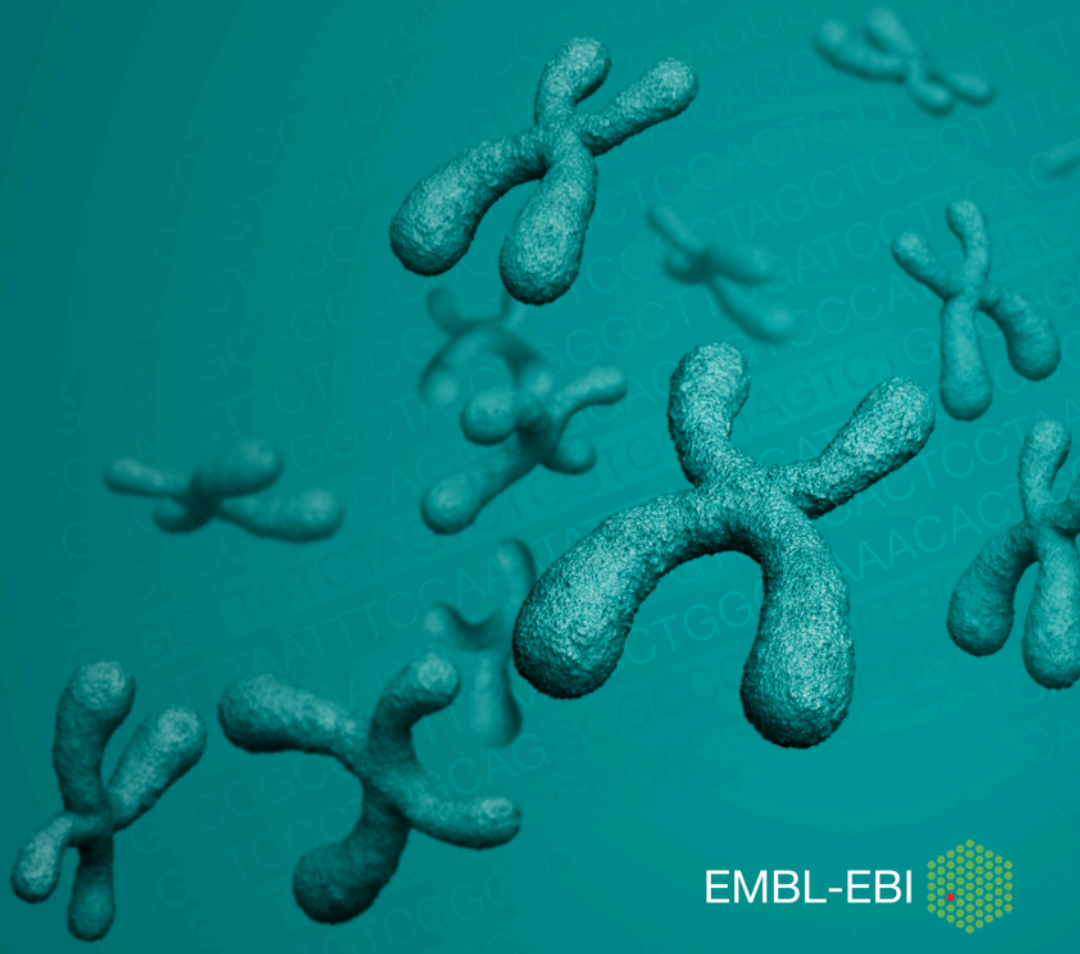
Sequencing communities at scale: dealing with the data

Guy Cochrane



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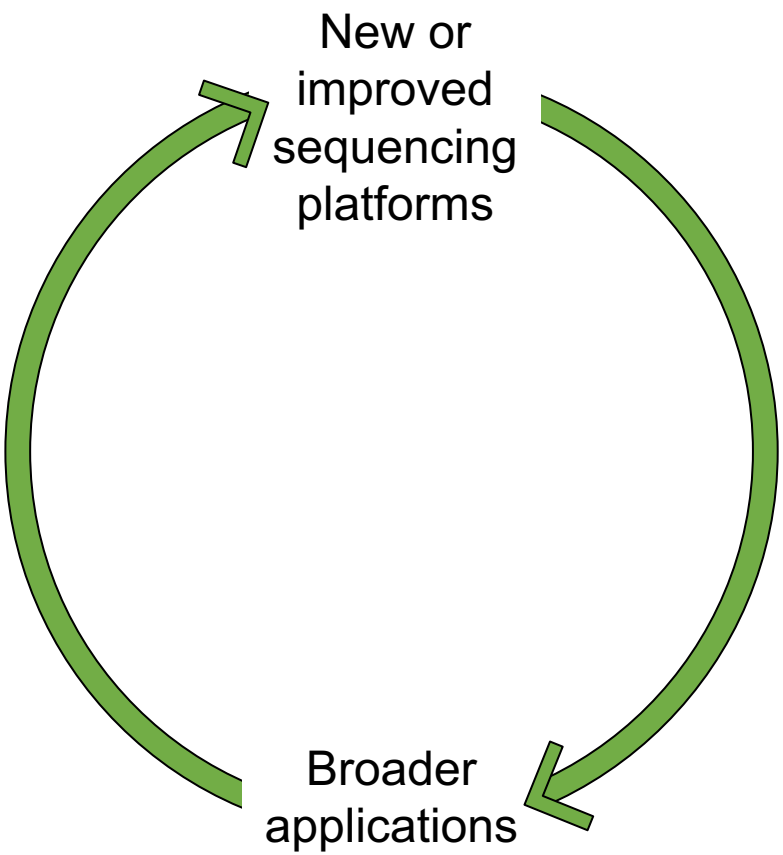

Data growth

Data diversification

Userbase growth

Public environmental sequencing data up to 2002

- Dominant data from small-scale 16S rDNA studies
- Single sequencing platform
- ~35k sequence records
- ~30 kilobase pairs; ~0.5 megabytes

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DT   10-MAR-2017 (Rel. 132, Last updated, Version 5)
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XX
KW   ENV.
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OS   uncultured archaeon ORGANIC1_A
OC   Archaea; Euryarchaeota; Halobacteria; Haloferacales; Halorubraceae;
OC   Halorubrum; environmental samples.
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RN   [1]
RP   1-914
RX   DOI; 10.1046/j.1462-2920.2000.00097.x.
RX   PUBMED; 11220308.
RA   Bowman J.P., Rea S.M., McCammon S.A., McMeekin T.A.;
RT   "Diversity and community structure within anoxic sediment from marine
RT   salinity meromictic lakes and a coastal meromictic marine basin, Vestfold
RT   Hilds, Eastern Antarctica";
RL   Environ. Microbiol. 2(2):227-237(2000).
XX
RN   [2]
RP   1-914
RA   Bowman J.P., McCammon S.A., McMeekin T.A.;
RT   ;
RL   Submitted (13-APR-1999) to the INSDC.
RL   School of Agricultural Science, University of Tasmania, GPO Box 252-54,
RL   Hobart, Tasmania 7001, Australia
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DR   SILVA-SSU; AF142985.
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//
```

Public environmental sequencing data in 2017

- 16,000 environmental sequencing studies
- 600,000 metagenomics samples
- diverse data
  - raw data
    - 454, Illumina, PacBio, Ion Torrent, ONT, etc.
    - sequenced libraries (600,000)
    - 30 terabase pairs, ~0.5 petabytes
  - shotgun metagenomics
  - metatranscriptomics
  - metagenome/metatranscriptome assemblies (1,100)
  - single cell genomes
  - reference data (e.g. 100,000 bacterial assemblies)
  - identification data (243)
  - gene catalogue (1)

Context

EMBL European Bioinformatics Institute

Genes, genomes & variation

European Nucleotide Archive
1000 Genomes
Ensembl
Ensembl Genomes
European Genome-phenome Archive
Metagenomics portal

Gene, protein & metabolite expression

ArrayExpress
Expression Atlas
Metabolights
PRIDE

Literature & ontologies

Europe PubMed Central
Gene Ontology
Experimental Factor Ontology

Protein sequences, families & motifs

InterPro
Pfam
UniProt

Molecular structures

Protein Data Bank in Europe
Electron Microscopy Data Bank

Chemical biology

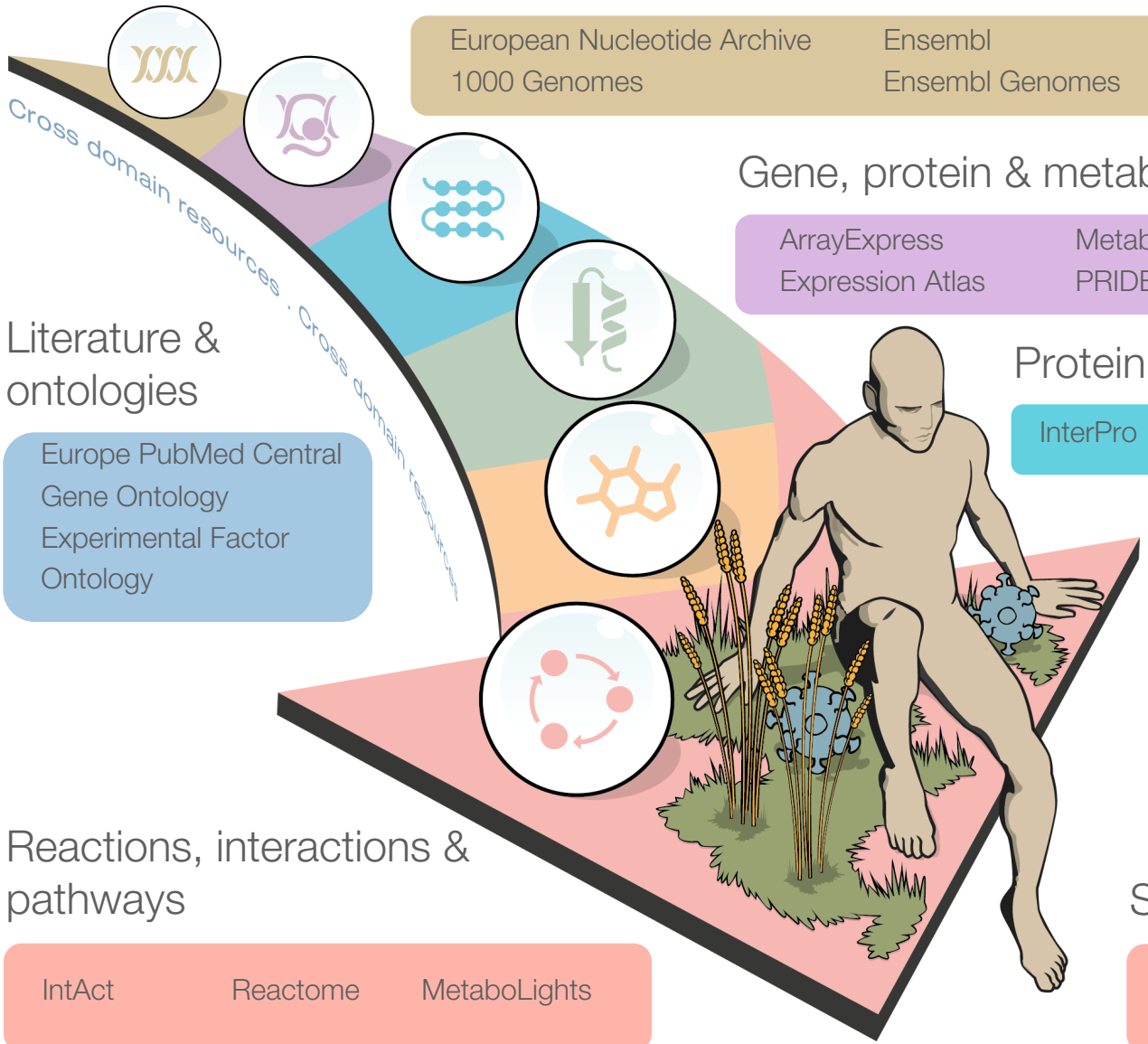
ChEMBL
ChEBI

Reactions, interactions & pathways

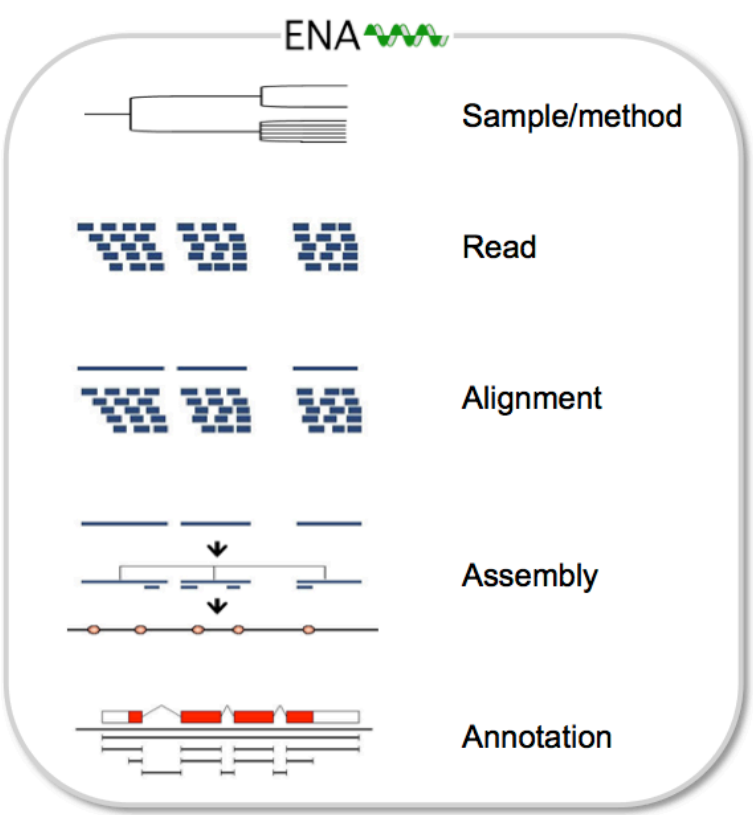
IntAct
Reactome
MetaboLights

Systems

BioModels
BioSamples
Enzyme Portal



European Nucleotide Archive (ENA)

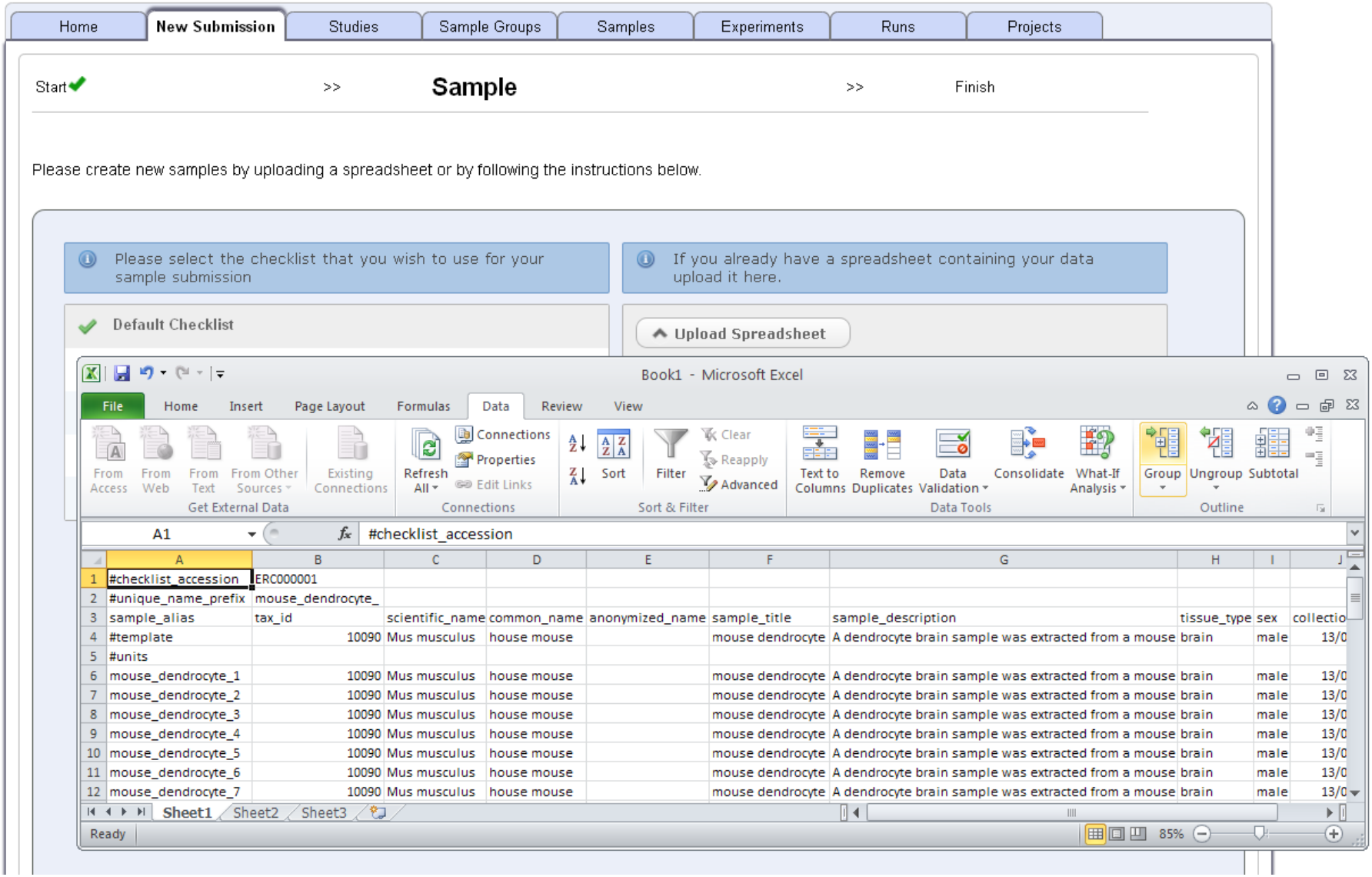


ENA

http://www.ebi.ac.uk/ena/

- **Globally comprehensive scientific record** and European node of **INSDC**
- A **broad platform** for the management, sharing, integration and dissemination of sequence data
- Established in the early 1980s, extended for **new technologies and applications**
- **Connectivity** with broader EMBL-EBI resources
- Sequence data **foundation**
- **Sustained** within EMBL-EBI under EMBL funding with additional support from EC, UK Research councils, Wellcome Trust, etc.
- **Substantial scale**: 1 submission every 6 minutes, 1.3 petabase pairs across 1.5 million taxa, 2,000-5,000 active data providers, global consumer userbase
- Rich submission, discovery and retrieval **software, tools and services**

Data validation and submissions



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5	#units									
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7	mouse_dendrocyte_2	10090	Mus musculus	house mouse		mouse dendrocyte	A dendrocyte brain sample was extracted from a mouse	brain	male	13/0
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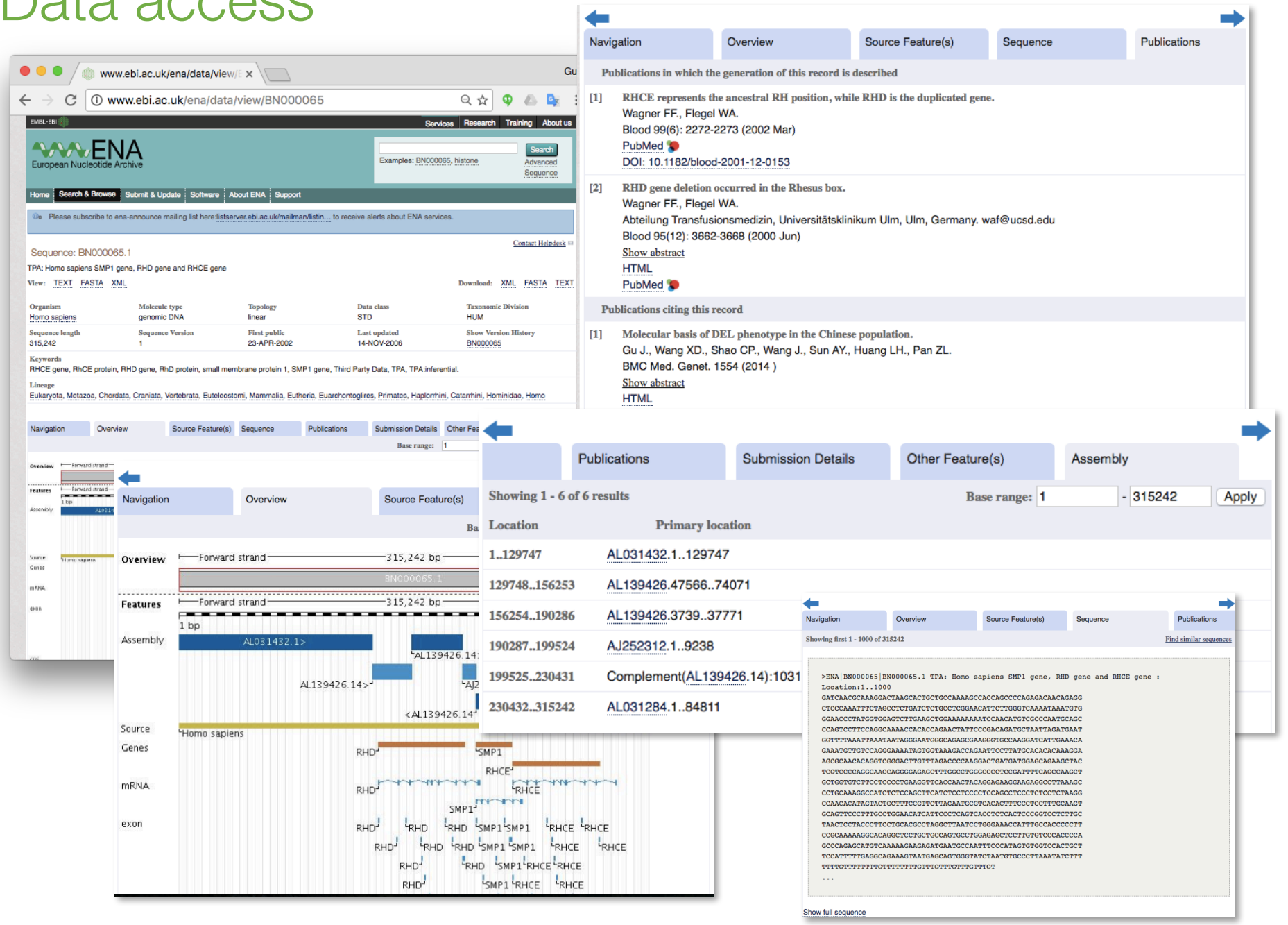
Data access


www.ebi.ac.uk/ena/data/view/BN000065
EMBL-EBI
Services
Research
Training
About us
ENA
European Nucleotide Archive
Search
Examples: BN000065, histone
Advanced Sequence
Home
Search & Browse
Submit & Update
Software
About ENA
Support
Please subscribe to ena-announce mailing list here:listserver.ebi.ac.uk/mailman/listin... to receive alerts about ENA services.
Contact Helpdesk
Sequence: BN000065.1
TPA: Homo sapiens SMP1 gene, RHD gene and RHCE gene
View: TEXT FASTA XML
Download: XML FASTA TEXT
Organism
Homo sapiens
Molecule type
genomic DNA
Topology
linear
Data class
STD
Taxonomic Division
HUM
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First public
23-APR-2002
Last updated
14-NOV-2006
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Eukaryota, Metazoa, Chordata, Craniata, Vertebrata, Euteleostomi, Mammalia, Eutheria, Euarchontoglires, Primates, Haplorrhini, Catarrhini, Hominidae, Homo
Navigation
Overview
Source Feature(s)
Sequence
Publications
Publications in which the generation of this record is described
[1] RHCE represents the ancestral RH position, while RHD is the duplicated gene.
Wagner FF., Flegel WA.
Blood 99(6): 2272-2273 (2002 Mar)
PubMed
DOI: 10.1182/blood-2001-12-0153
[2] RHD gene deletion occurred in the Rhesus box.
Wagner FF., Flegel WA.
Abteilung Transfusionsmedizin, Universitätsklinikum Ulm, Ulm, Germany. waf@ucsd.edu
Blood 95(12): 3662-3668 (2000 Jun)
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PubMed
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[1] Molecular basis of DEL phenotype in the Chinese population.
Gu J., Wang XD., Shao CP., Wang J., Sun AY., Huang LH., Pan ZL.
BMC Med. Genet. 1554 (2014)
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Genes
RHD
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mRNA
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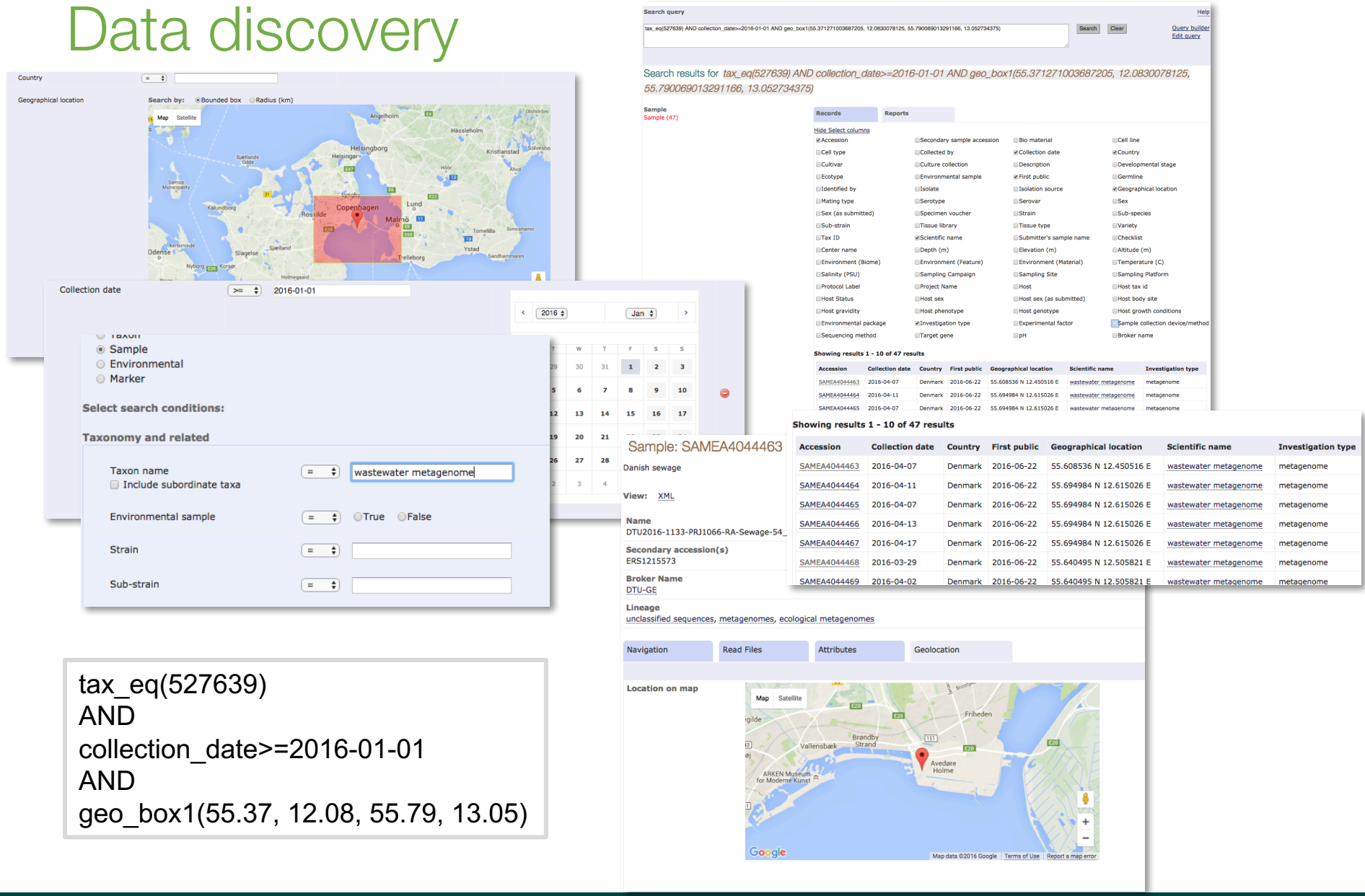
Show full sequence

Data discovery



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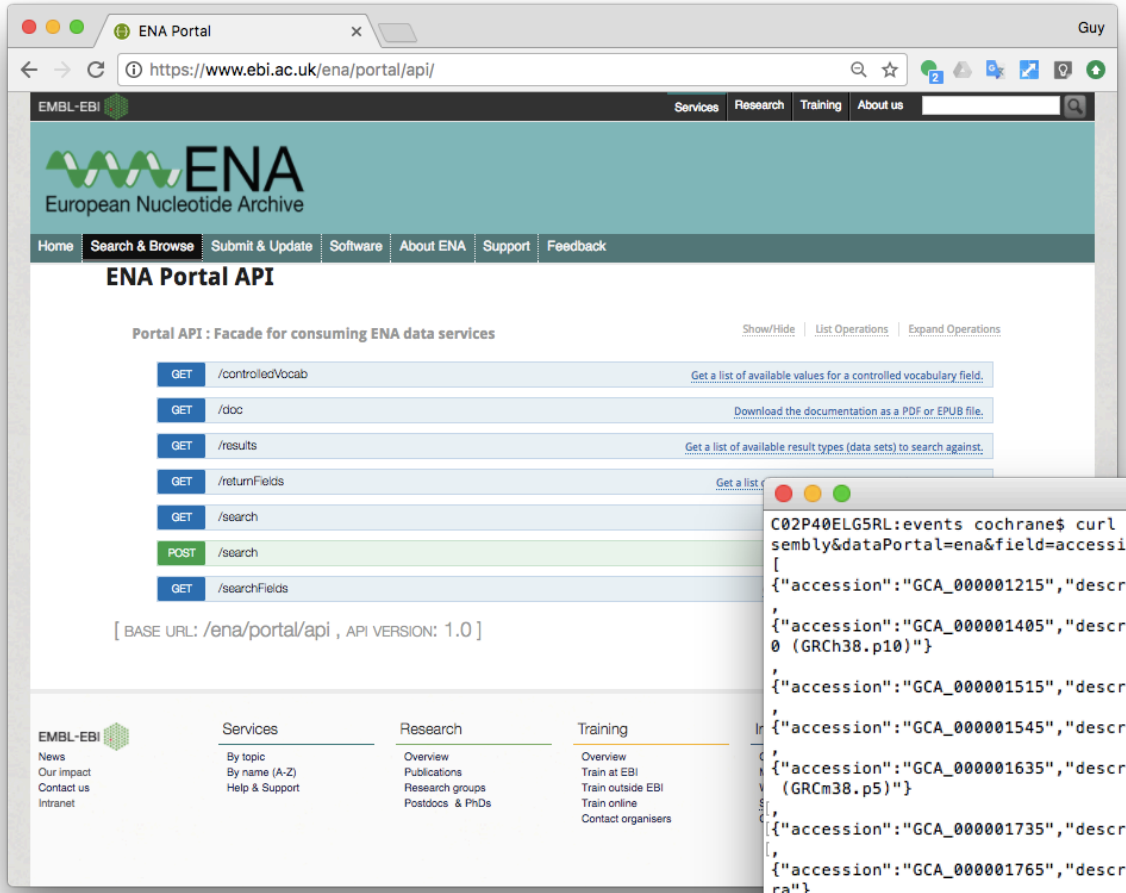
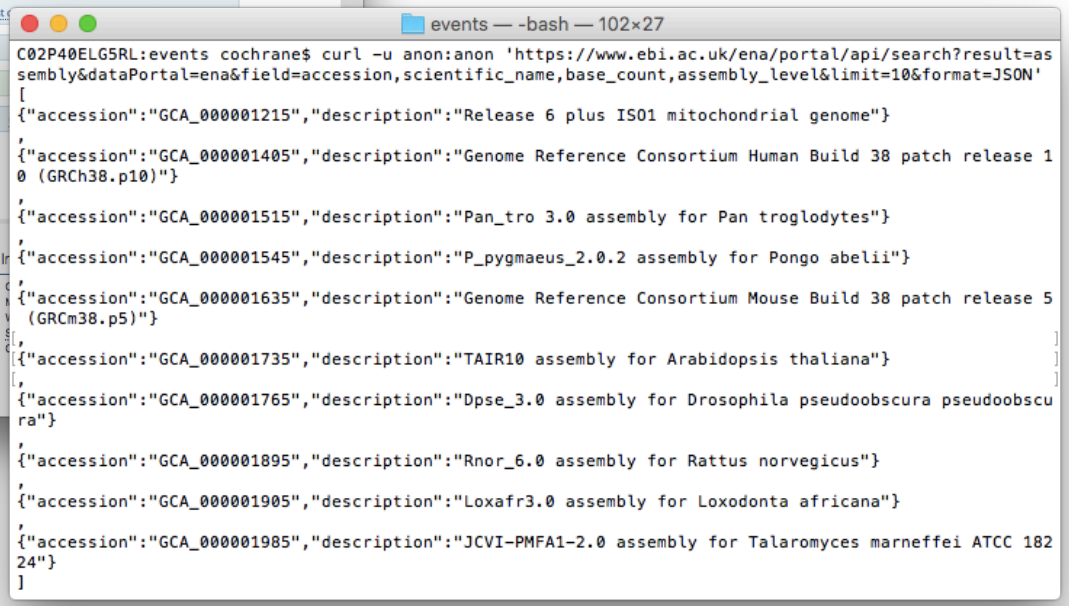
EMBL-EBI

Programmatic access





- ENA discovery API
  - RESTful
  - Entire ENA content
  - Logical searches across data types
  - TSV/JSON

https://www.ebi.ac.uk/ena/portal/api

Public environmental sequencing data in 2017

- 16,000 environmental sequencing studies
- 600,000 metagenomics samples
- diverse data
  - raw data
    - 454, Illumina, PacBio, Ion Torrent, ONT, etc.
    - sequenced libraries (600,000)
    - 30 terabase pairs, ~0.5 petabytes
  - shotgun metagenomics
  - metatranscriptomics
  - metagenome/metatranscriptome assemblies (1,100)
  - single cell genomes
  - reference data (e.g. 100,000 bacterial assemblies)
  - identification data (243)
  - gene catalogue (1)

ENA as data management platform for metagenomics

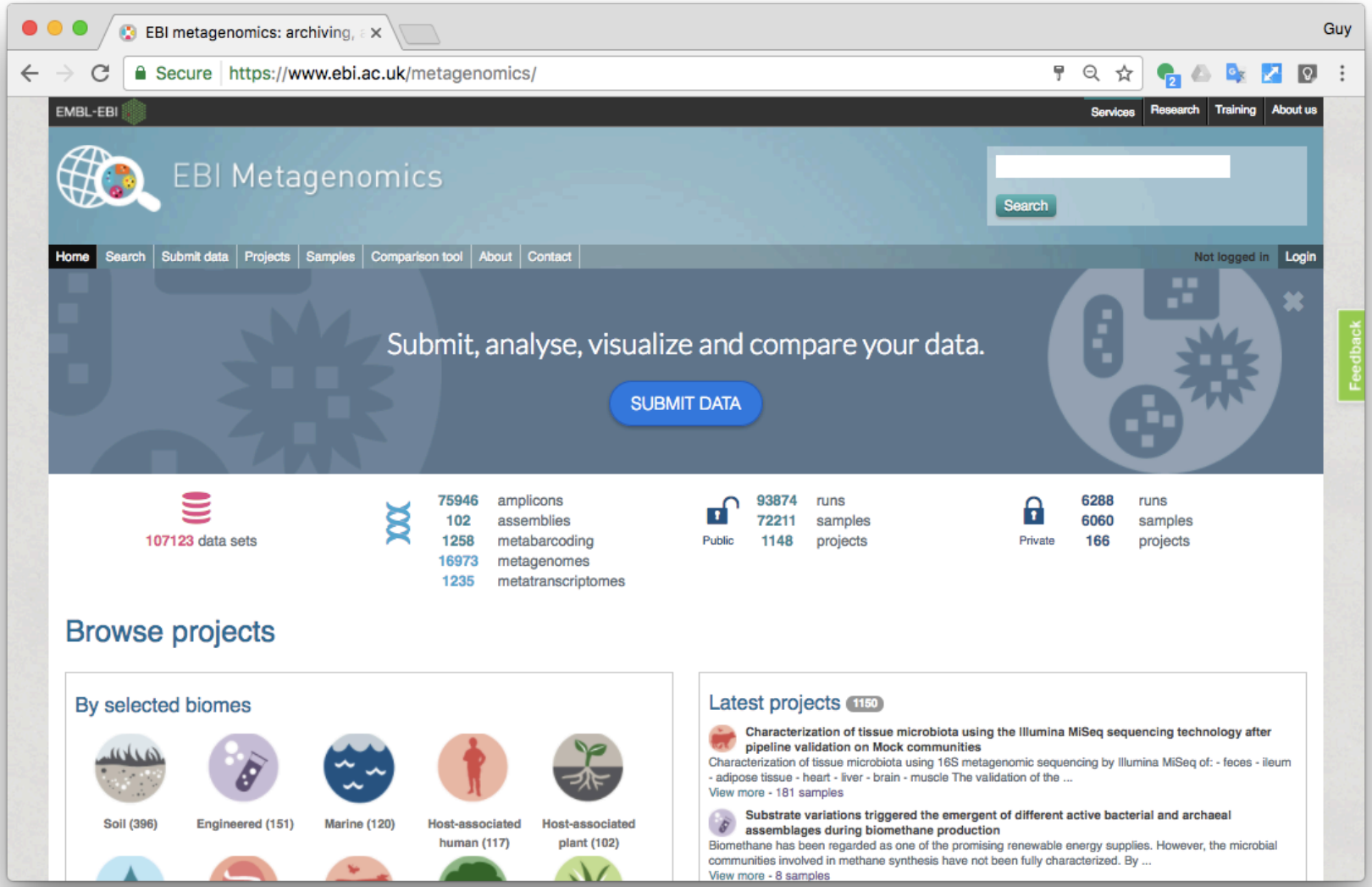
- In-project data sharing
- Data validation
- Dissemination and publishing
- Data coordination

- for customers small....,

- medium...

UniEuk

… and large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Secure
https://www.ebi.ac.uk/metagenomics/
EMBL-EBI
Services
Research
Training
About us
EBI Metagenomics
Search
Home
Search
Submit data
Projects
Samples
Comparison tool
About
Contact
Not logged in
Login
Submit, analyse, visualize and compare your data.
SUBMIT DATA
Feedback
107123 data sets
75946 amplicons
102 assemblies
1258 metabarcoding
16973 metagenomes
1235 metatranscriptomes
Public
93874 runs
72211 samples
1148 projects
Private
6288 runs
6060 samples
166 projects
Browse projects
By selected biomes
Soil (396)
Engineered (151)
Marine (120)
Host-associated human (117)
Host-associated plant (102)
Latest projects
1150
Characterization of tissue microbiota using the Illumina MiSeq sequencing technology after pipeline validation on Mock communities
Characterization of tissue microbiota using 16S metagenomic sequencing by Illumina MiSeq of: - feces - ileum - adipose tissue - heart - liver - brain - muscle The validation of the ...
View more - 181 samples
Substrate variations triggered the emergent of different active bacterial and archaeal assemblages during biomethane production
Biomethane has been regarded as one of the promising renewable energy supplies. However, the microbial communities involved in methane synthesis have not been fully characterized. By ...
View more - 8 samples

Standards

Standards through the data journey

Scientist generating data

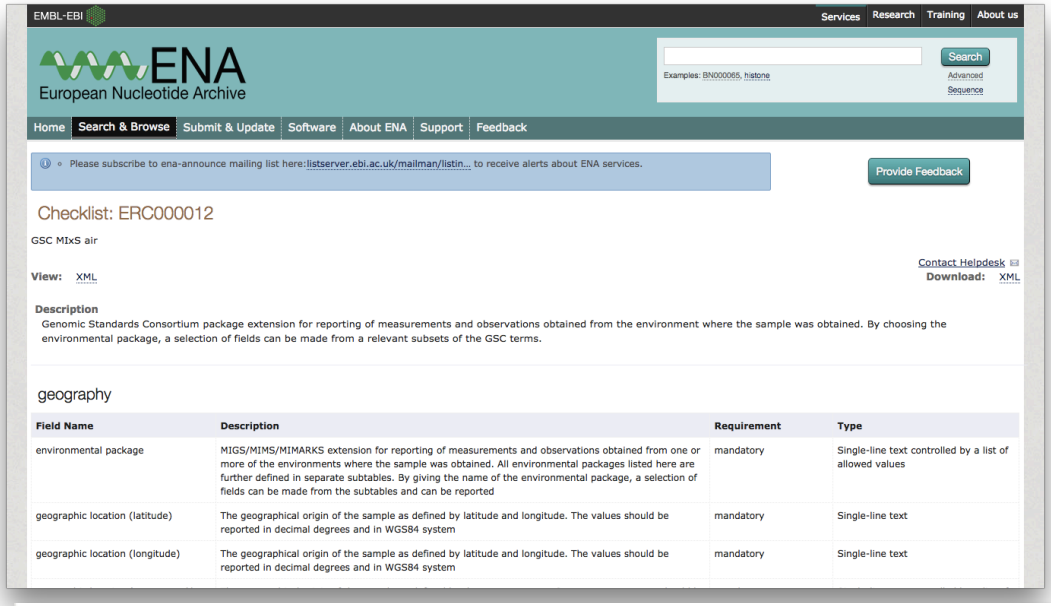
- Study design
- Data capture

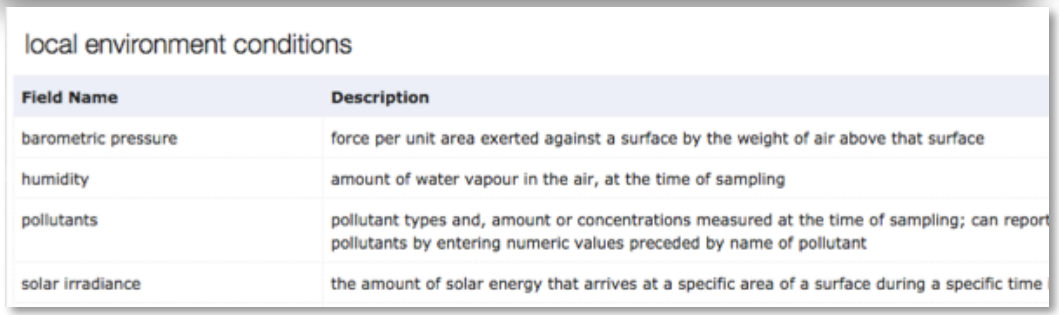
ENA

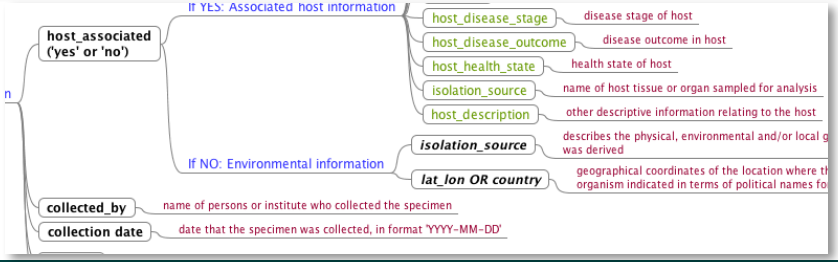
- Submission
- Validation
- Discovery
- Presentation

Scientist consuming data

- Interpretation

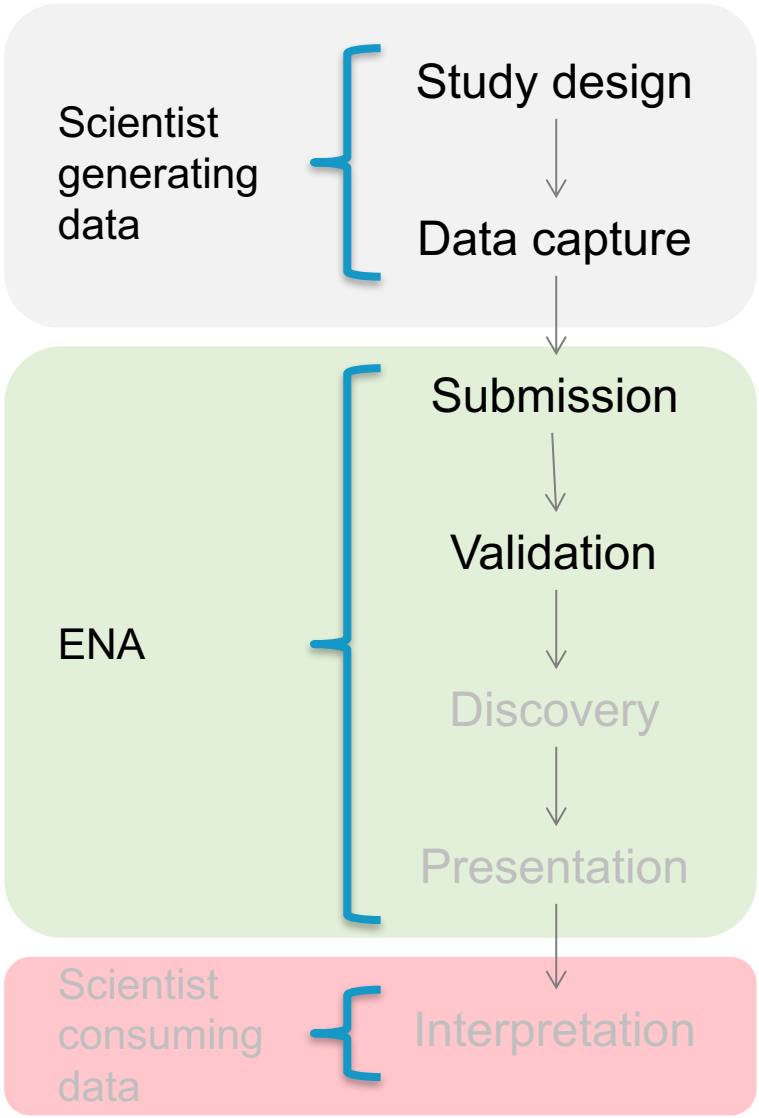


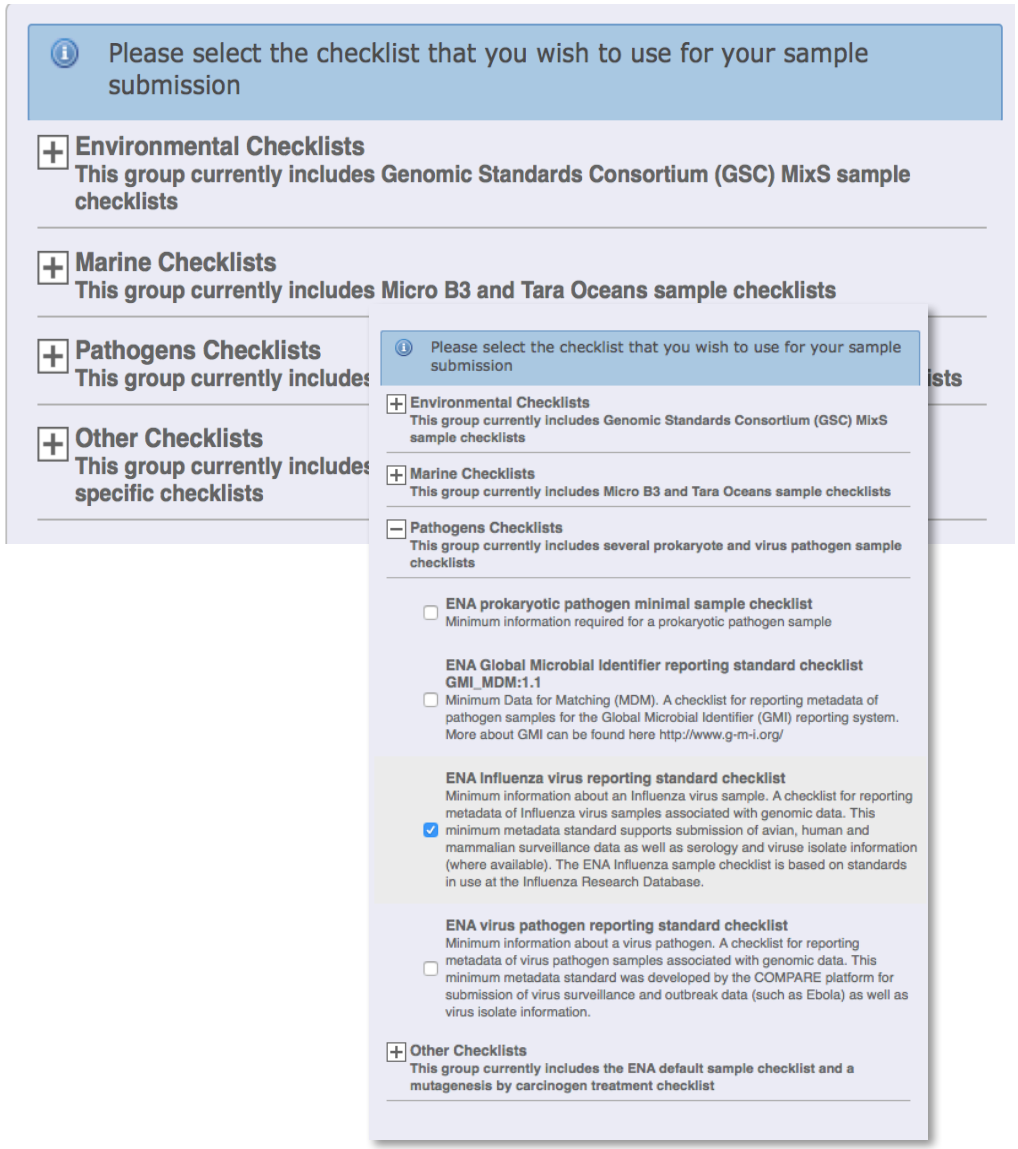




EMBL-EBI

Standards through the data journey





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ENA

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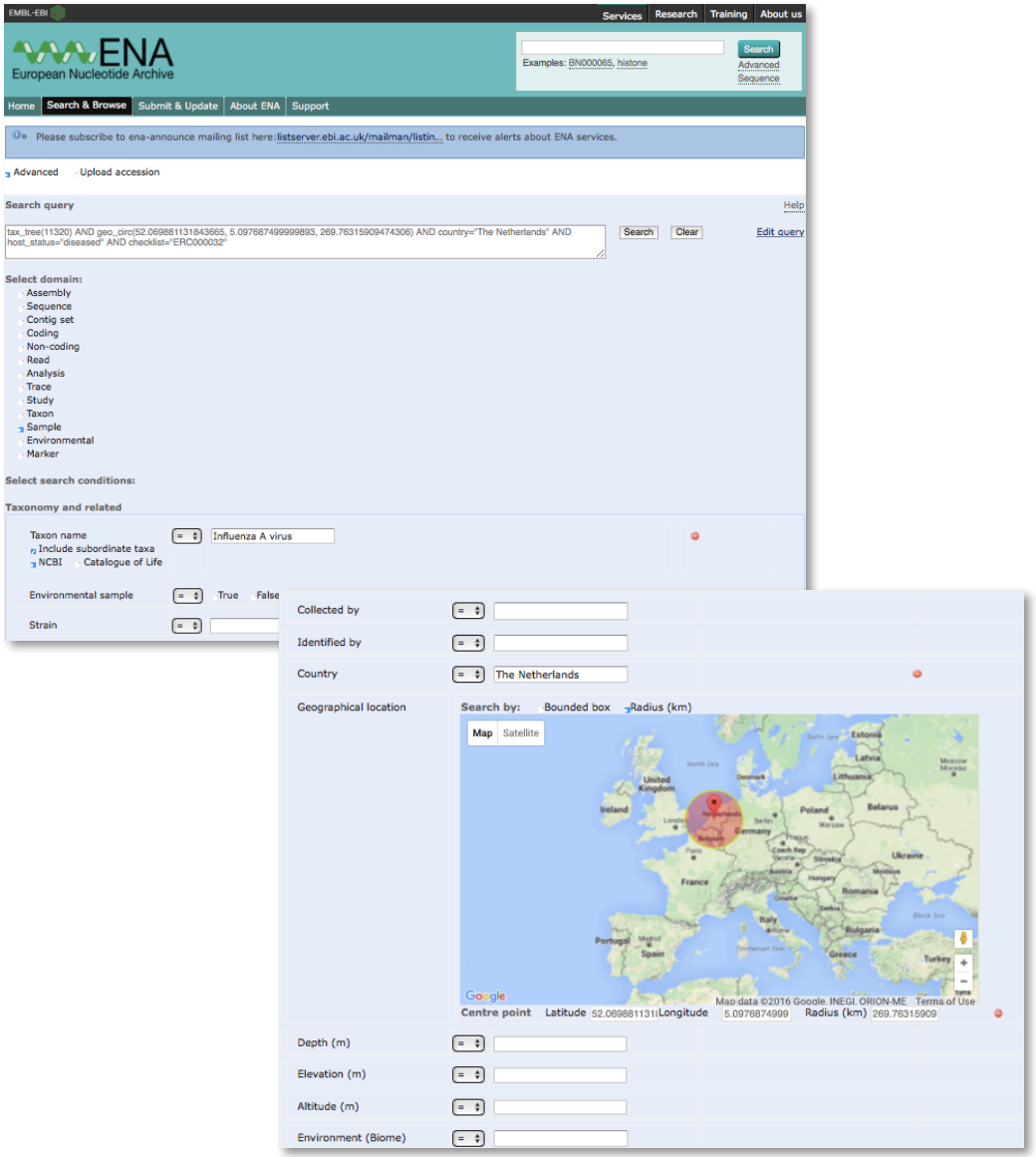
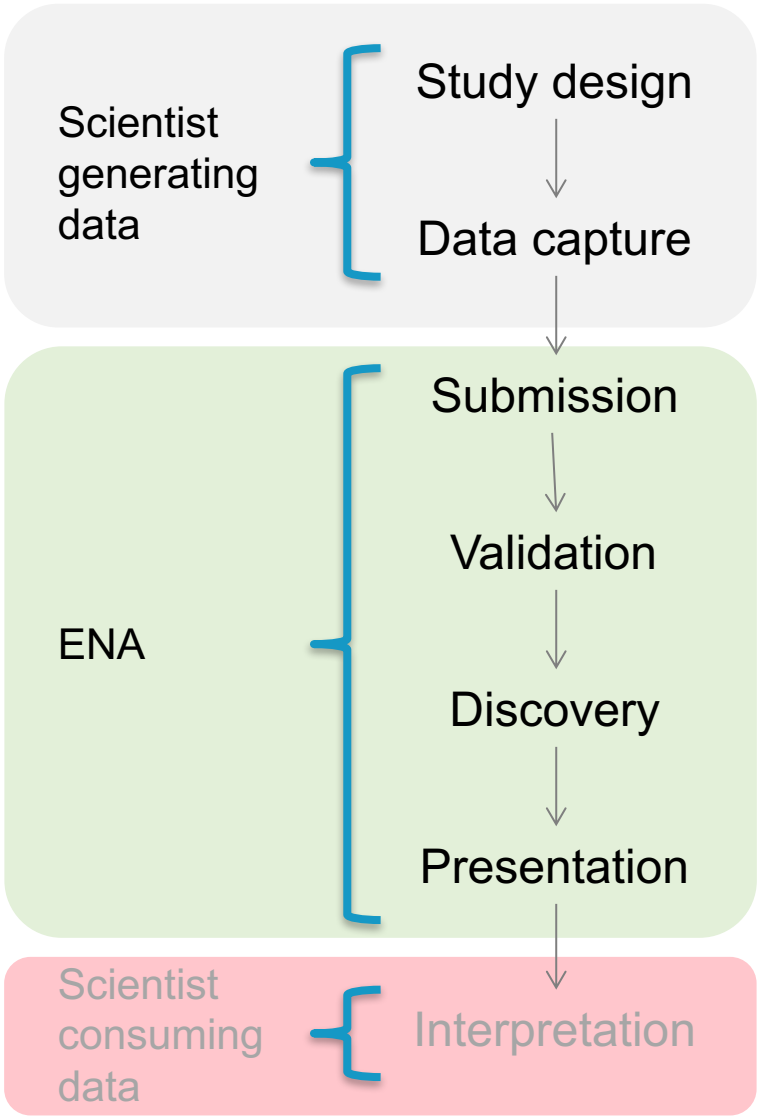


EMBL-EBI

Standards through the data journey



Please subscribe to ena-announce mailing list here:listserver.ebi.ac.uk/mailman/listin... to

Sample: SAMEA3493153

Influenza A virus; Initial sample from November H5N8 outbreak in UK

View: XML

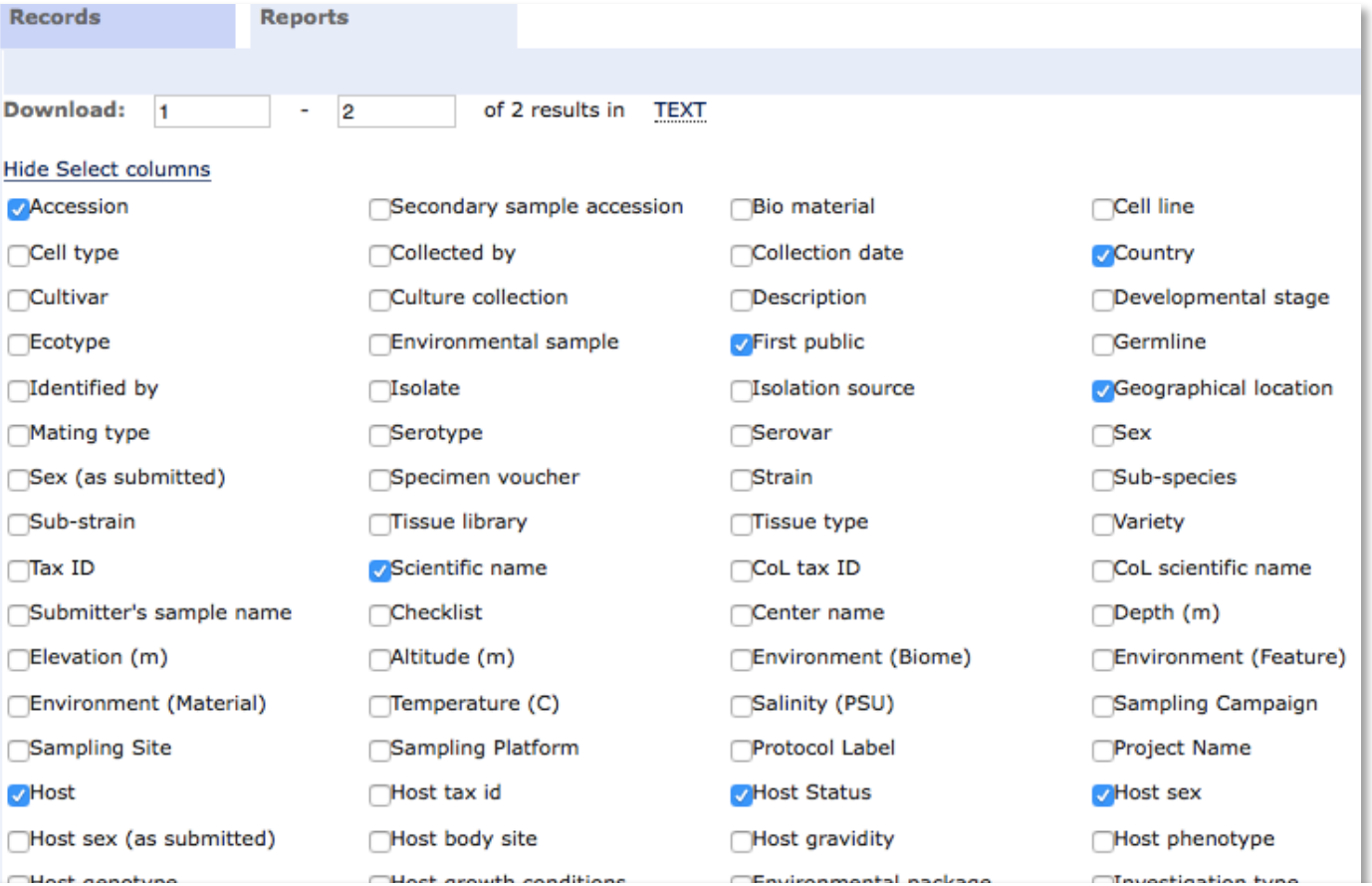
Submitting Centre	Organism
Animal and Plant Health Agency (APHA)	Influenza A virus

Secondary accession(s)
ERS800302

Lineage
Viruses, ssRNA viruses, ssRNA negative-strand viruses, Orthomyxoviridae, Influenzavirus A

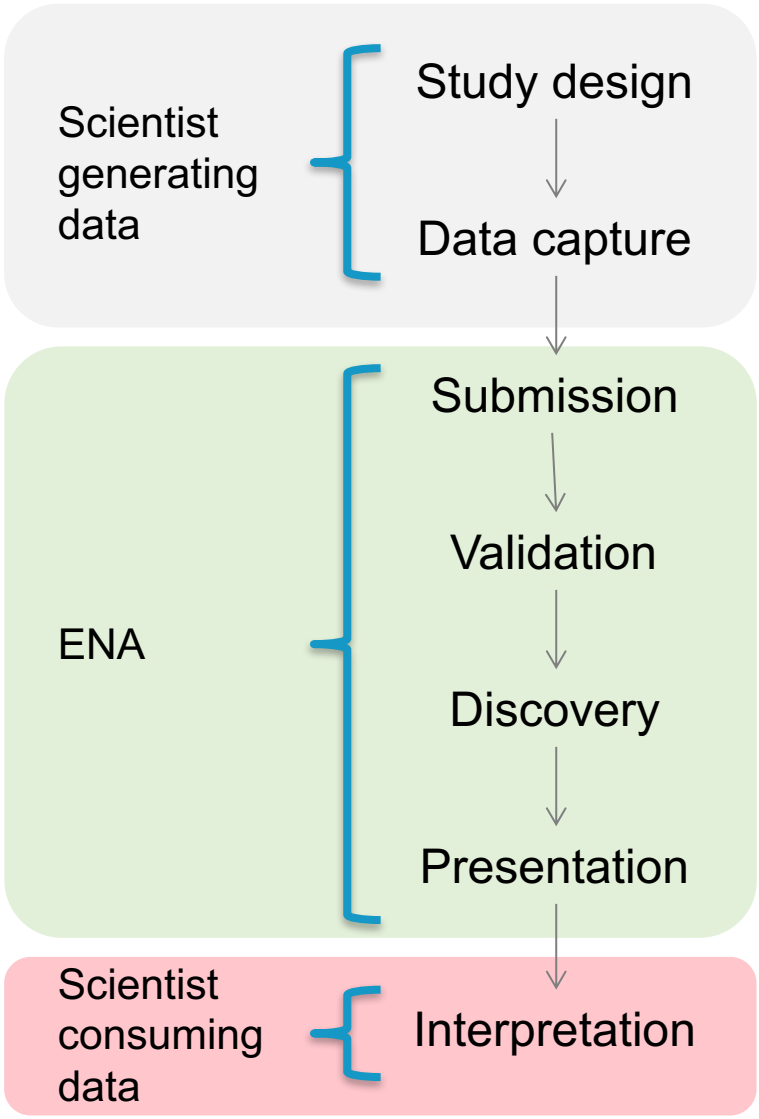
Navigation | Read Files | Attributes | Geolocation

host scientific name	Anas platyrhynchos
host common name	Domestic duck
host subject id	#1
host health state	diseased
host disease outcome	dead
host age	60 weeks
host sex	female
host behavior	domestic
host habitat	domestic:indoor farm
isolation source host-associated	pooled intestines
collector name	APHA



Accession	Collection date	Country	First public	Geographical location	Scientific name	Submitter's sample name	Host	Host Status	Host sex
SAMEA3493153	2014-11-14	United Kingdom	2016-02-17	54.001 N 0.434 W	Influenza A virus	AVP-14-036255	Anas platyrhynchos	diseased	female
SAMEA3860663	2014-11-04	Germany	2016-02-17		Influenza A virus	A/turkey/Germany/AR2485-L01478/2014	Meleagris gallopavo	diseased	

Standards through the data journey



Please subscribe to ena-announce mailing list here:listserver.ebi.ac.uk/mailman/listin... to

Sample: SAMEA3493153

Influenza A virus; Initial sample from November H5N8 outbreak in UK

View: XML

Submitting Centre	Organism
Animal and Plant Health Agency (APHA)	Influenza A virus

Secondary accession(s)
ERS800302

Lineage
Viruses, ssRNA viruses, ssRNA negative-strand viruses, Orthomyxoviridae, Influenzavirus A

Navigation | Read Files | Attributes | Geolocation

host scientific name	Anas platyrhynchos
host common name	Domestic duck
host subject id	#1
host health state	diseased
host disease outcome	dead
host age	60 weeks
host sex	female
host behavior	domestic
host habitat	domestic:indoor farm
isolation source host-associated	pooled intestines
collector name	APHA

Look out for…

ACCEPTED MANUSCRIPT

The metagenomic data life-cycle: standards and best practices

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Abstract

Metagenomics data analyses from independent studies can only be compared if the analysis workflows are described in a harmonised way. In this overview, we have mapped the landscape of data standards available for the description of essential steps in metagenomics: (1) material
quencing (3) data analysis and (4) data archiving
arine research, we summarise essential variables
sampling processes and sequencing procedures
iment. These aspects of metagenomics dataset generation have been to some extent addressed by the scientific

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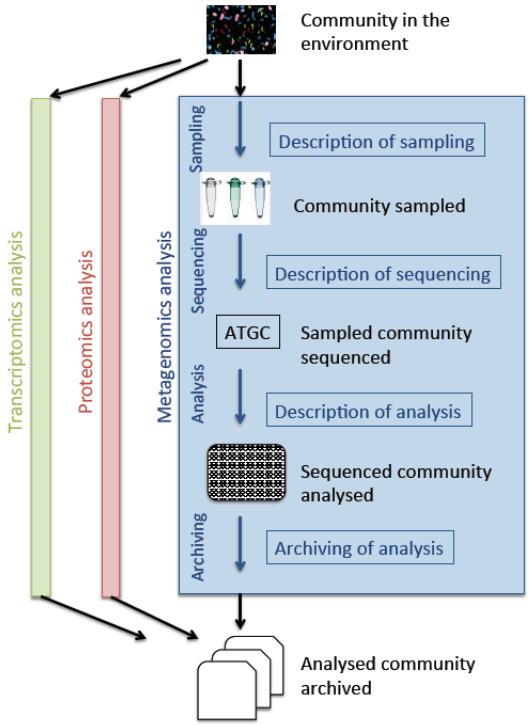
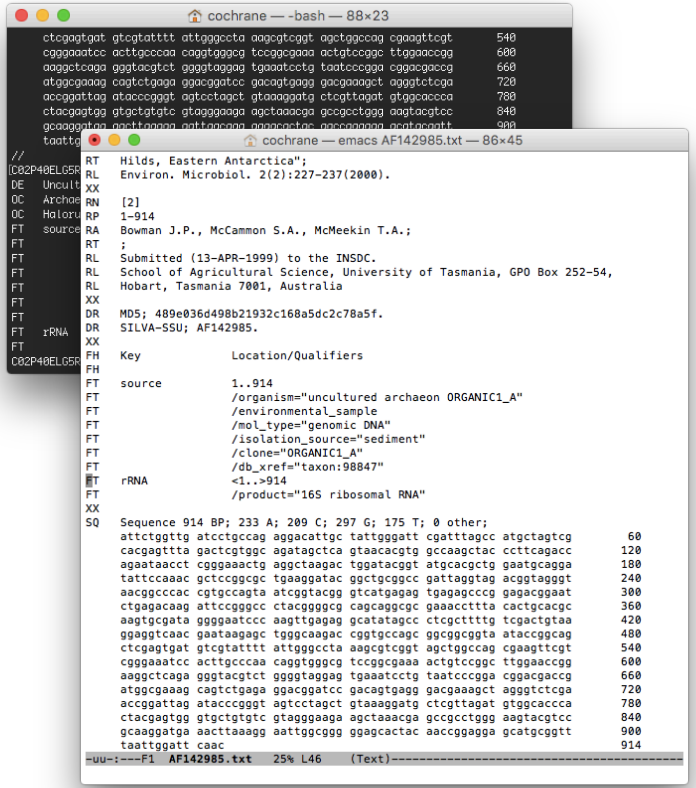
- Authors from 9 institutions, lead author Petra ten Hoopen, input from marine-community@elixir-europe.org
- Covers full workflow from sampling, though sequencing, analysis and result publication
- Promotes systematic archiving of analysis outputs



Scaling: internal tools

Sustainable biocuration

From…



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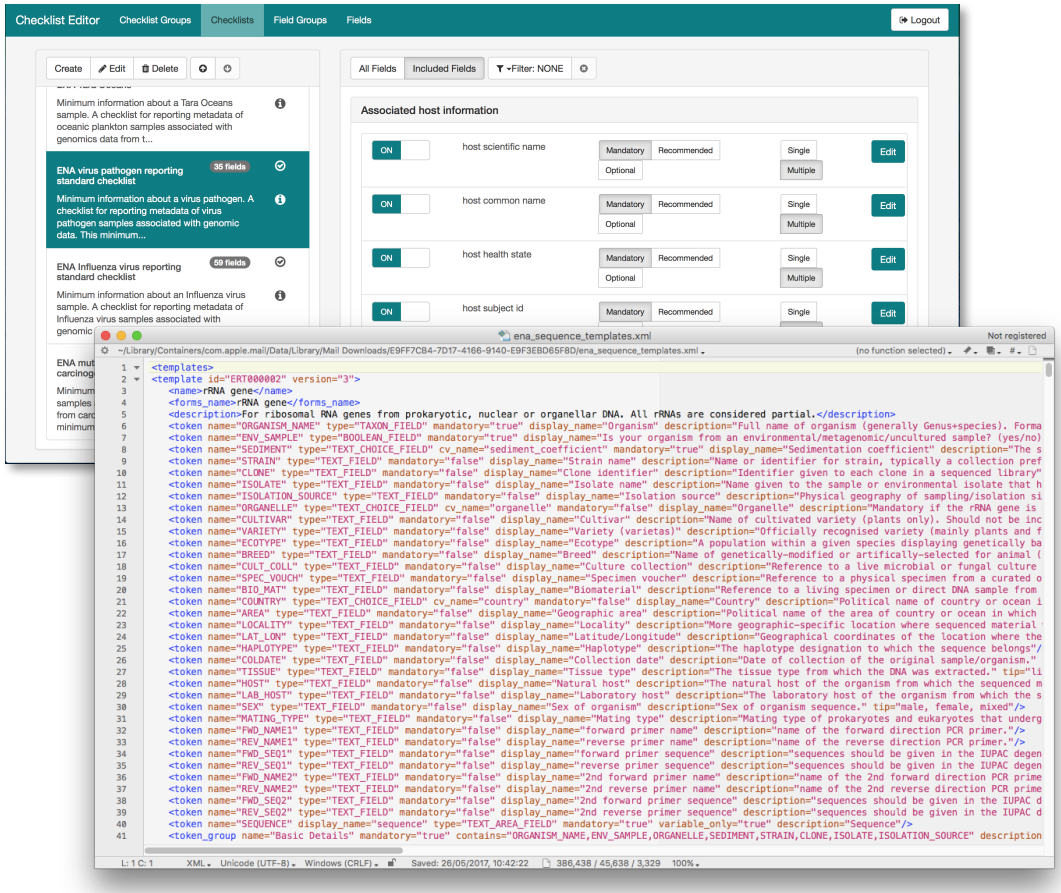

- Submission-level processing
- Class-level insertion of scientific organisation

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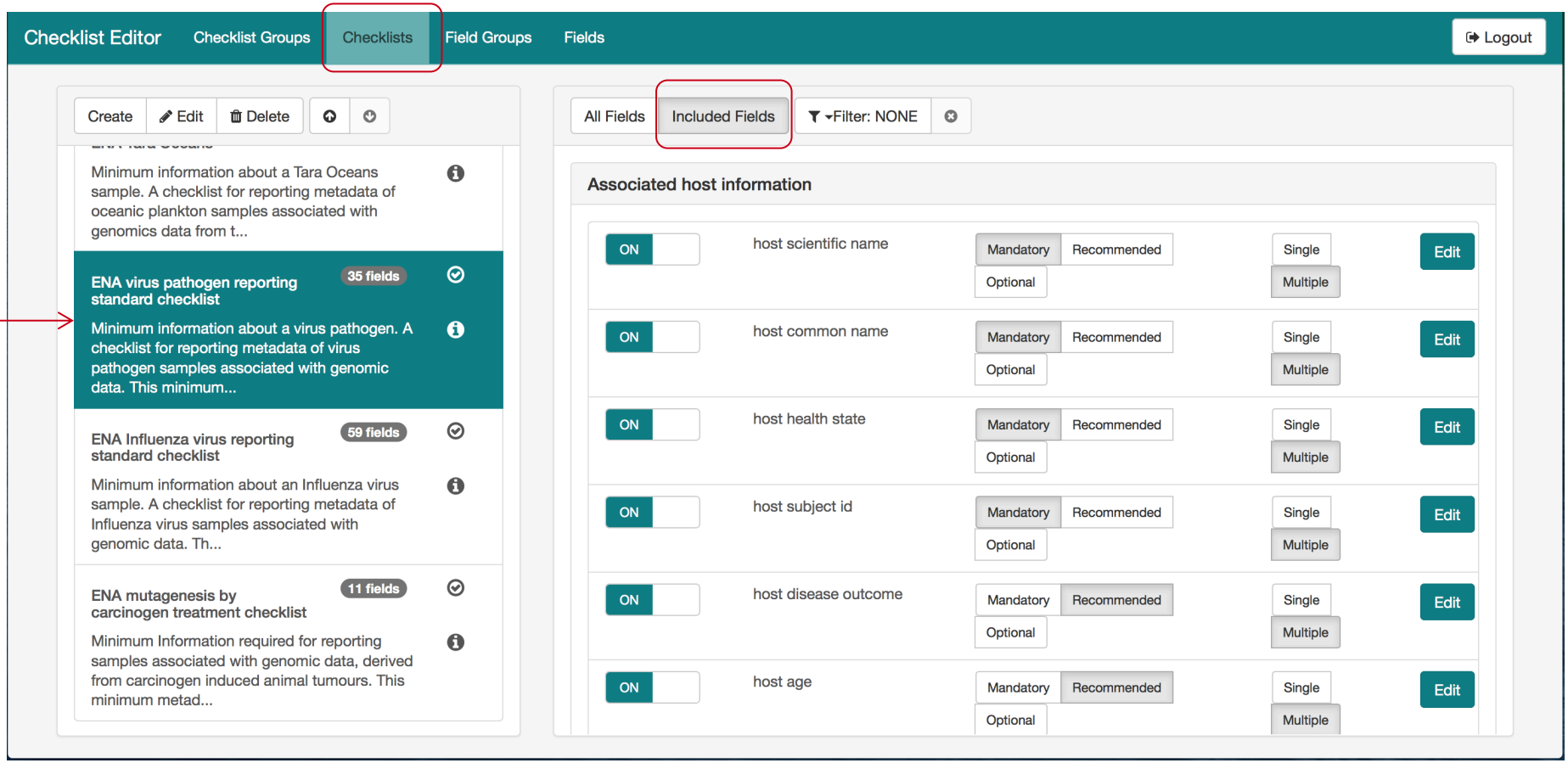
Checklist Editor

fields
- name
- description
- syntax

→ groups
- name
- description

→ checklists
- name
- description

→ implementation
- tools
- services
- content

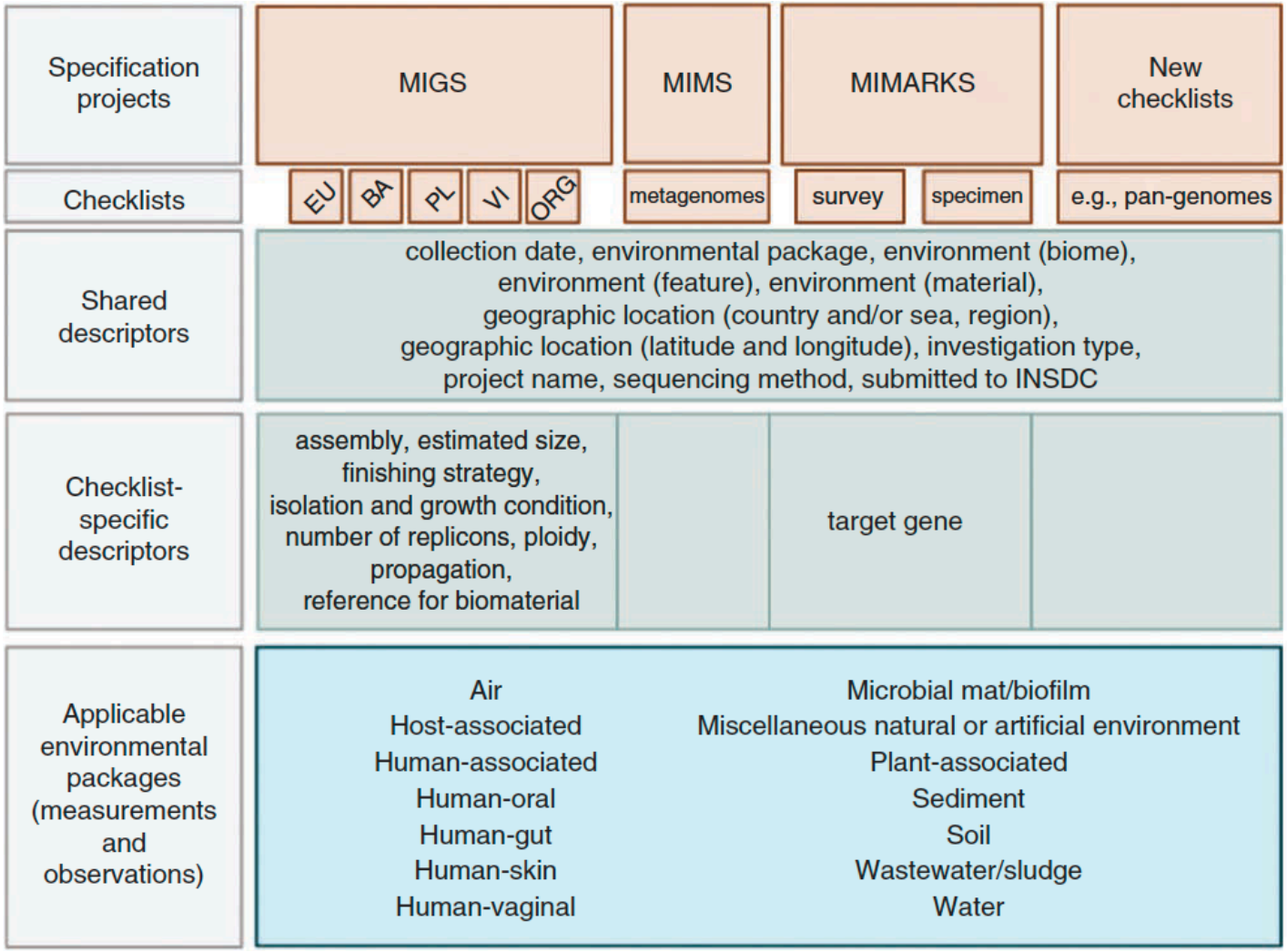


Scaling: community engagement

MIxS family of standards

genomic STANDARDS consortium

http://gensc.org



Yilmaz et al.
Nature Biotech.
2011; 29:415-420

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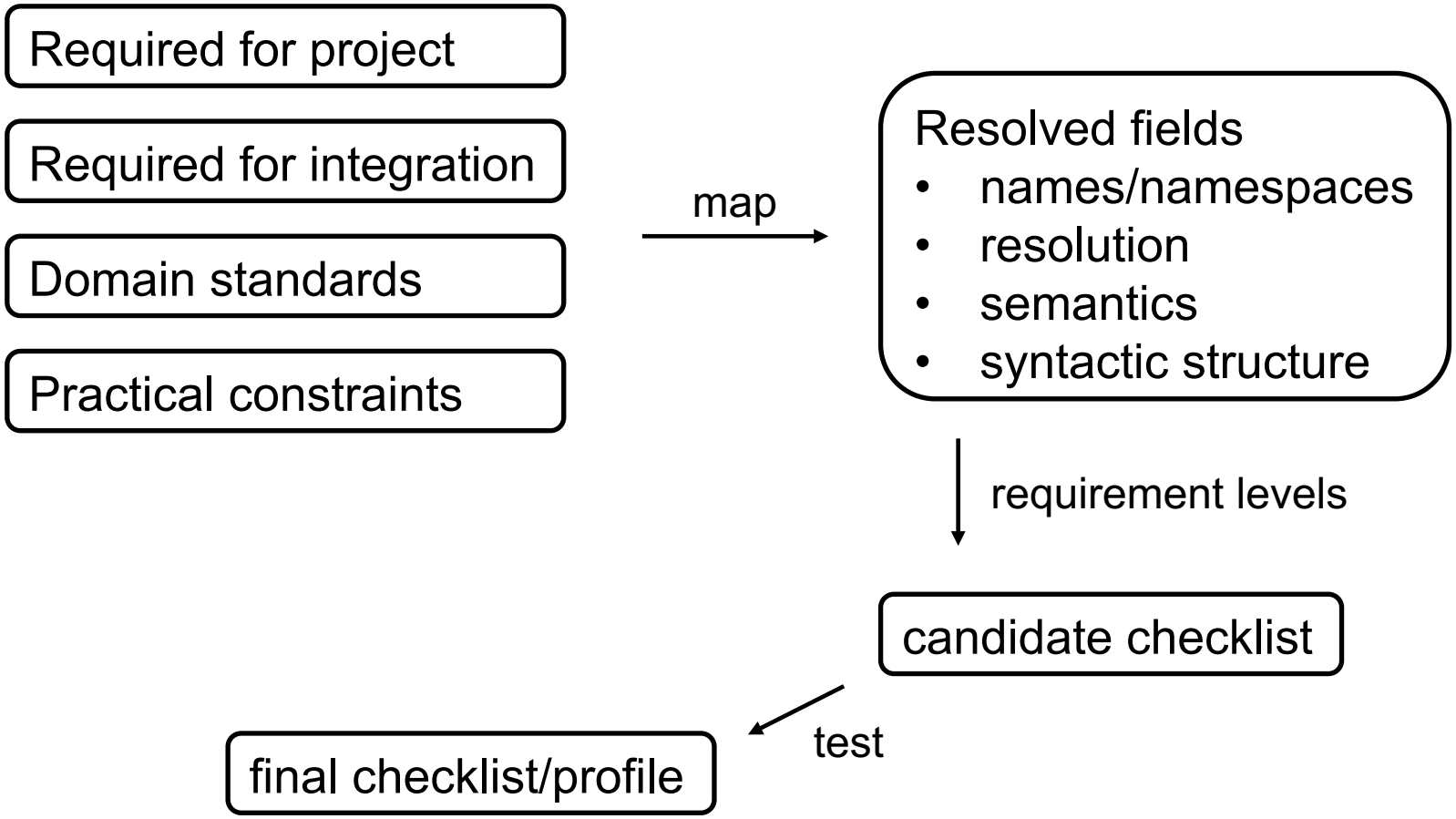
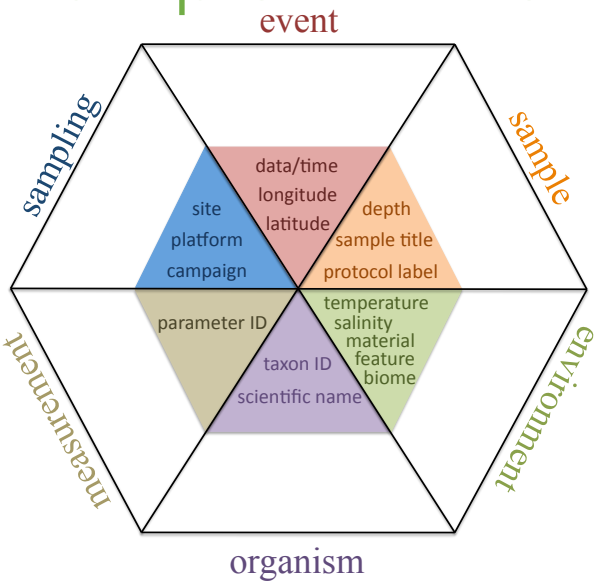
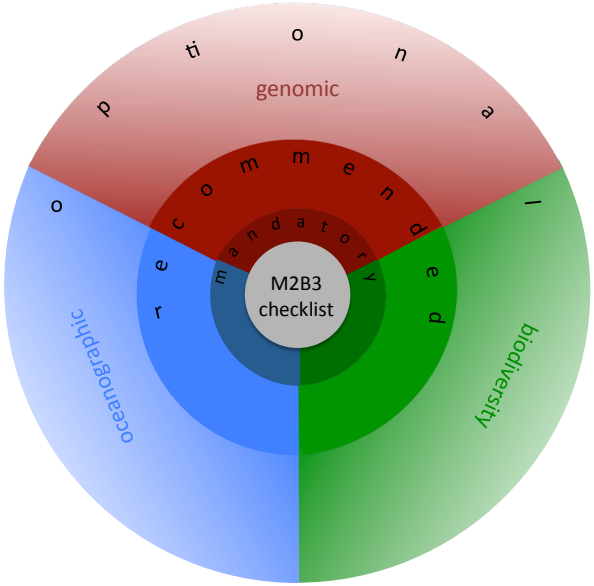
Standards development workflow



Example: M2B3





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Standards in Genomic Sciences

COMMENTARY Open Access

Marine microbial biodiversity, bioinformatics and biotechnology (M2B3) data reporting and service standards

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Abstract

Contextual data collected concurrently with molecular samples are critical to the use of metagenomics in the fields of marine biodiversity, bioinformatics and biotechnology. We present here Marine Microbial Biodiversity, Bioinformatics and Biotechnology (M2B3) standards for *"Reporting"* and *"Serving"* data. The M2B3 Reporting Standard (1) describes minimal mandatory and recommended contextual information for a marine microbial sample obtained in the epipelagic zone, (2) includes meaningful information for researchers in the oceanographic, biodiversity and molecular disciplines, and (3) can easily be adopted by any marine laboratory with minimum sampling resources. The M2B3 Service Standard defines a software interface through which these data can be discovered and explored in data repositories. The M2B3 Standards were developed by the European project Micro B3, funded under 7th Framework Programme "Ocean of Tomorrow", and were first used with the Ocean Sampling Day initiative. We believe that these standards have value in broader marine science.

Keywords: Data standard, Marine, Molecular, Biodiversity, Microbial, Bioinformatics, Reporting, Interoperability

Background

An immense wealth of genetic, functional and morphological diversity in marine ecosystems remains unexplored, offering the potential for substantial scientific and biotechnological discoveries. Indeed, significant interest in this area has led to large-scale initiatives, such as Tara Oceans [1], the Global Ocean Survey [2] and Malaspina [3], that target the exploration of marine biodiversity on planetary scales. While the shared goal of such initiatives is the development of an understanding of the compos-

biotechnology will derive benefit. Prerequisite for the successful exploitation of acquired data are standards that enable interoperability in the data infrastructure.

Just as marine studies span many disciplines (e.g. biological, oceanographic, molecular), use of data from marine studies requires approaches that traverse the many disciplines, asking questions, for example, of species distribution, physical oceanographic parameters, molecular biology and data licensing. Each discipline has established infrastructure and best practice for the dissemin-

positories,
d analysis
when data
a lack of

explorations and will continue to build a powerful marine data infrastructure from which ecosystems biology and

of a consistent environment for the discovery and retrieval of data.

The Marine Microbial Biodiversity, Bioinformatics, Biotechnology Project (Micro B3) [4] unites intensive oceanographic monitoring, thorough biodiversity studies

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micro B3 Biodiversity Bioinformatics Biotechnology

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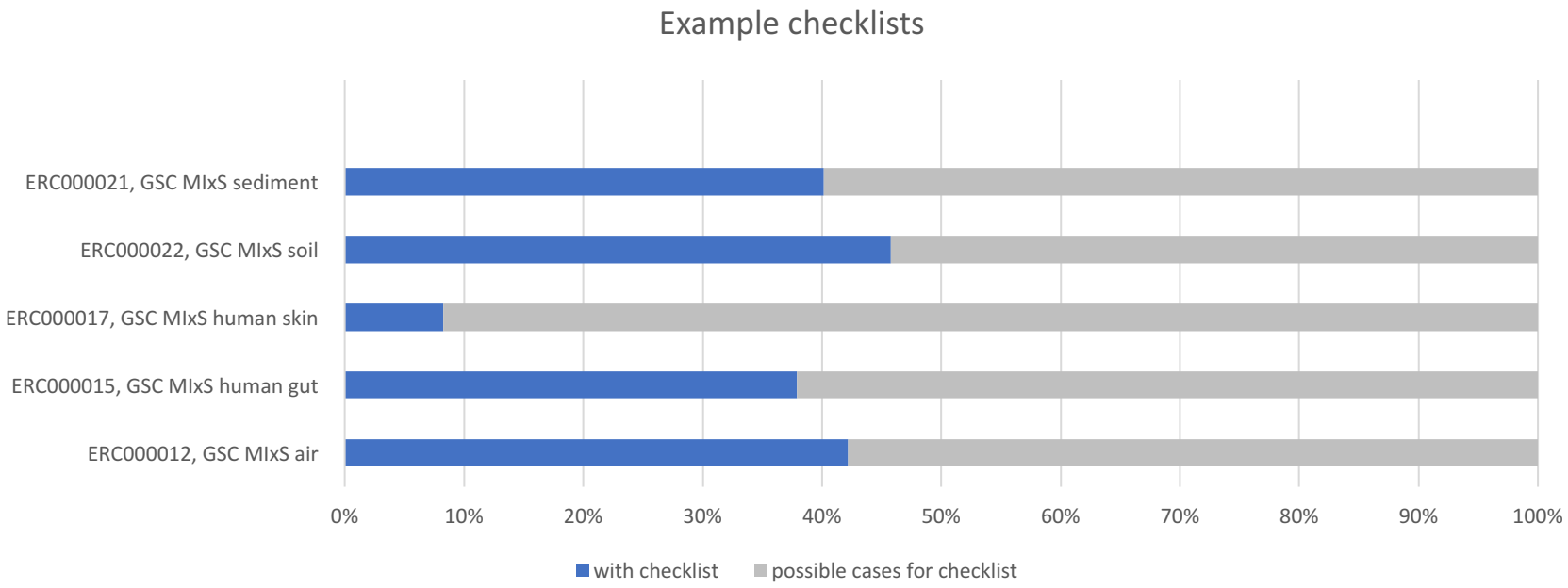
Uptake

- **51%** (100,366/195,702) of metagenomics-related samples use appropriate checklists
- (**18%** (188,213/1,059,594) overall usage of MIxS and MIxS-informed checklists)



- Uptake of individual fields may be greater

*includes pre-publication data

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