

# How to identify the relevant metadata standard (for Life Sciences)?



#### Marta Eide

Data & Models senior adviser Centre for Digital Life Norway

#### Korbinian Bösl

Data management coordinator ELIXIR Norway & Centre for Digital Life Norway

## **ELIXIR** Europe

'Data for Life'



#### Mission:

To operate a sustainable European infrastructure for biological information, supporting life-science research and its translation to society, the bio-industries, environment and medicine

#### **ELIXIR Members**



Portugal

**United Kingdom** 

Spain

Sweden

#### **ELIXIR Observers**





Slovenia

Switzerland





### Data deposition:

ENA, EGA, PDBe, EuropePMC, ...



### Data management:

Genome annotation
Data management plans



### Data deposition:

ENA, EGA, PDBe, EuropePMC, ...



### Data management:

Genome annotation Data management plans



## Added value data:

UniProt, Ensembl, OrphaNet, ...



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### Data Interoperability:

FAIRSharing, identifiers.org, OLS, Bioschemas, ...



Data deposition: ENA, EGA, PDBe, EuropePMC, ...



Compute:

Secure data transfer, cloud computing, AAI



Data management:

Genome annotation
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Bioinformatics tools:

Bio.tools, Benchmarking: OpenEBench



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Industry:

Innovation and SME programme Bespoke collaborations



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Bio.tools, Benchmarking: OpenEBench



Industry:

Innovation and SME programme Bespoke collaborations



Training:

TeSS, Data Carpentry, eLearning

## RDMkit



#### Your problem

Compliance monitoring

Data analysis

Data management plan

Data organisation

Data protection

Data publication

Data quality

Data storage

Data transfer

Identifiers

Licensing

Metadata management

Sensitive data



rdmkit.elixir-europe.org

Distributed national Research Infrastructure

~ 34 FTE/a - funded RCN, universities & users



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Training events on bioinformatics & RDM

last 1.5a: ~330 registrations



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Dedicated data storage & analysis platform

Norwegian e-Infrastructure for Life Sciences - **NeLS** 



Distributed national Research Infrastructure

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Deliverables to ELIXIR Europe

Tools and databases

















## $\begin{array}{c} \textbf{Filled questionnaire} \rightarrow \textbf{Template} \rightarrow \textbf{DMP in various formats} \\ \text{once} \\ \\ \textbf{per funding body} \\ \\ \textbf{.docx, .tex, .html, .jso} \\ \end{array}$

#### Full compliance:





https://github.com/ds-wizard

elixir-no.ds-wizard.org



## $\begin{array}{c} \textbf{Filled questionnaire} \rightarrow \textbf{Template} \rightarrow \textbf{DMP in various formats} \\ \text{once} \\ \\ \textbf{per funding body} \\ \textbf{.docx, .tex, .html, .jso} \\ \end{array}$

Adapted for Norwegian users

elixir-no.ds-wizard.org

#### Full compliance:





https://ds-wizard.org https://github.com/ds-wizard



## Filled questionnaire $\rightarrow$ Template $\rightarrow$ DMP in various formats once per funding body .docx, .tex, .html, .jso

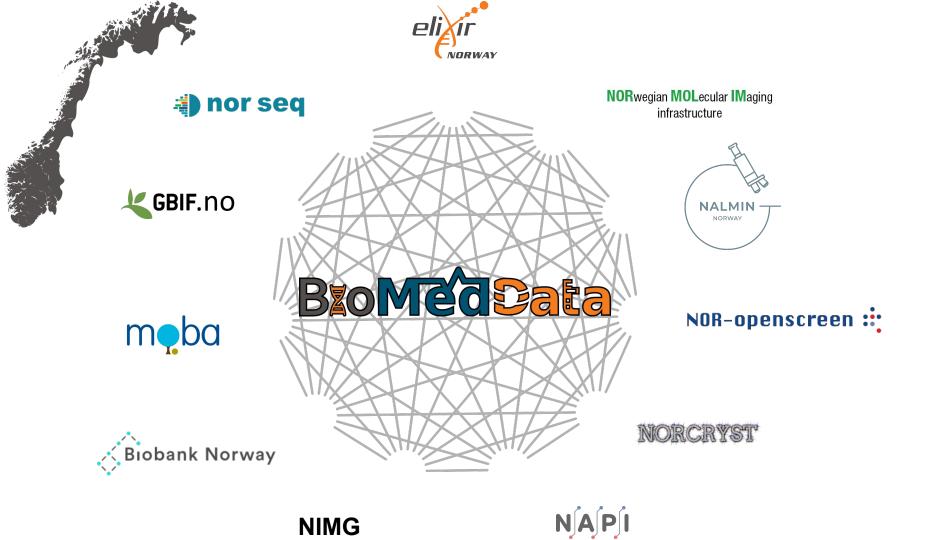


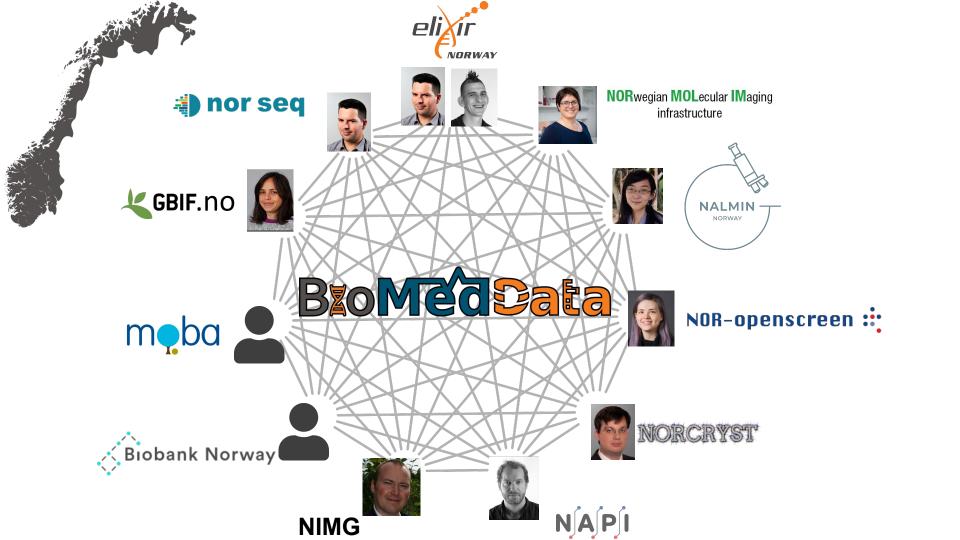
#### Full compliance:





https://ds-wizard.org https://github.com/ds-wizard







273 model/formats standards



273 model/formats standards

Technology & domain specific

## Investigation



273 model/formats standards

Technology & domain specific

## Investigation



Study(s)

273 model/formats standards

Technology & domain specific

## Investigation



Study(s)

273 model/formats standards

Technology & domain specific

Assay(s)

## Investigation

Persons
Organizations
Publications



Study(s)

273 model/formats standards

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273 model/formats standards

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Study(s)

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Design Factor Protocol

## Investigation

Persons Organizations Publications



Study(s)

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273 model/formats standards

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Assay(s)

Measurement Technology Materials Data

## Investigation

Persons Organizations Publications



Study(s)

Design
Factor
Protocol

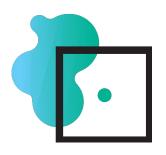
Controlled Vocabularies
Ontologies
Standards

Technology & domain specific

273 model/formats standards

Assay(s)

Measurement Technology Materials Data



# Centre for Digital Life Norway (DLN 2.0) facilitates transdisciplinary research, innovation, and education in Life Science



Transdisciplinary collaborations

www.digitallifenorway.org



Education and career development



Responsible research and innovation



Innovation and commercialisation



Data management





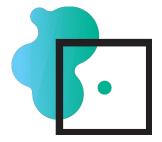








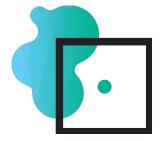




35 transdisciplinary biotechnology projects all over the country.

Biotechnology with digital technology: health, aquaculture, agriculture & industrial biotechnology.

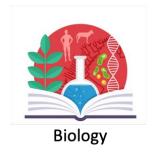




35 transdisciplinary biotechnology projects all over the country.

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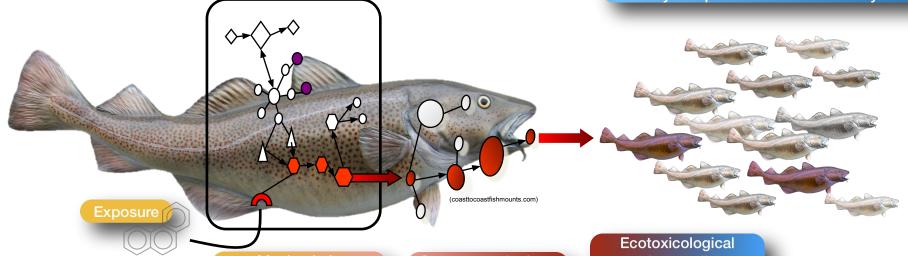


Responsible research and innovation (RRI)

## Systems toxicology



Evolutionary and comparative aspects: Why do species behave differently?

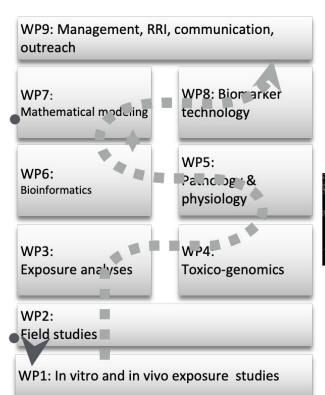


Mechanistic understanding: Where does it start Systems toxicology understanding:
What does it lead to?

understanding:
What are the ultimate consequences?



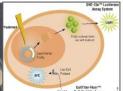
And: How can we use this knowledge to develop tools for monitoring environmental and human health?











Genome mining

Transcriptomics

**Proteomics** 

Metabolomics - lipidomics

### In our breakout:

#### Metadata standards

Structure and content of a metadata standard on one specific example

Brief overview of other metadata standards used in ELIXIR repositories



Tools to navigate standards and ontologies: FAIRsharing, Data Stewardship Wizard, OLS



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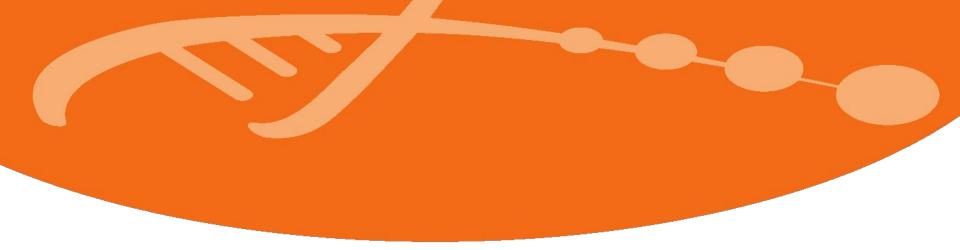
#### How to track metadata

What kind of tools are out there?

SEEK: one possible solution (not only for Life Sciences)

Examples & Experiences from the dCod1.o project





# How to identify the relevant metadatastandard (for Life Sciences)?

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Find

Recommendations

Standards and/or databases recommended by journal or funder data policies.

© Collections

Standards and/or databases grouped by domain, species or organization.



https://fairsharing.org/askFAIRsharing/wizard



	Are you looking for a database, policy, and/or standard?					
	Step 1 Registr	<u> </u>	$\overline{}$			
		Step 1 of	ı			
Registry:	☐ Databases ☐ Policies ☐ Standards					
	Please choose in which registry/registries you would like	e to search.				

https://fairsharing.org/askFAIRsharing/wizard

RDMkit



inbuilt curated resources:

Repositories & Metadata standards

FAIRsharing



rdmkit.elixir-europe.org

RDMkit



inbuilt curated resources:

Repositories & Metadata standards

FAIRsharing

**Software** 





rdmkit.elixir-europe.org

## RDMkit



inbuilt curated resources:

Repositories & Metadata standards

FAIRsharing

**Software** 



**Training** 

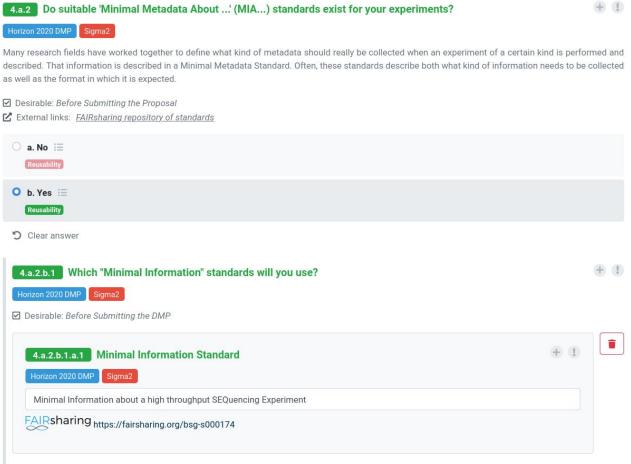




rdmkit.elixir-europe.org



Build your DMP by following a decision tree with defined questions



elixir-no.ds-wizard.org

### **Example MINSEQ - for quantitative sequencing**

Minimum Information about a high-throughput nucleotide SEQuencing Experiment

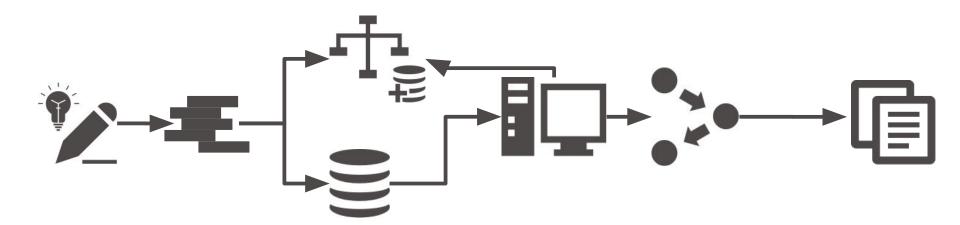
Established 2012

Extension of MIAME (for Arrays)

Governed by Functional Genomics Data Society

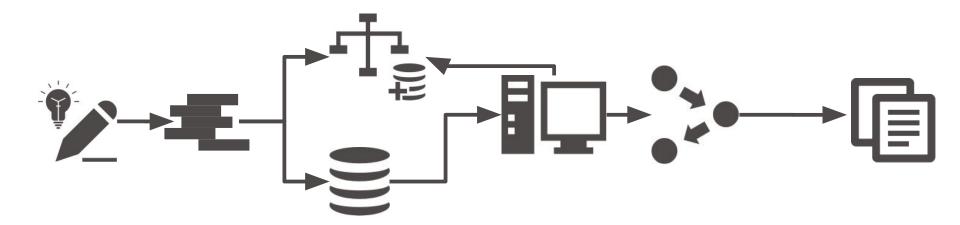


### **MINSEQE**



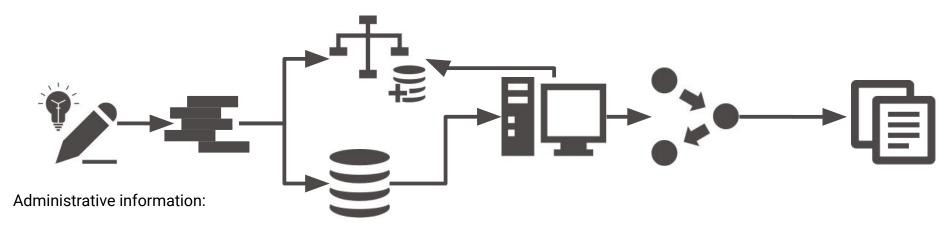
### **MINSEQE**





### **MINSEQE**



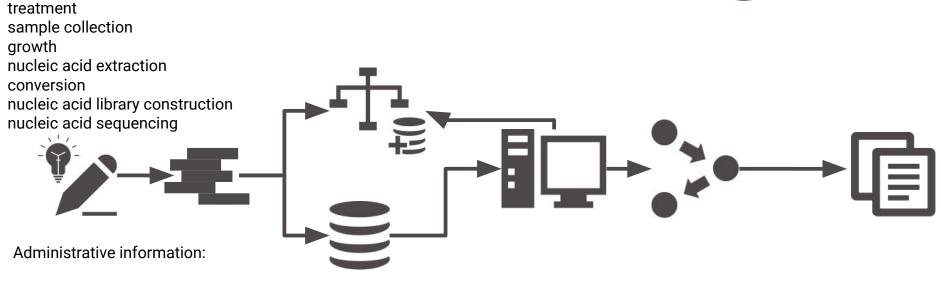


Persons Organizations Publications Experimental conditions/design

protocols: MINSEQE







Persons Organizations Publications Experimental conditions/design

protocols:

treatment

growth

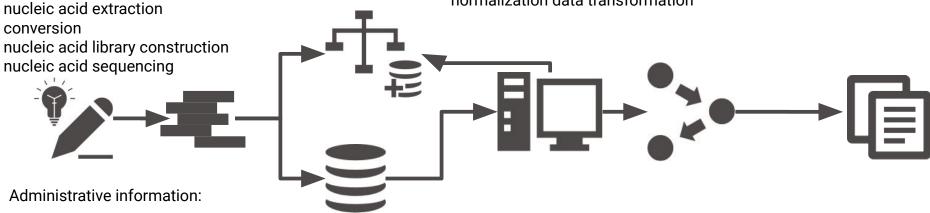
sample collection

**MINSEQE** 



protocols:

high throughput sequence alignment normalization data transformation



Persons Organizations Publications

fastq bam csv/tsv Experimental conditions/design

protocols:

treatment

growth

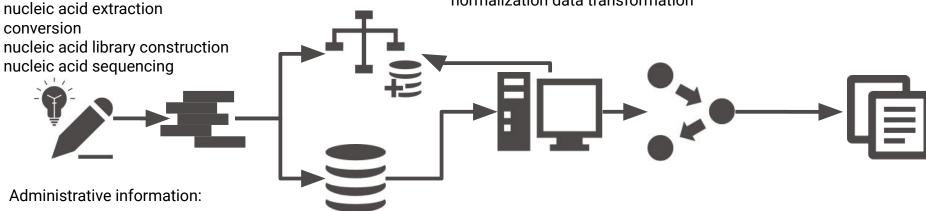
sample collection

**MINSEQE** 



protocols:

high throughput sequence alignment normalization data transformation



Persons Organizations Publications

Experimental conditions/design **MINSEQE ArrayExpress** protocols: protocols: treatment sample collection high throughput sequence alignment growth normalization data transformation nucleic acid extraction conversion nucleic acid library construction nucleic acid sequencing Administrative information: Ensembl ID

RefSeq ID

fastq

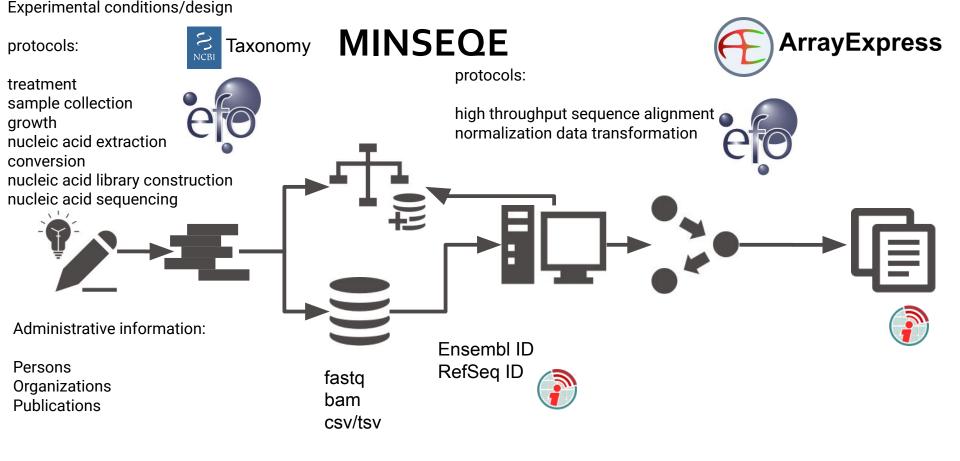
bam

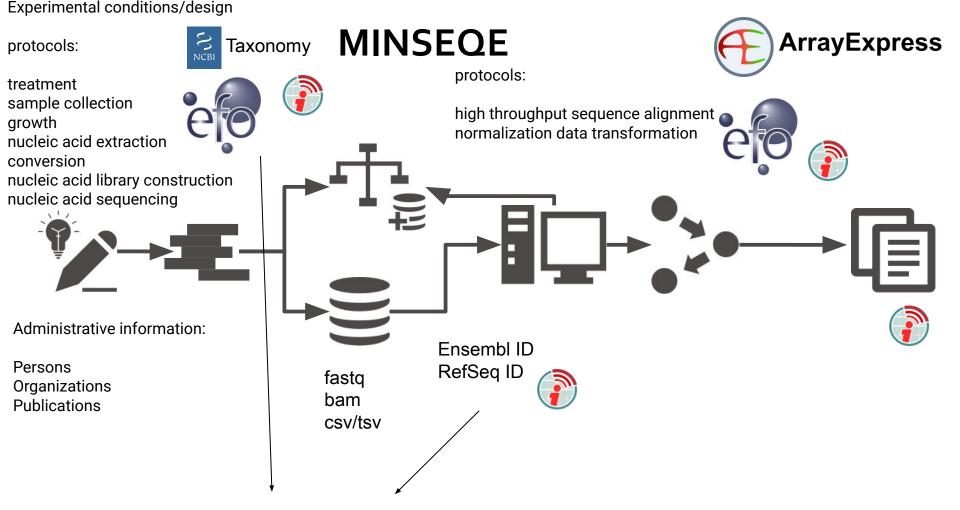
csv/tsv

Persons

Organizations

**Publications** 





Interlinking with other resources

# How many way can you say "female"?

# How many way can you say "female"?

18-day pregnant females	female (lactating)	individual female	worker caste (female)
2 yr old female	female (pregnant)	lgb*cc females	sex: female
400 yr. old female	female (outbred)	mare	female, other
adult female	female parent	female (worker)	female child
asexual female	female plant	monosex female	femal
castrate female	female with eggs	ovigerous female	3 female
cf.female	female worker	oviparous sexual females	female (phenotype)
cystocarpic female	female, 6-8 weeks old	worker bee	female mice
dikaryon	female, virgin	female enriched	female, spayed
dioecious female	female, worker	pseudohermaprhoditic female	femlale
diploid female	female(gynoecious)	remale	metafemale
f	femele	semi-engorged female	sterile female
famale	female, pooled	sexual oviparous female	normal female
femail	femalen	sterile female worker	sf
female	females	strictly female	vitellogenic replete female
female - worker	females only	tetraploid female	worker
female (alate sexual)	gynoecious	thelytoky	hexaploid female
female (calf)	healthy female	female (gynoecious)	female (f-o)

probably female (based on morphology)

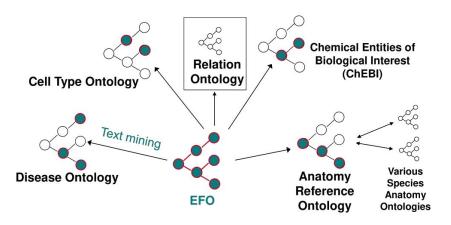
hen

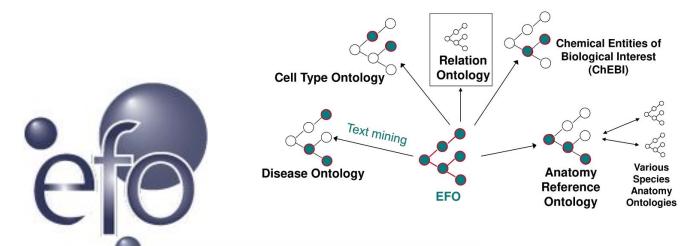
female (note: this sample was originally provided as a \"male\" sample to us and therefore labeled this way in the brawand et al. paper and original geo submission; however, detailed data analyses carried out in the meantime clearly show that this sample stems from a female individual)"

Courtesy of N. Silvester, European Nucleotide Archive, EMBL-EBI









- experimental factor
  - material property
    - **⊟**-quality
      - =-sex

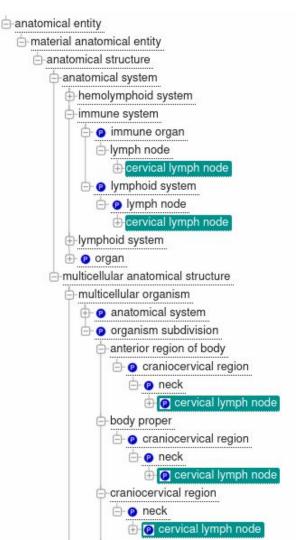
-female

### database cross reference

- MSH:D005260
- MO:506
- NClt:C16576
- SNOMEDCT:248152002
- CARO:0000028
- PATO:0000383

## • ŭ Uberon

Onthologies enable hierarchical searches



#### Welcome to the EMBL-EBI Ontology Lookup Service

Search OLS...

Search

Examples: diabetes, GO:0098743

Looking for a particular ontology?



The Ontology Lookup Service (OLS) is a repository for biomedical ontologies that aims to provide a single point of access to the latest ontology versions. You can browse the ontologies through the website as well as programmatically via the OLS API. OLS is developed and maintained by the Samples, Phenotypes and Ontologies Team (SPOT) at EMBLEBI.

https://www.ebi.ac.uk/ols/index



In addition to OLS the SPOT team also provides the OxO, Zooma and Webulous services. OxO provides cross-ontology mappings between terms from different ontologies. Zooma is a service to assist in mapping data to ontologies in OLS and Webulous is a tool for building ontologies from spreadsheets.

#### A Report an Issue

For feedback, enquiries or suggestion about OLS or to request a new ontology please use our GitHub issue tracker. For announcements relating to OLS, such as new releases and new features sign up to the OLS announce mailing list

#### ■ Data Content

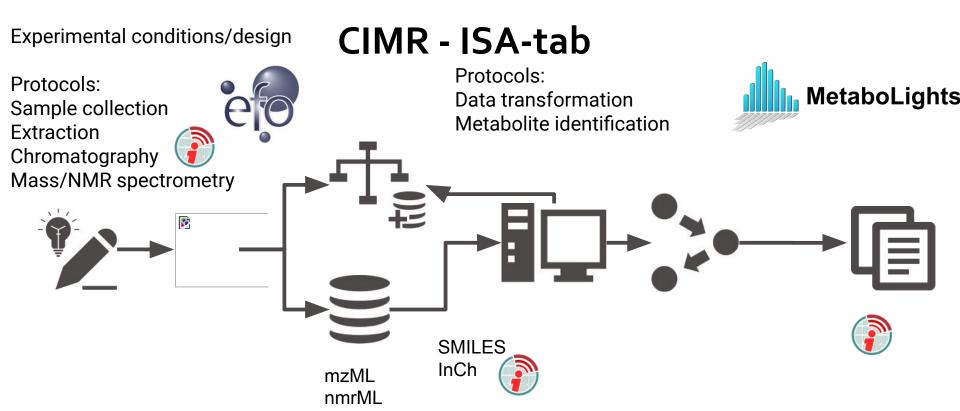
#### Updated 28 May 2021 08:03

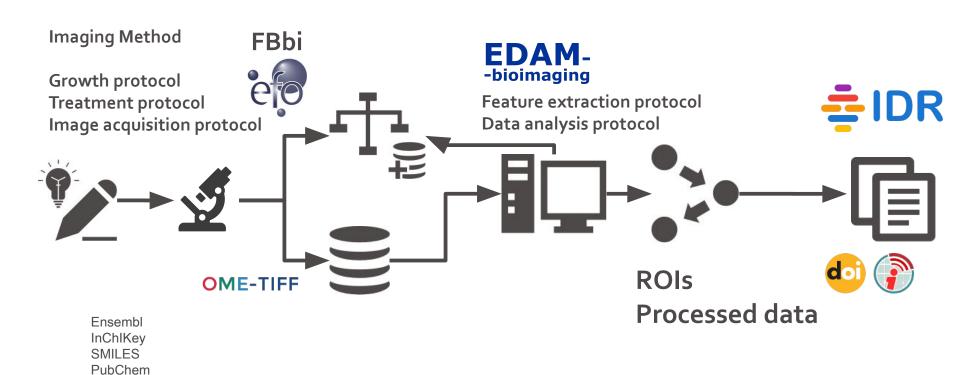
- · 264 ontologies
- 6,460,093 terms
- 32,279 properties
- 497,528 individuals



elijir

The Ontology Lookup Service is part of the ELIXIR infrastructure





**ChEBI** 

# Where to deposit data?



















# Where to deposit data?















https://www.ebi.ac.uk/submission/

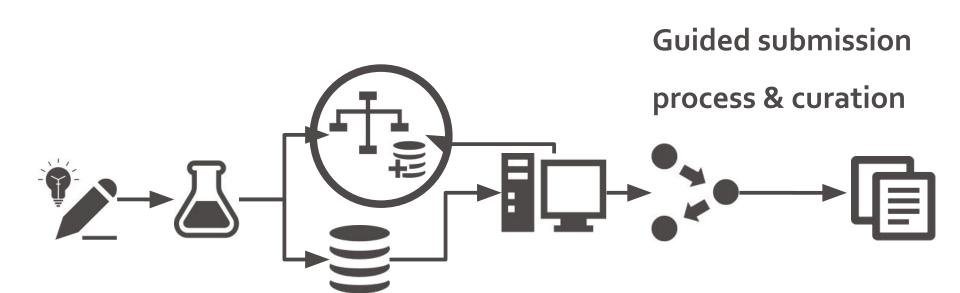




### **Guided submission**

process & curation

Process & curation



# Metadata tracking platforms

### Domain specific:

**COPO** for plant sciences

**MOLGENIS** for biobanking

. . .





# Metadata tracking platforms

### **Domain specific:**

**COPO** for plant sciences

**MOLGENIS** for biobanking

. . .





Adaptable (configuration requires domain knowledge):

Proprietary ELNs/LIMS - often poor support for ontologies

openBIS - open source ELN/LIMS

SEEK





# Challenges

Standards & Repositories historically grown:

... some predate CC licenses (terms of usage ≈ public domain)

... some standards predate DDI, datacite, dublin core

... own PID system (identifiers.org), not all repos issue DOIs (yet)



→ searchability can depend on dataset search engine

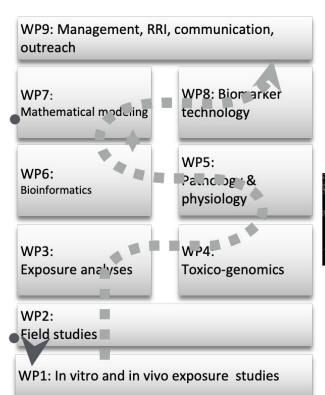
... large curation effort for legacy data >160 PB (EBI repos 2018)

... parallel development: certification procedures: EDD|ECR vs CoreTrustSeal

## Experiences from dCod 1.0 and SEEK



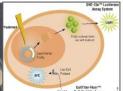












Genome mining

Transcriptomics

**Proteomics** 

Metabolomics - lipidomics







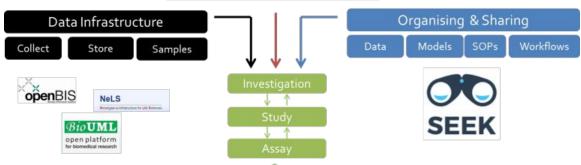




#### **FAIRDOM** integration







fair-dom.org seek4science.org - github.com/seek4science/seek rightfield.org.uk - github.com/myGrid/RightField

Metadata Management

RightField :



but often following the same concept:

## Investigation

Persons Organizations Publications



Study(s)

Design
Factor
Protocol

Controlled Vocabularies
Ontologies
Standards

Technology & domain specific

273 model/formats standards

Assay(s)

Measurement Technology Materials Data

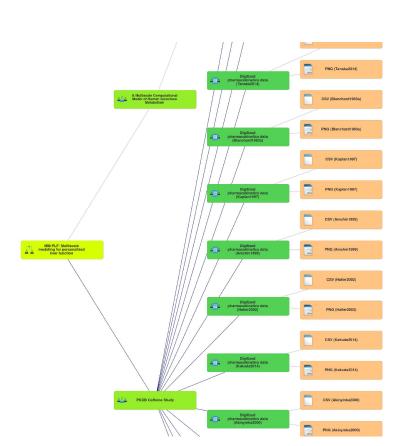


# Investigation

Study

**A**ssay

https://seek4science.org/ https://fairdomhub.org/



## ISA example of dCod 1.0

Study In vivo I-VIII Metabolic reconstruction etc.

AAA PKDB Caffeine Study

Data Link to NeLS Link to GEO Metadata SBML model **Publications** etc.

PNG (Tanaka2014)

PNG (Blanchard1983a)

CSV (Kaplan1997)

Investigation

Ex vivo In vivo In silico Field studies etc.

**Assay** 

Biometric data

Hormone levels

**Omics** 

etc.

Digitized

A Digitized pharmacokinetics data
(Tanaka2014)

□ Digitized
pharmacokinetics data
(Blanchard1983a)

Digitized

△Ⅲ△ pharmacokinetics data
(Kakuda2014)

Digitized

☐ pharmacokinetics data
(Kaplan1997) PNG (Kaplan1997)

CSV (Amchin1999)

PNG (Amchin1999)

CSV (Haller2002)

PNG (Haller2002)

PNG (Kakuda2014)

CSV (Akinyinka2000)

**Programme** dCod 1.0

**Project** 

Systems toxicology



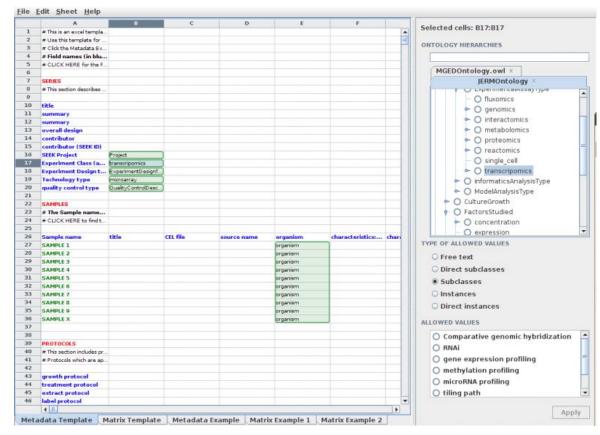


https://seek4science.org/ https://fairdomhub.org/

# RightField 1/3







# Integration of SEEK and









Reference data in NeLS in SEEK



Access data in NeLS through SEEK



Save Metadata to SEEK through NeLS

#### **Galaxy** Days/Weeks nature **Publications Months NeLS** Norwegian e-Infrastructure for Life Sciences ola@uib.no 🛭 store / **Years SEEK** ola@uib.no Open registration **Decades** NORSTORE RESEARCH DATA ARCHIVE

### Administrate access

Sharing ▲

Here you can specify who can view the summary of, get access to the content of, and edit the SOP.

	No Access	View	Download	Edit	Manage	
Public	×	0	0			
■ FAIRDOM	0	✓	4	0	0	
	0	1	0	0	0	×
Stuart Owen	0	4	4	4	4	×
Natalie Stanford	0	<	4	4	0	×

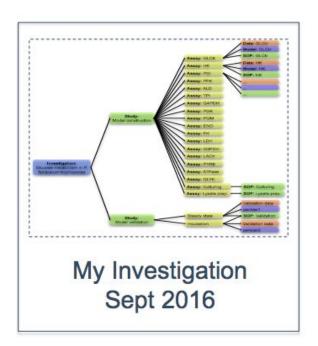
Share with a person

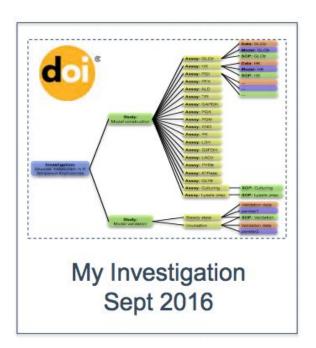
Share with a project/institution

Share with a programme

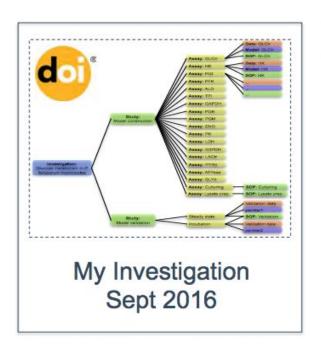
## Generate snapshots and assign DOIs

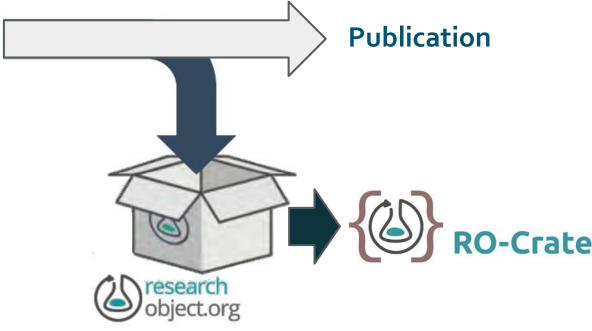






## Package snapshot as a Research Object







#### In vivo Nord 1: Chlorpyrifos-methyl



Ø Add new ▼
 ⑥ Actions ▼

Aim: To investigate whether Atlantic cod that feed close to aquatic breeding facilities are affected by chlorpyrifos-methyl. Feeding experiment with chlorpyrifos-methyl, an organophosphorous pesticide detected in plant based salmon feed. Based on previous experiments using salmon.

Doses: 0, 0.5, 5.0, 25 mg/kg) chlorpyrifos-methyl. Duration: 30 days Set-up: Three tanks per treatment (12 in total)

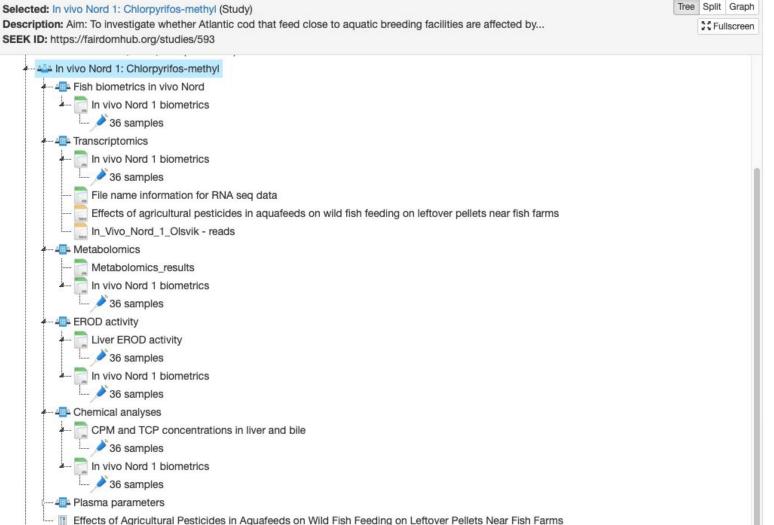
Samples include: Liver, plasma, bile, brain. Analysis include: - Have RNAseq and metabolomics from 36 liver samples - Plasma cholinesterase, cortisol, ASAT, ALAT, and total protein (36 samples) - EROD on liver samples (36 samples) - Chemical levels of chlorpyrifos-methyl and main metabolite TCP in liver and bile (36 samples) - Hypoxia stress test (72 samples)

SEEK ID: https://fairdomhub.org/studies/593

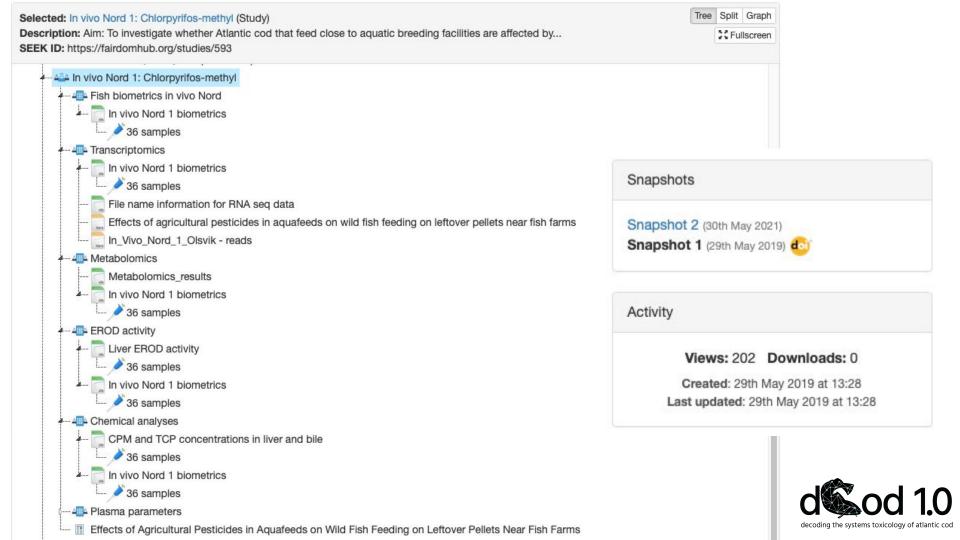
Investigation: In vivo - Exposure studies on living Atlantic cod

Projects: Systems toxicology of Atlantic cod







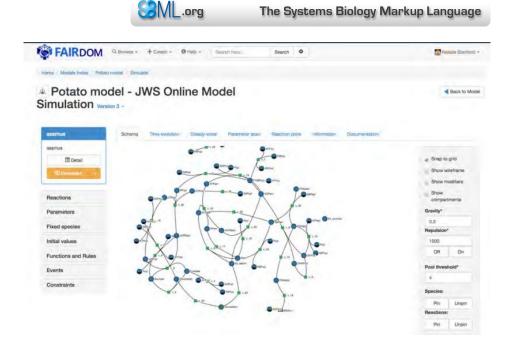


#### **Models in SEEK**

Integrated support for SBML models (Systems Biology Markup Language)

Allows for online simulations (JWS Online)

Reproduction of simulations (SED-ML)

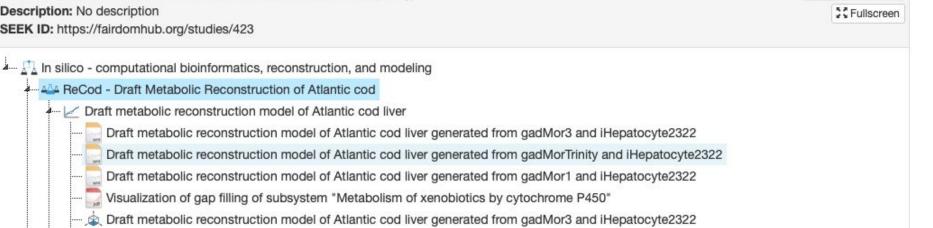




Selected: ReCod - Draft Metabolic Reconstruction of Atlantic cod (Study)

**Description:** No description

SEEK ID: https://fairdomhub.org/studies/423



🛮 🏖 Draft metabolic reconstruction model of Atlantic cod liver generated from gadMorTrinity and iHepatocyte2322 Draft metabolic reconstruction model of Atlantic cod liver generated from gadMor1 and iHepatocyte2322 ReCodLiver0.9: Overcoming Challenges in Genome-Scale Metabolic Reconstruction of a Non-model Species

Split Grap

## Experiences from dCod 1.0



- Little data management experience
  - traditional repositories (like GEO and ArrayExpress)
- No allocated funds in project budget
  - no specified data manager
  - ...but received funding from DLN for getting started and coursing

## Experiences from dCod 1.0



- Little data management experience
  - traditional repositories (like GEO and ArrayExpress)
- No allocated funds in project budget
  - no specified data manager
  - ...but received funding from DLN for getting started and coursing
- Transdisciplinary projects need good data management!
  - An eye-opener for the possibilities of data management
- How to change old (bad) habits?
  - Support
  - Clear guidelines and expectations
  - O Carrots?

khrono.no, 12.12.2020



eksempel på at god datahåndtering er livsviktig, skriver kronikkforfatterne.



### **DMP** writing workshops

15-16th of June - free spots!

## **BxoMed**Cata







#### **DM** implementation course

TBA

online

#### NeLS/usegalaxy.no

Q3/21

online

digitallifenorway.org









CONVERGE



















Norwegian University of Life Sciences

The Data Steward Wizard is provided by:











