



DIGITAL INTEGRATION HUB

**Implementing the Allotrope Framework  
at Biotechs - A case study between  
Macromoltek and ZONTAL**

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**Allotrope Connect**

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**Turn Data into Corporate Assets - Make Data Available for Reuse –  
Secure Compliance & Data Integrity**

# OVERVIEW

OUR **VISION** IS TO CHANGE *DRUG DISCOVERY* TO *DRUG DESIGN*, ELIMINATING LUCK FROM THE PROCESS

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Software enabled biotech company  
focused on *de novo in silico* antibody design

We have developed an advanced AI platform  
to design potent and novel antibodies

**We support our partners in addressing unmet needs in  
biotechnology and molecular bioscience**

# ABOUT US

First to computationally design an antibody

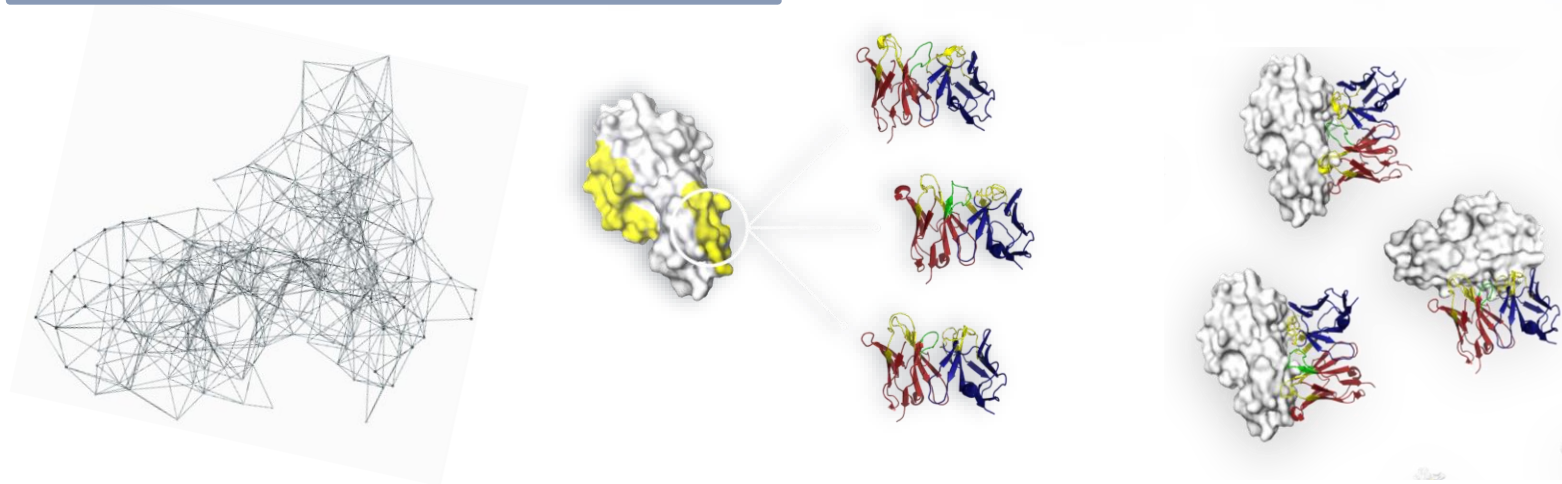
Built design algorithms entirely in-house

Our algorithms rely on decades of structural and sequence data

Highly experienced cross-disciplinary team

Computer science, machine learning, biology, engineering, therapeutic development

# WHAT WE DO



**TARGET  
STRUCTURE**

**DESIGN  
ALGORITHM**

**POST-PROCESSING  
AND SELECTION**

**LAB TESTING**

**NN MODELS**

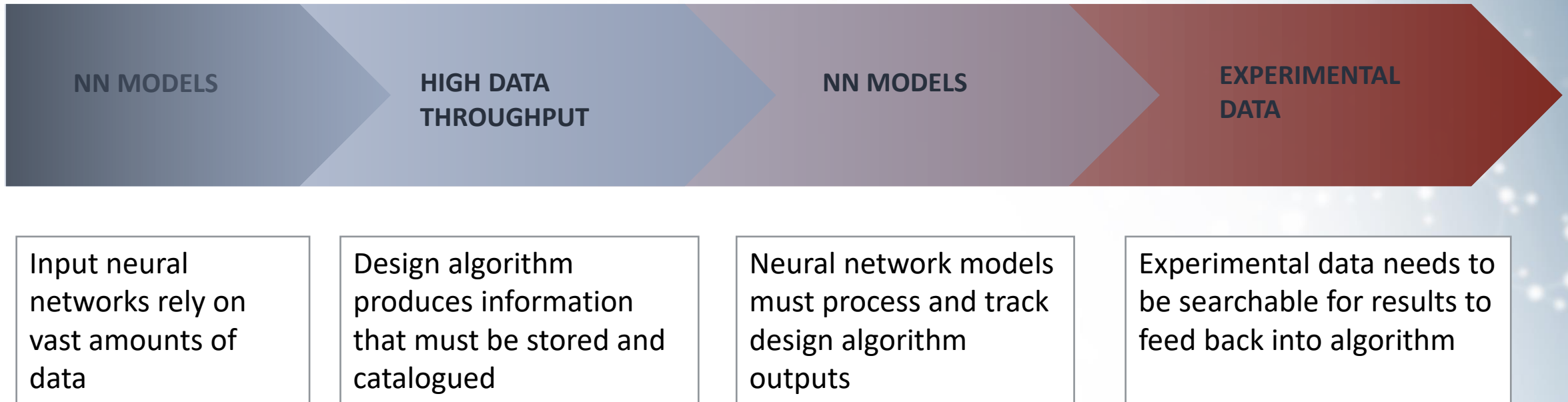
**HIGH DATA  
THROUGHPUT**

**NN MODELS**

**EXPERIMENTAL  
DATA**

# NEED FOR DATA PIPELINE

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We need a **consistent data pipeline** which tracks from the earliest stages through to validated antibodies in order to **continuously improve algorithms**

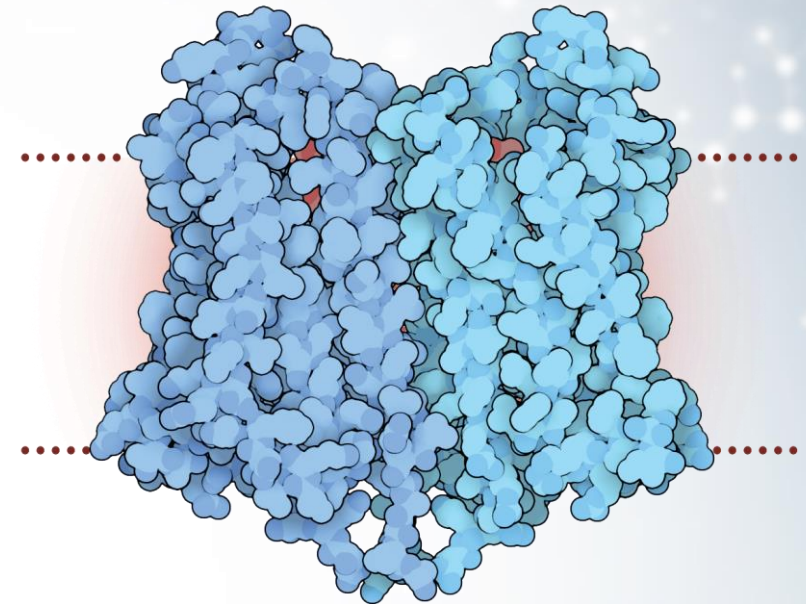
## Current Challenges

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Finding data

Preserving data

Cross project analysis



# Biotechs need FAIR data – can we use Allotrope?

Current schools of thought:

Result in:

Build complex ontological graph models

Long project runtimes before ADF can be created, most complete representation of universe

Build tabular models

Easy to create and align with SMEs, limited descriptive power

Leverage data cubes and limit semantics

Standardized data representation, but limited contextual info

Use ADF data package as audit trailed Zip folder

Instant ADF with limited data genealogy

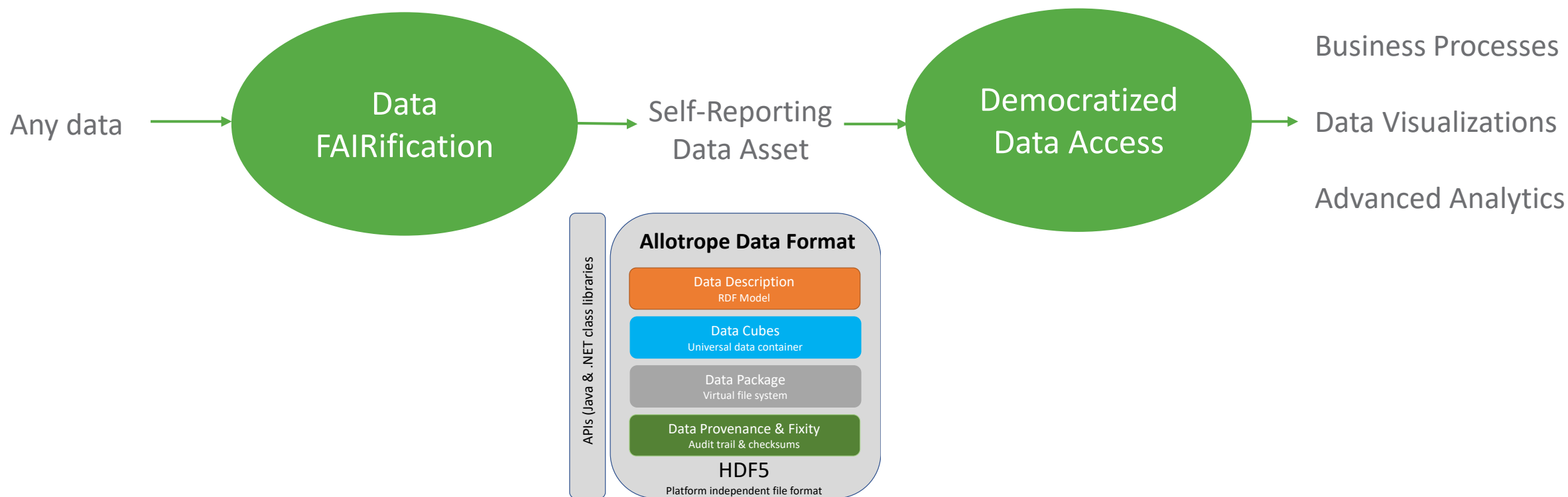
Ignore all semantics and use data abstractions (like json) instead of ADF

ADF is only created as an afterthought



# Productionalize ADF Generation and Reuse

Fit for purpose selection of ADF features

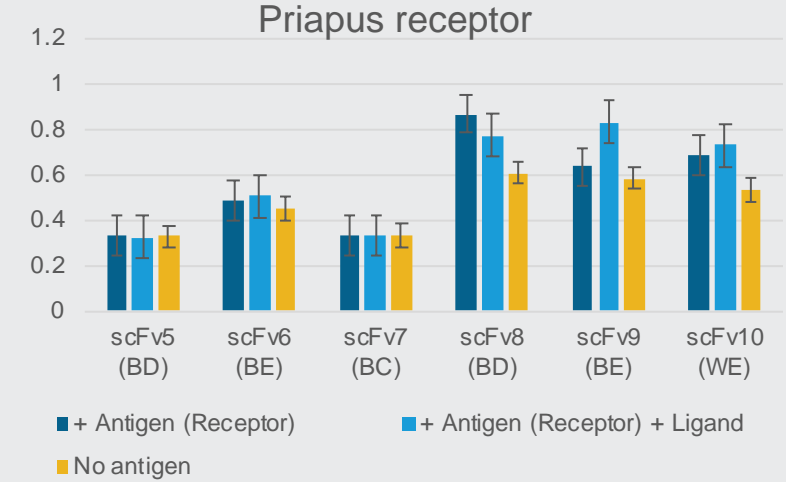


ZONTAL is the first Digital Hub that produces ADF on demand and delivers ADF to any consumer!



# Elisa Assay – Allotrope based Datamodel for Translational Analysis

## Before Zontal:

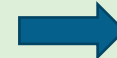
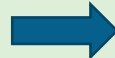
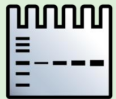


Elisa assay

produces one excel

that results in one plate analysis

## With Zontal:



Multiple assays

are mapped

Data stored in ADF based  
upon ZONTAL Datamodel

and made accessible

for project wide analysis

# Self-Reporting Data Assets

## Map from Raw data and experiment to ELISA Data model

Excel based raw data

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1														
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19														



priapus-4.json — Edited

```
{
  "antigen": "priapus",
  "antigenConcentration": "1ng",
  "bufferSolution": "PBS",
  "note": "Test to Zontal Priapus-4",
  "results": [
    {
      "plasmid": "pM0PAC54 - p54",
      "project": "priapus",
      "labName": "priapus-4",
      "concentrations": [
        "2 ng",
        "0.632456 ng",
        "0.200000 ng",
        "0.063246 ng",
        "0.020000 ng",
        "0.006325 ng",
        "2 ng",
        "0.632456 ng",
        "0.200000 ng",
        "0.063246 ng",
        "0.020000 ng",
        "0.006325 ng"
      ]
    }
  ]
}
```

JSON based experiment description

ADF explorer

Tree View

- Data Description
  - Default
  - adf/dd/annotations
  - Data Package
    - Ingest4.json
    - Audit Trail

Tab 1

Data Description Table [C:\Users\della\Downloads\Elisa-Example-4.adf]

Named Set: Default

Search

☒ Subject ☒ Predicate ☒ Object

Drag a column header here to group by that column

Subject	Predicate	Object
37a2c8e31746b13fae8-74e6	http://mlins.com/foaf/0.1/accountName	demo/boss_admin
37a2c8e31746b13fae8-74e5	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://www.w3.org/2000/01/rdf-schema#Resource
37a2c8e31746b13fae8-74e5	http://purl.org/dc/terms/identifier	2203a2c-cd9-47a7-a52e-650367b2980b
37a2c8e31746b13fae8-74e5	http://purl.org/pav/importedOn	2020-09-08T12:37:39.959Z
37a2c8e31746b13fae8-74e5	http://purl.org/pav/importedBy	https://demo.zontal.space/api/users/boss_admin
Elisa-Example-4	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	http://purl.zontal.io/ontologies/space/information-object#InformationPackage
Elisa-Example-4	http://purl.org/dc/terms/title	Elisa-Example-4
Elisa-Example-4	http://purl.org/pav/version	1
Elisa-Example-4	http://www.w3.org/2004/02/skos/core#prefLabel	Elisa-Example-4
Elisa-Example-4	http://www.w3.org/2004/02/skos/core#prefLabel	Elisa-Example-4
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#representedBy	37a2c8e31746b13fae8-74e5
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#createdOn	2020-09-08T12:37:05.933Z
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#createdBy	https://demo.zontal.space/api/users/boss_admin
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#hasInformationPackageProfile	https://demo.zontal.space/api/informationPackageProfiles/14680GHMVEQ-HD04RL2D...
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#hasInformationCollection	https://demo.zontal.space/api/informationCollections/MWIS4XF33RZVLCK7VPWGMPEM...
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#hasLifecycleStatus	https://purl.zontal.io/codelists/space/lifecycle-status#Archived
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#hasDataOwnerPerson	https://demo.zontal.space/api/users/zontal_space_bot
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#hasDataOwnerGroup	https://demo.zontal.space/api/groups/software_bots
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#hasDataOwnerOrganization	https://purl.zontal.io/ontologies/space/information-object#hasDataOwnerOrganization
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#contentIdentifier	2203a2c-cd9-47a7-a52e-650367b2980b
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#submittedOn	2020-09-08T12:38:08.154Z
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#submittedBy	https://demo.zontal.space/api/users/boss_admin
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#archivedOn	2020-09-08T12:38.11438Z
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#archivedBy	https://demo.zontal.space/api/users/boss_admin
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#expirationReviewedOn	2020-09-08T12:38.11438Z
Elisa-Example-4	http://purl.zontal.io/ontologies/space/information-object#expirationReviewedBy	https://demo.zontal.space/api/users/boss_admin
urn:uuid:811b8c26-2813-4733-871a-d77e06110e4	http://www.w3.org/1999/02/22-rdf-syntax-ns#type	Results Filename
urn:uuid:811b8c26-2813-4733-871a-d77e06110e4	http://purl.allotrope.org/ontologies/property#AFX_0000690	Priapus-4/Priapus-4-RawData.xlsx
urn:uuid:7a7b96c-d441-4b69-8cbe-c8a767b49657	https://www.w3.org/1999/02/22-rdf-syntax-ns#type	Result

Count: 5969

ZONTAL creates ADF file to store raw Elisa data

# Deriving Value from a collection of ADF

**ZONTAL** is the first enterprise scale product that allows effective SQL search on ADF information

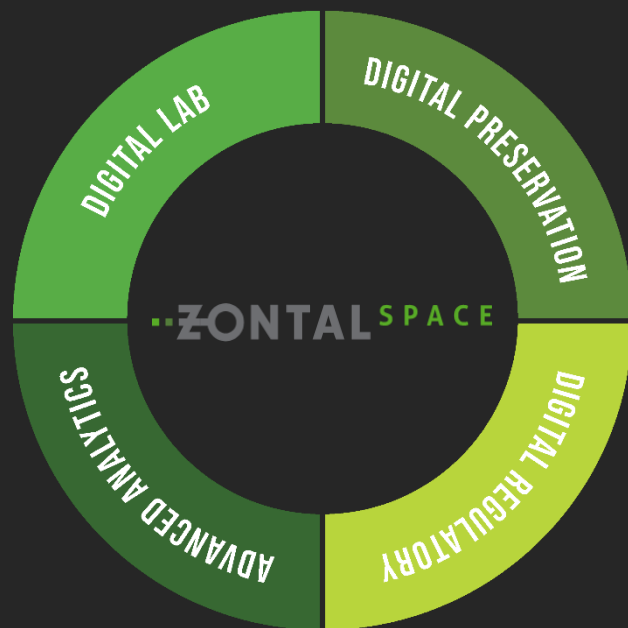
Hold Light



Live Demo!

# ..ZONTAL SPACE

The first FAIR Digital Data Integration &  
Data Lifecycle Management Platform



## Summary

ZONTAL offers ADF creation on  
demand

ZONTAL powers visualization on ADF  
Data

ADF can bring high value to biotechs

Questions?

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