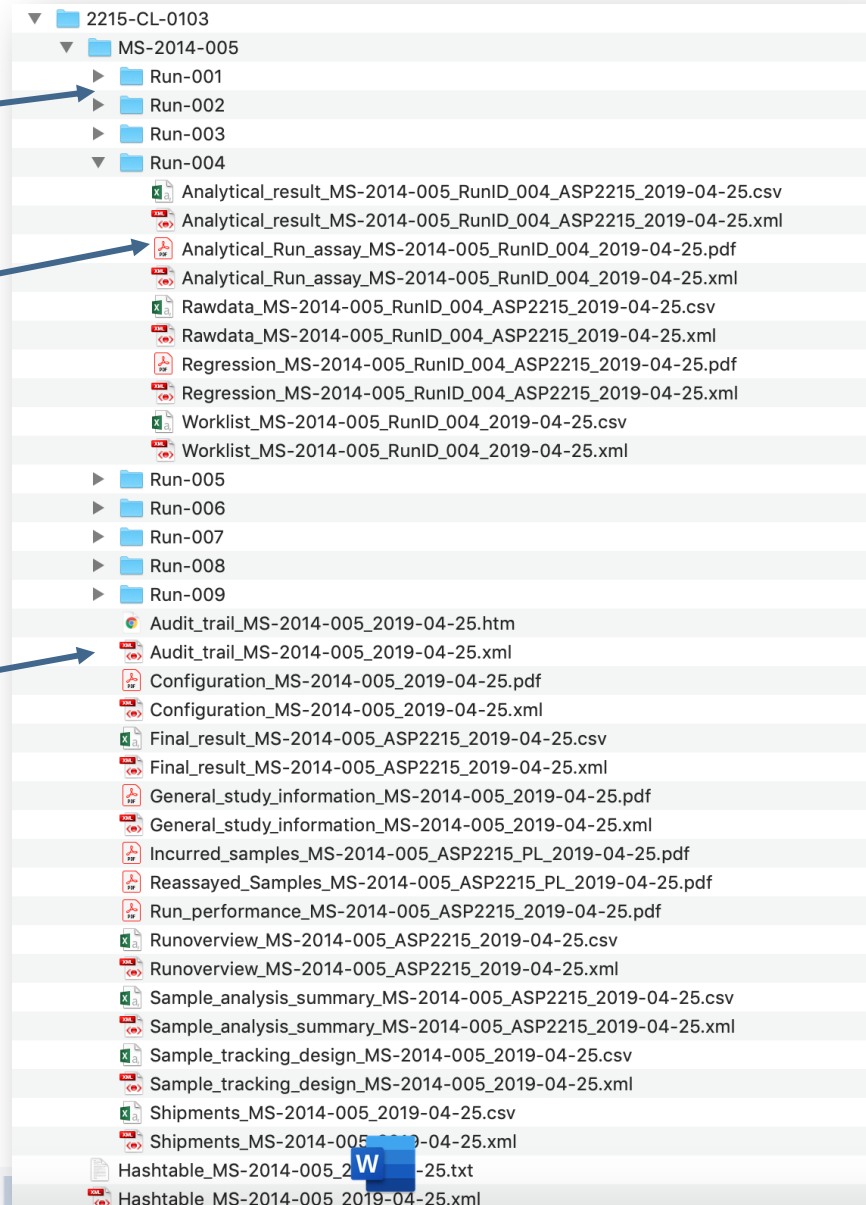
Mission: A New Approach to Archiving

Study Archiving Framework

- Refer to <https://www.fda.gov/media/75414/download>
- US FDA Guidance for Industry: „21 CFR Part 11; Electronic Records; Electronic Signatures; Maintenance of Electronic Records“ was **withdrawn** (line 100)
 - Section 11.10 (b) was requesting: “The ability to generate accurate and complete copies of records in **both human readable and electronic** form suitable for inspection, review, and copying by the agency“
 - Replaced with **recommendation** (line 284ff):
 - “We recommend that you supply **copies of electronic records** by: ...
Using established automated conversion or export methods, where available, to make copies **in a more common format** (examples of such formats include, but are not limited to, PDF, XML, or SGML).
...
In each case, we recommend that the copying process used produces copies that preserve the content and meaning of the record. ...”
- Case Study: Create Study Archive mechanism that is
 - human readable for fast review without addtl. software
 - consistent with prior submission documents (statistics, comments, ...)
 - as light-weight as possible
 - makes all data accessible to be further processed without knowledge of any software

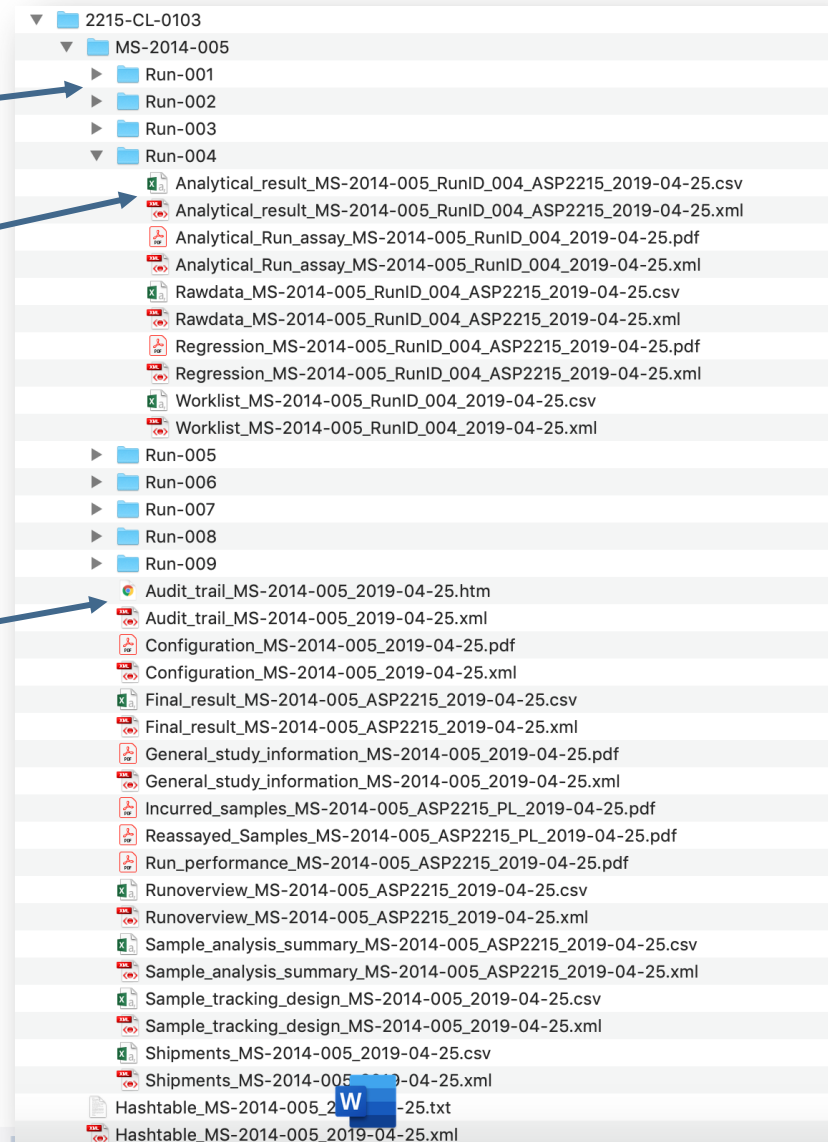
Human Readable

- PDF document stack
 - Structure by RUN
- Individual analyte reports
 - with "raw" response value tabulation
 - calibration data (regression info)
 - processing information
 - ...
- Structure by STUDY
 - Audit trail
 - ...



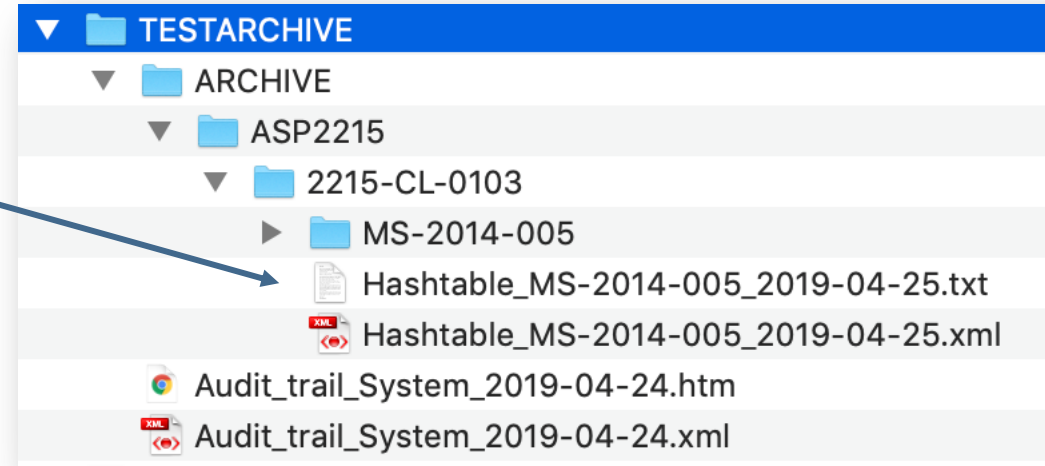
Accessible Data

- XML and/or CSV file stack
 - Structure by RUN
- Individual analyte data
 - with "raw" response value tabulation
 - calibration data (regression info)
 - processing information
 - ...
- Structure by STUDY
 - Audit trail



Data Integrity

- File with checksum of all files
 - Hash-values of files
- Checksum of this file in processing protocol
 - Hash of Hashes



Algorithm	Hash	Path
SHA256	8e8b22f10cf4516115796809041a2e54df9970a3520ee7ada03dd38056577530	ASP2215\2215-CL-0103\MS-2014-005\Run-001\Analytical_Run_assay_MS-2014-005_RunID_001_2019-04-25.pdf
SHA256	c4dadba6c5234df7d299c914348e9ec537fc5842266b03453cb4f240ea072fc7	ASP2215\2215-CL-0103\MS-2014-005\Run-001\Analytical_Run_assay_MS-2014-005_RunID_001_2019-04-25.xml
SHA256	8b51c10e1746a14fa46085fa067b16a01293765e6dc904cc27a37d3c2aab03a0	ASP2215\2215-CL-0103\MS-2014-005\Run-002\Analytical_Run_assay_MS-2014-005_RunID_002_2019-04-25.pdf
SHA256	adb248c5c4f4d788817f9464786d9dbd562917881714ea11736a8eed6d1bc78	ASP2215\2215-CL-0103\MS-2014-005\Run-002\Analytical_Run_assay_MS-2014-005_RunID_002_2019-04-25.xml
SHA256	98364a74f43e9105604166c1f33da8f0dbdf5b33ca953e59be7c1db5c86448	ASP2215\2215-CL-0103\MS-2014-005\Run-003\Analytical_Run_assay_MS-2014-005_RunID_003_2019-04-25.pdf
SHA256	83e10afa4adb3b5a79880bfaa7d7764343b8cfc23a5e5d0708b3784cce9bb	ASP2215\2215-CL-0103\MS-2014-005\Run-003\Analytical_Run_assay_MS-2014-005_RunID_003_2019-04-25.xml
SHA256	5c6045a2c5f6824363619d18d424e63fa8177f184bce4a01dedcb24f332424b1	ASP2215\2215-CL-0103\MS-2014-005\Run-004\Analytical_Run_assay_MS-2014-005_RunID_004_2019-04-25.pdf
SHA256	3fcd126fb6f0fb01d467b3ab97e16b992647b098e41a2ab6b84f0f9ad5d12001	ASP2215\2215-CL-0103\MS-2014-005\Run-004\Analytical_Run_assay_MS-2014-005_RunID_004_2019-04-25.xml
SHA256	4f2726ea14f1f639f0a5f24f0b8f144b0a0f782b97444395080c4dd987cd1421	ASP2215\2215-CL-0103\MS-2014-005\Run-005\Analytical_Run_assay_MS-2014-005_RunID_005_2019-04-25.pdf
SHA256	7b5ee1be9c160e74bcd5d387935534055a6f02aa5420541c316ee5fe793ce16c	ASP2215\2215-CL-0103\MS-2014-005\Run-005\Analytical_Run_assay_MS-2014-005_RunID_005_2019-04-25.xml
SHA256	fc8ed60f0024733c2af619474843808bb574cdf9da4767ddab84d9c4a3594cb0	ASP2215\2215-CL-0103\MS-2014-005\Run-006\Analytical_Run_assay_MS-2014-005_RunID_006_2019-04-25.pdf
SHA256	b2c7f88286b9a852cfb4bb52972926a587bb955b060b5903670739682c4f8ff6	ASP2215\2215-CL-0103\MS-2014-005\Run-006\Analytical_Run_assay_MS-2014-005_RunID_006_2019-04-25.xml
SHA256	47293e719e61a39eff593fb833cfff1613de1a7d34de293724105fc49ca89958f	ASP2215\2215-CL-0103\MS-2014-005\Run-007\Analytical_Run_assay_MS-2014-005_RunID_007_2019-04-25.pdf
SHA256	6e10ecdffa1a49a4760ca9d5cfe7f6e4fd08a85c8501ed7ad28a7f8005b2a60c	ASP2215\2215-CL-0103\MS-2014-005\Run-007\Analytical_Run_assay_MS-2014-005_RunID_007_2019-04-25.xml
SHA256	0755d7cf2d11eb67ee1c3e9f034bbb7331b1cb4785c6c3061bccaba67e40df38	ASP2215\2215-CL-0103\MS-2014-005\Run-008\Analytical_Run_assay_MS-2014-005_RunID_008_2019-04-25.pdf
SHA256	41252d64c88711b5024f0e22e086b11820d4f32f01e552866ab0150406dc	ASP2215\2215-CL-0103\MS-2014-005\Run-008\Analytical_Run_assay_MS-2014-005_RunID_008_2019-04-25.xml

Contact for questions/comments

Norbert Bittner
up to data GmbH
Energie-Allee 1
D-55286 Woerrstadt

norbert.bittner@uptodata.com

