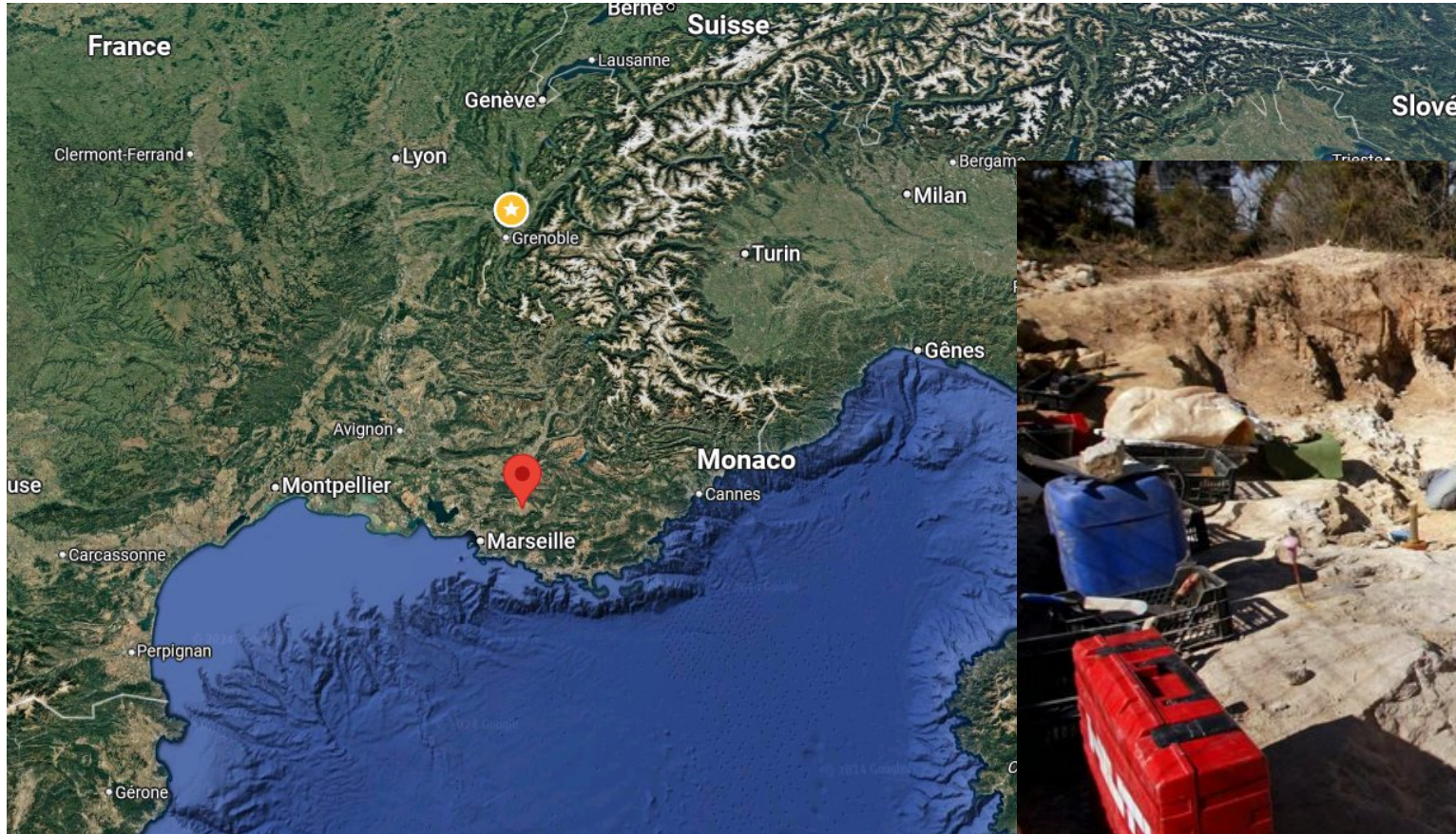


Datasets metadata

Renaud DUYME - ESRF
NOBUGS - 2024/09/27

Dinosaur Story

2006/07 – bones found during highway 8 roadworks



Thierry Tortosa

Photo J.-E.Ely

2014 – a new dinosaur : “Arcovenator Escotae”



Annales de Paléontologie
Volume 100, Issue 1, January–March 2014, Pages 63–86

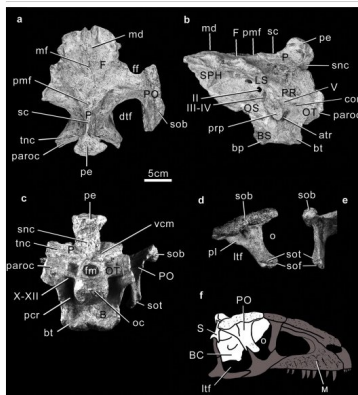


Original article

A new abelisaurid dinosaur from the Late Cretaceous of southern France: Palaeobiogeographical implications

Thierry Tortosa ^{a b} ✉, Eric Buffetaut ^a, Nicolas Vialle ^b, Yves Dutour ^b, Eric Turini ^b, Gilles Cheylan ^b

<https://doi.org/10.1016/j.annpal.2013.10.003>



“Arc” => Nearby river

“venator” => Latin for “hunter”

“Escotae” => ESCOTA french highway company



Société des Autoroutes
Estérel, Côte d'Azur,
Provence, Alpes

 ESCOTA



2014 - Official ICZN-ZooBank identifier



International Commission on
Zoological Nomenclature

ZooBank

about conta

Search

Arcovenator escotae Tortosa, Buffetaut, Vialle, Dutour, Turini & Cheylan, 2013

LSID urn:lsid:zoobank.org:act:1E903E97-E98B-4BB2-8031-65BF0E232FB6

Rank: Species

Parent: [Arcovenator Tortosa, Buffetaut, Vialle, Dutour, Turini & Cheylan, 2013](#)

Specific Name: escotae

Authorship: Tortosa, Buffetaut, Vialle, Dutour, Turini & Cheylan

Publication: [Tortosa, Thierry, Eric Buffetaut, Nicolas Vialle, Yves Dutour, Eric Turini & Gilles Cheylan. 2013 A new abelisaurid dinosaur from the Late Cretaceous of southern France: Palaeobiogeographical implications. *Annales de Paléontologie*.](#)

Page: 3

Figure(s): 2-6

Type Specimen(s): MHNA-PV-2011.12.1

Type Locality: Jas Neuf Sud (Var, France)

Fossil: No

<https://zoobank.org/NomenclaturalActs/1e903e97-e98b-4bb2-8031-65bf0e232fb6>

2011 - Specimen stored in museum

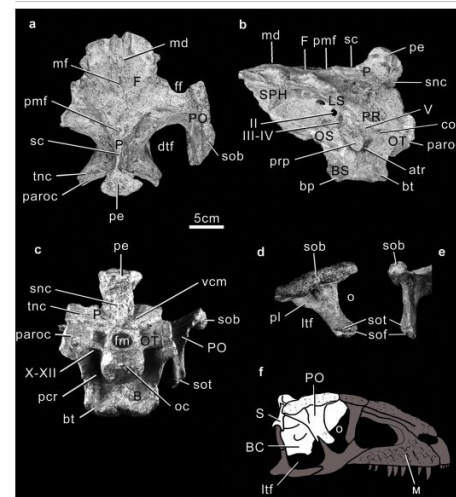


- Specimens are housed in the *Muséum d'Histoire Naturelle d'Aix-en-Provence* (MHNA), France. (MHNA-PV-2011.12.1 to 12.5)

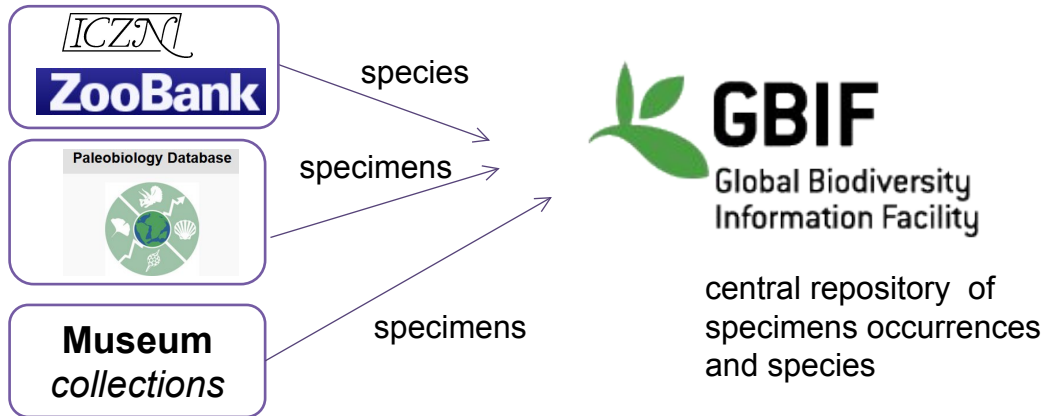
Paleobiology Database



- Specimens digitally tracked in PBDB
https://paleobiodb.org/classic/checkTaxonInfo?taxon_no=285749



GBIF : Species PID - Specimen PID



OCCURRENCE | UNKNOWN DATE
Arcovenator escotae Tortosa, Buffetaut, Vialle, Dutour, Turini & Cheylan, 2013

Recorded in France
 Animalia > Chordata > Abelisauridae > Arcovenator

DETAILS

Species: *Arcovenator escotae* Tortosa, Buffetaut, Vialle, Dutour, Turini & Cheylan, 2013
 Location: Europe > France
 Basis of record: Material citation

Dataset: Paleobiology Database
 Publisher: Paleobiology Database



Occurrence	
Term	Interpreted
Occurrence ID	pbdb:occ:1188017
Occurrence remarks	Specimens in Aix-en-Provence Natural History Museum

Location	
Term	Interpreted
Continent	EUROPE
Coordinate precision	0.0166667
Country or area	France
Country code	FR
County	Var
Decimal latitude	43.5
Decimal longitude	5.733333
Geodetic datum	WGS84
Georeference remarks	based on nearby landmark
Higher geography	FR Provence-Alpes-Côte d'Azur Var

Locality	near the village of Pourrières; two distinct localities but no further details given. One is Pourrières-Les Eysarettes (titanosaur)
State province	Provence-Alpes-Côte d'Azur

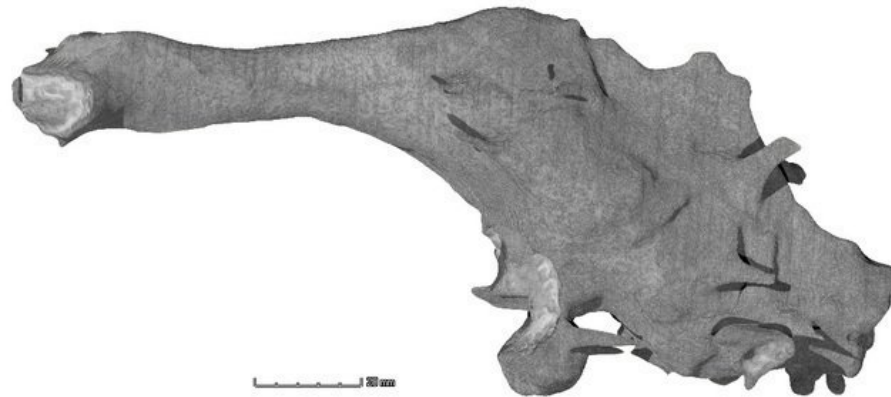
Taxon	
Term	Interpreted
Kingdom	Animalia
Phylum	Chordata
Class	
Family	Abelisauridae
Genus	Arcovenator
Specific epithet	escotae
Generic name	Arcovenator
Higher classification	Chordata Saurischia Abelisauridae Arcovenator
Name published in year	2013
Nomenclatural code	ICZN

Scientific name	<i>Arcovenator escotae</i> Tortosa, Buffetaut, Vialle, Dutour, Turini & Cheylan, 2013
Scientific name authorship	
Taxon concept ID	285749
Taxon ID	285749
Rank	Species

<https://www.gbif.org/fr/occurrence/1699073315>
<https://api.gbif.org/v1/occurrence/1699073315/>

2019 Arcovenator at ESRF

- A few years later... 2019. Arcovenator escotae specimen parts are scanned at ESRF on BM05 beamline.
- Technique used :
 - Propagation Phase Contrast Synchrotron X-ray Microtomography
 - PPC-SR μ CT



scientific reports

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[nature](#) > [scientific reports](#) > [articles](#) > [article](#)

Article | [Open access](#) | Published: 25 July 2019

Multiphase progenetic development shaped the brain of flying archosaurs

[Vincent Beyrand](#), [Dennis F. A. E. Voeten](#) , [Stanislav Bureš](#), [Vincent Fernandez](#), [Jiří Janáček](#), [Daniel Jirák](#), [Oliver Rauhut](#) & [Paul Tafforeau](#)

[Scientific Reports](#) **9**, Article number: 10807 (2019) | [Cite this article](#)

Dataset : <https://doi.org/10.15151/esrf-dc-1634316333>

Publication : <https://doi.org/10.1038/s41598-019-46959-2>

PaNET - Photon and Neutron Experimental Techniques

PaNET - Ontology

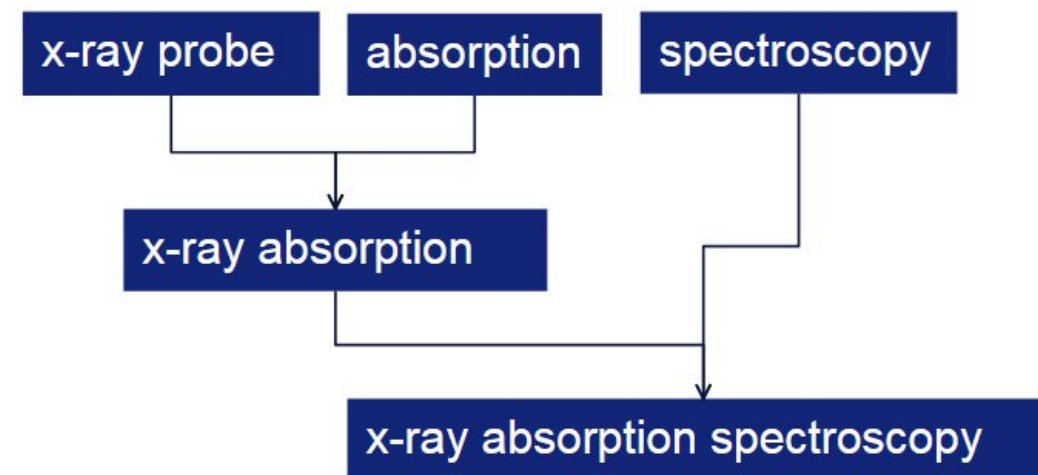
The PaNET ontology provides a taxonomy (classification) and thesaurus (synonyms and acronyms) of Photon and Neutron Experimental Techniques.



EXAFS	EXAFS	extended x-ray absorption fine structure	PaNET01198
FT-SSX	FT-SSX	fixed target serial synchrotron crystallography	PaNET01310
FTIR	FTIR	fourier transform infrared spectroscopy	PaNET01320
GISANS	GISANS	grazing incidence small angle neutron scattering	PaNET01276
GISAS	GISAS	grazing incidence small angle scattering	PaNET01099
GISAXS	GISAXS	grazing incidence small angle x-ray scattering	PaNET01162
GIWAXS	GIWAXS	grazing incidence wide angle scattering	PaNET01316
GIXD	GIXD	grazing incidence x-ray diffraction	PaNET01161
HAXPES	HAXPES	hard x-ray photoelectron spectroscopy	PaNET01103
WAXS	WAXS	wide angle x-ray scattering	PaNET01191
XAFS	XAFS	x-ray absorption fine structure	PaNET01197
XANES	XANES	x-ray absorption near edge structure	PaNET01199
XAS	XAS	x-ray absorption spectroscopy	PaNET01196

PaNET Ontology (not just taxonomy but relations as well)

- x-ray probe (PaNET01012)
- spectroscopy (PaNET01125)
- absorption technique (PaNET00202)
- x-ray absorption (PaNET01227)
- x-ray absorption spectroscopy (PaNET01196) - XAS



Courtesy : Wout de Nolf (ESRF)

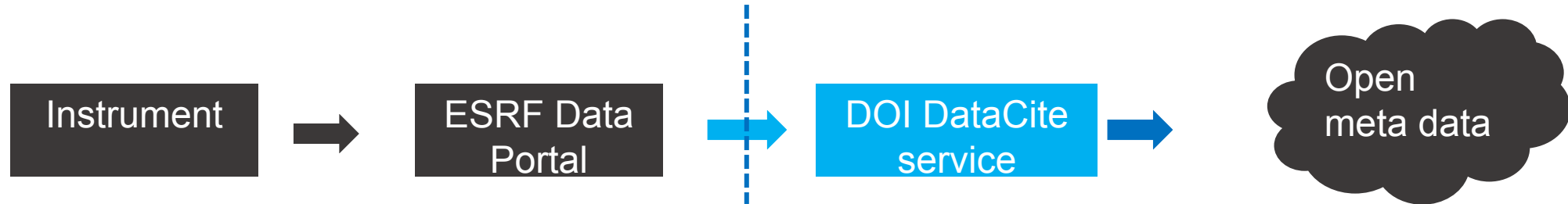
You are welcome !



contact : panet-maintenance@desy.de

DataCite

DataCite - DOI metadata enhancements



Step 0

.....>
Link available data : author orcid, author affiliations, proposal Id...)

Step 1

.....>
Add Photon and Neutron Experimental technique(ex : PPC-SR μ CT)

Next steps

.....>
Add thematic metadata (GBIF Id, Wikidata Id ...)



User input required at sample or dataset creation

ESRF Dataset – enhancement with PaNET

propagation phase contrast microtomography^C

IRI: <http://purl.org/pan-science/PaNET/PaNET01210>



has super-classes Synonyms : PPC-SR μ CT
[microscopy](#)^C, [propagation phase contrast tomography](#)^C

Data Collection

Open access

Arcovenator escotae MHNA-PV-2011-1

Paul Tafforeau; Vincent Beyrand

3D reconstruction for Arcovenator escotae MHNA-PV-2011-1. For further details regarding samples, measurements and data analysis, refer to the files and the article.

Experimental Data

The data can be accessed by clicking on the link below

Access data

Experimental Report

No report was found for IH-ES-132. Proposers and session participants may submit it via the [ESRF User Portal](#).

Metadata

Identifier

DOI [10.15151/ESRF-DC-1634316333](https://doi.org/10.15151/ESRF-DC-1634316333)

Proposals

IH-ES-132

Beamlines

[BM05](#)

Public release year

2024

Publisher

[European Synchrotron Radiation Facility](#)

PaNET Technique PPC-SR μ CT



PaNET
Ontology
term

<https://doi.org/10.15151/esrf-dc-1634316333>

ESRF Dataset – enhancement with GBIF

specimen : <https://www.gbif.org/en/occurrence/1699073315> : MHNA-PV2011-1
species : <https://www.gbif.org/fr/species/8704992> : Arcovenator escotae



<https://doi.org/10.15151/esrf-dc-1634316333>

Data Collection

Open access

Arcovenator escotae MHNA-PV-2011-1

Paul Tafforeau; Vincent Beyrand

3D reconstruction for Arcovenator escotae MHNA-PV-2011-1. For further details regarding samples, measurements and data analysis, refer to the files and the article.

Experimental Data

The data can be accessed by clicking on the link below

Access data

Experimental Report

No report was found for IH-ES-132. Proposers and session participants may submit it via the [ESRF User Portal](#).

Metadata

Identifier

DOI [10.15151/ESRF-DC-1634316333](https://doi.org/10.15151/ESRF-DC-1634316333)

Proposals

IH-ES-132

Beamlines

[BM05](#)

Public release year

2024

Publisher

[European Synchrotron Radiation Facility](#)

PaNET Technique

PPC-SR μ CT

GBIF Species

Arcovenator escotae

GBIF Specimen

MHNA-PV-2011-1



GBIF PID

Datacite metadata json API

<https://data.esrf.fr/doi/10.15151/ESRF-DC-1634316333>

Data Collection **Open access**

Arcovenator escotae MHNA-PV-2011-1

Paul Tafforeau; Vincent Beyrand

3D reconstruction for Arcovenator escotae MHNA-PV-2011-1. For further details regarding samples, measurements and data analysis, refer to the files and the article.

Experimental Data

The data can be accessed by clicking on the link below

[Access data](#)

Experimental Report

No report was found for IH-ES-132. Proposers and session participants may submit it via the [ESRF User Portal](#).

Metadata

Identifier
DOI [10.15151/ESRF-DC-1634316333](https://doi.org/10.15151/ESRF-DC-1634316333)

Proposals IH-ES-132 Beamlines [BM18](#)

Public release year
2024

Publisher
[European Synchrotron Radiation Facility](#)

<https://api.datacite.org/does/10.15151/esrf-dc-1634316333>

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attributes:
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  prefix: "10.15151"
  suffix: "esrf-dc-1634316333"
  identifiers: []
  alternateIdentifiers: []
  creators:
    0:
      name: "Tafforeau, Paul"
      nameType: "Personal"
      givenName: "Paul"
      familyName: "Tafforeau"
      affiliation: []
      nameIdentifiers: []
  titles:
    0:
      title: "Arcovenator escotae MHNA-PV-2011-1"
      publisher: "European Synchrotron Radiation Facility"
```



DataCite Metadata Schema

DataCite

4.5

Search docs

Introduction

DataCite Metadata Properties	
Overview	10. ResourceType
1. Identifier	11. AlternateIdentifier
2. Creator	12. RelatedIdentifier
3. Title	13. Size
4. Publisher	14. Format
5. PublicationYear	15. Version
6. Subject	16. Rights
7. Contributor	17. Description
8. Date	18. GeoLocation
9. Language	19. FundingReference
	20. RelatedItem

DataCite API metadata - Subjects

▼ attributes:

```
doi: "10.15151/esrf-dc-1634316333"
prefix: "10.15151"
suffix: "esrf-dc-1634316333"
identifiers: []
alternateIdentifiers: []
▼ creators:
  ▼ 0:
    name: "Tafforeau, Paul"
    nameType: "Personal"
    givenName: "Paul"
    familyName: "Tafforeau"
    affiliation: []
    nameIdentifiers: []
  ▼ 1:
    name: "Beyrand, Vincent"
    nameType: "Personal"
    givenName: "Vincent"
    familyName: "Beyrand"
    affiliation: []
    nameIdentifiers: []
▼ titles:
  ▼ 0:
    title: "Arcovenator escotae MHNA-PV-2011-1"
    publisher: "European Synchrotron Radiation Facility"
    container: {}
    publicationYear: 2024
  ▼ subjects:
    ▼ 0:
      subject: "IH-ES-132"
      subjectScheme: "Proposal"
    ▼ 1:
      subject: "BM05"
      subjectScheme: "Instrument"
```

<https://api.datacite.org/doi/10.15151/esrf-dc-1634316333>



PaNET

```
"subjects": [
  {
    "subject": "propagation phase contrast microtomography",
    "valueUri": "http://purl.org/pan-science/PaNET/PaNET01210",
    "schemeUri": "http://purl.org/pan-science/PaNET/",
    "subjectScheme": "PaNET"
  }
]
```



GBIF
Global Biodiversity
Information Facility

```
"subjects": [
  {
    "subject": "Arcovenator escotae",
    "valueUri": "https://www.gbif.org/species/8704992",
    "schemeUri": "https://www.gbif.org/species",
    "subjectScheme": "GBIF species"
  }
]
```


DataCite API metadata – Related Identifiers

DataCite Metadata Properties	
Overview	10. ResourceType
1. Identifier	11. AlternateIdentifier
2. Creator	12. RelatedIdentifier
3. Title	13. Size
4. Publisher	14. Format
5. PublicationYear	15. Version
6. Subject	16. Rights
7. Contributor	17. Description
8. Date	18. GeoLocation
9. Language	19. FundingReference
	20. RelatedItem

Controlled List Values:

- **IsCitedBy**
- Cites
- IsSupplementTo
- IsSupplementedBy
- IsContinuedBy
- Continues
- IsDescribedBy
- Describes
- HasMetadata
- IsMetadataFor
- HasVersion
- IsVersionOf
- IsNewVersionOf
- IsPreviousVersionOf
- IsPartOf
- HasPart
- IsPublishedIn
- IsReferencedBy
- References
- IsDocumentedBy
- Documents
- IsCompiledBy
- Compiles
- IsVariantFormOf
- IsOriginalFormOf
- IsIdenticalTo
- IsReviewedBy
- Reviews
- **IsDerivedFrom**
- IsSourceOf
- IsRequiredBy
- Requires
- IsObsoletedBy
- Obsoletes
- **IsCollectedBy**
- Collects

relatedIdentifierType

- ARK
- arXiv
- bibcode
- DOI
- EAN13
- EISSN
- Handle
- **IGSN**
- ISBN
- ISSN
- ISTC
- LISSN
- LSID
- PMID
- PURL
- UPC
- URL
- URN
- w3id

```
"relatedIdentifiers": [  
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    "relatedIdentifierType": "DOI",  
    "relationType": "IsCitedBy",  
    "resourceTypeGeneral": "JournalArticle"  
  }  
]
```



```
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    "relationType": "IsCollectedBy",  
    "resourceTypeGeneral": "Instrument"  
  }  
]
```



```
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    "relatedIdentifierType": "URL",  
    "relationType": "IsDerivedFrom",  
    "resourceTypeGeneral": "PhysicalObject"  
  }  
]
```



DataCite API metadata – Related Identifiers

DataCite Metadata Properties

Overview

1. Identifier

2. Creator

3. Title

4. Publisher

5. PublicationYear

6. Subject

7. Contributor

8. Date

9. Language

10. ResourceType

11. AlternateIdentifier

12. RelatedIdentifier

13. Size

14. Format

15. Version

16. Rights

17. Description

18. GeoLocation

19. FundingReference

20. RelatedItem

Controlled List Values:

- [IsCitedBy](#)
- [Cites](#)
- [IsSupplementTo](#)
- [IsSupplementedBy](#)
- [IsContinuedBy](#)
- [Continues](#)
- [IsDescribedBy](#)
- [Describes](#)
- [HasMetadata](#)
- [IsMetadataFor](#)
- [HasVersion](#)
- [IsVersionOf](#)
- [IsNewVersionOf](#)
- [IsPreviousVersionOf](#)
- [IsPartOf](#)
- [HasPart](#)
- [IsPublishedIn](#)
- [IsReferencedBy](#)
- [References](#)
- [IsDocumentedBy](#)
- [Documents](#)
- [IsCompiledBy](#)
- [Compiles](#)
- [IsVariantFormOf](#)
- [IsOriginalFormOf](#)
- [IsIdenticalTo](#)
- [IsReviewedBy](#)
- [Reviews](#)
- [IsDerivedFrom](#)
- [IsSourceOf](#)
- [IsRequiredBy](#)
- [Requires](#)
- [IsObsoletedBy](#)
- [Obsoletes](#)
- [IsCollectedBy](#)
- [Collects](#)

"relatedIdentifiers": [

{

"schemeUri": "http://www.fao.org/plant-treaty/areas-of-work/global-information-system/descriptors",

"schemeType": "XML",

"relationType": "HasMetadata",

"relatedIdentifier": "https://glis.fao.org/glisapi/v1/pgrfas?doi=10.18730/1M80VH",

"relatedIdentifierType": "URL",

"relatedMetadataScheme": "GLIS Descriptors"

}

]



Documentation

GLIS technical documentation

DataCite API metadata - Proposal

<https://api.datacite.org/doi/10.15151/esrf-dc-1634316333>

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  ▼ 0:
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    nameType: "Personal"
    givenName: "Paul"
    familyName: "Tafforeau"
    affiliation: []
    nameIdentifiers: []
  ▼ 1:
    name: "Beyrand, Vincent"
    nameType: "Personal"
    givenName: "Vincent"
    familyName: "Beyrand"
    affiliation: []
    nameIdentifiers: []
▼ titles:
  ▼ 0:
    title: "Arcovenator escotae MHNA-PV-2011-1"
    publisher: "European Synchrotron Radiation Facility"
    container: {}
    publicationYear: 2024
▼ subjects:
  ▼ 0:
    subject: "IH-ES-132"
    subjectScheme: "Proposal"
  ▼ 1:
    subject: "BM05"
    subjectScheme: "Instrument"
```

```
"fundingReferences": [
  {
    "awardUri": "[N/A for ESRF]",
    "awardTitle": "Flying archosaurs project",
    "funderName": "European Synchrotron Radiation Facility",
    "awardNumber": "IH-ES-132",
    "funderIdentifier": "https://ror.org/02550n020",
    "funderIdentifierType": "ROR"
  },
]
```



DataCite API metadata - affiliation

▼ attributes:

```
doi: "10.15151/esrf-dc-1634316333"
prefix: "10.15151"
suffix: "esrf-dc-1634316333"
identifiers: []
alternateIdentifiers: []
▼ creators:
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    name: "Tafforeau, Paul"
    nameType: "Personal"
    givenName: "Paul"
    familyName: "Tafforeau"
    affiliation: []
    nameIdentifiers: []
  ▼ 1:
    name: "Beyrand, Vincent"
    nameType: "Personal"
    givenName: "Vincent"
    familyName: "Beyrand"
    affiliation: []
    nameIdentifiers: []
▼ titles:
  ▼ 0:
    title: "Arcovenator escotae MHNA-PV-2011-1"
    publisher: "European Synchrotron Radiation Facility"
    container: {}
    publicationYear: 2024
▼ subjects:
  ▼ 0:
    subject: "IH-ES-132"
    subjectScheme: "Proposal"
  ▼ 1:
    subject: "BM05"
    subjectScheme: "Instrument"
```

<https://api.datacite.org/doi/10.15151/esrf-dc-1634316333>

```
"affiliation": [
  {
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    "affiliationIdentifier": "https://ror.org/02ma7yv75",
    "affiliationIdentifierScheme": "ROR"
  }
],
"nameIdentifiers": [
  {
    "nameIdentifier": "0000-0002-1808-2206",
    "nameIdentifierScheme": "ORCID"
  }
]
```

Datacite updates



Support for instruments

- Addition of [Instrument](#) to the [resourceTypeGeneral](#) controlled list values.
 - This value may be used in [10.a resourceTypeGeneral](#) and other places where resourceTypeGeneral is used ([12.f resourceTypeGeneral](#), [20.a relatedItemType](#)).
- Addition of new [relationType](#) pair: [IsCollectedBy](#) and [Collects](#)
- To enhance support for instruments, addition of new mapping: [PIDINST Schema Mapping](#)



RDAs Working Group PIDINST

Persistent Identification of Instruments
<https://docs.pidinst.org/>

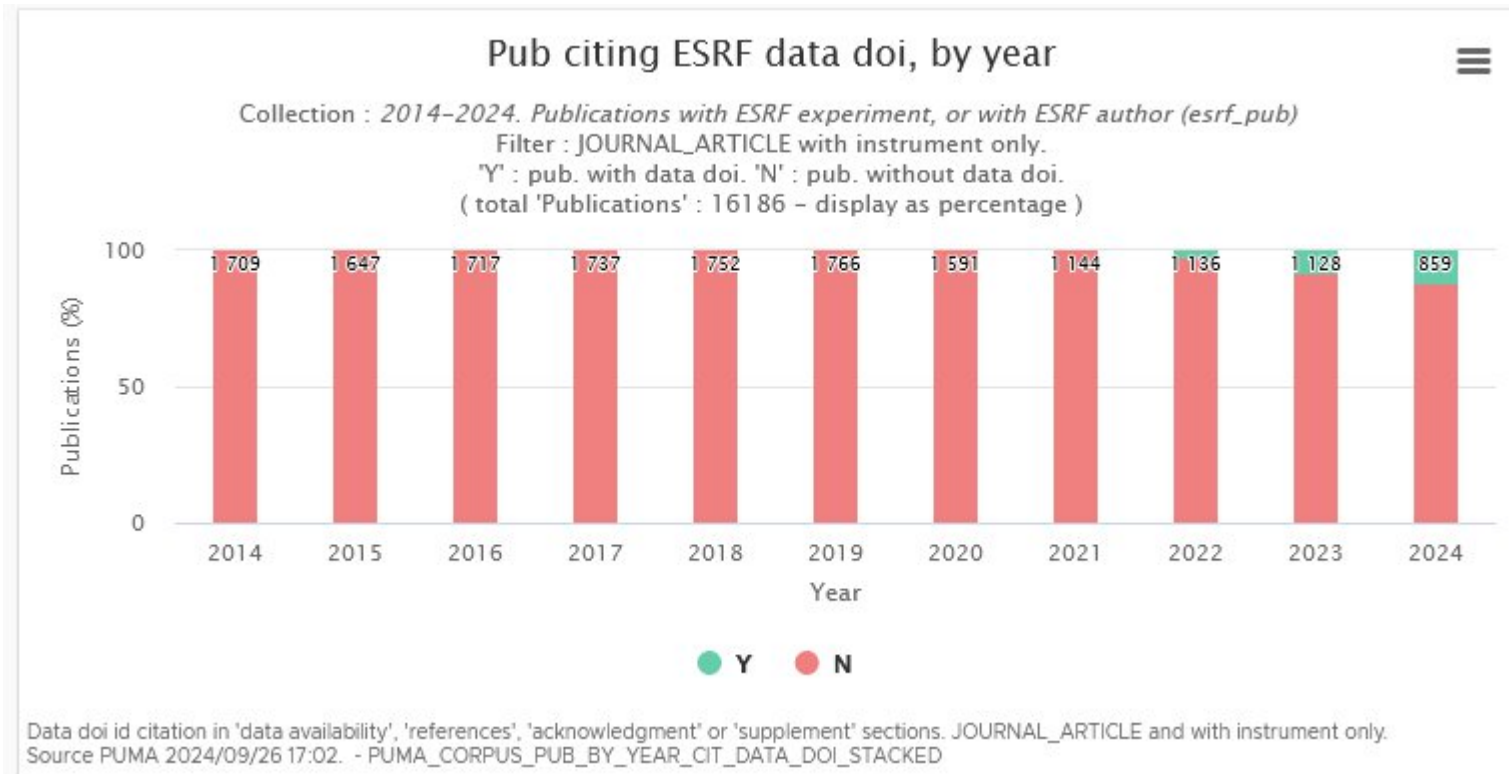
Updated PhysicalObject definition

- Change to the definition of [PhysicalObject](#) in support of samples.

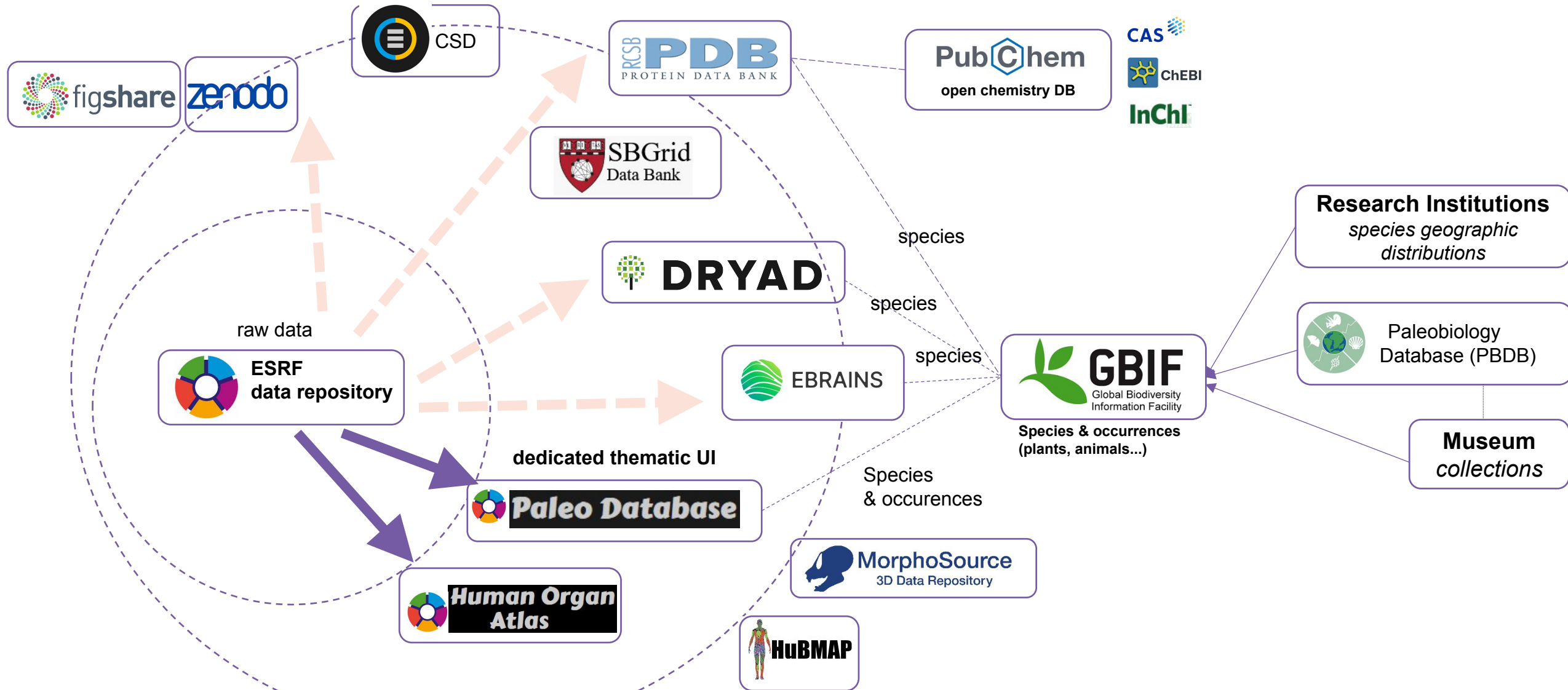
Processed data

Example 1/3

Where is the ESRF processed data ??



Where is our processed data ?



Data aggregators are emerging



“The DiSSCO infrastructure will connect historical collection data with specimen-derived data emerging from new technologies, e.g., DNA barcodes, whole genome sequences, proteomics and metabolomics data, chemical data, trait data, and imaging data (computer-assisted tomography (CT) and Synchrotron data). This integration will combine earlier investments in data interoperability practices with technological advancements in digitisation, cloud services and semantic linking.”

Physical Object



Digital Specimen
digital object



Example link to external data



ESRF
data repository

<https://doi.org/10.15151/ESRF-DC-1089735712>

Data Collection

Open access

Raw data (diffraction images) for **PDB entry 8CJE** "AETF, A SINGLE-COMPONENT FLAVIN-DEPENDENT TRYPTOPHAN HALOGENASE, IN COMPLEX WITH L-TRYPTOPHAN"

Simon Gäfe; Hartmut H. Niemann

Data set exhibiting non-merohedral twinning with high twin fraction of 0.4. The point group appears to be 422 but the space group is actually P212121. The publication describing the experiment can be accessed via the PDB entry.

Metadata

Identifier

DOI [10.15151/ESRF-DC-1089735712](https://doi.org/10.15151/ESRF-DC-1089735712)

Proposals

MX-2393

Beamlines

[ID30B](#)

Public release year

2023

Publisher

[European Synchrotron Radiation Facility](#)

Licence (for files)

[Creative Commons Attribution 4.0](#)

Proteins - PDB – processed/derived Data



<https://doi.org/10.2210/pdb8CJE/pdb>

Structure Summary | Structure | Annotations | Experiment | Sequence | Genome | Ligands | Versions

Biological Assembly 1

8CJE

AetF, a single-component flavin-dependent tryptophan halogenase, in complex with L-tryptophan

PDB DOI: <https://doi.org/10.2210/pdb8CJE/pdb>

Classification: FLAVOPROTEIN
Organism(s): Aetokthonos hydrillicola Thurmond2011
Expression System: Escherichia coli BL21(DE3)
Mutation(s): No

Deposited: 2023-02-13 Released: 2023-06-14
Deposition Author(s): Cafe, S., Niemann, H.H.
Funding Organization(s): Not funded

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 1.80 Å
R-Value Free: 0.188
R-Value Work: 0.160
R-Value Observed: 0.181

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree		0.187
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		2.9%
RSRZ outliers		0.9%

Explore in 3D: Structure | Sequence | Annotations | Electron Density | Validation Report | Ligand Interaction (FAD)

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Monomer - A1

Find Similar Assemblies

Biological assembly 1 assigned by authors.

Small Molecules

Ligands 2 Unique

InChI

ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
FAD (Subject of Investigation/LOI) Query on FAD	E [auth A], G [auth B], I [auth C], K [auth D]	FLAVIN-ADENINE DINUCLEOTIDE C ₂₇ H ₃₃ N ₉ O ₁₅ P ₂ VWWQXMAJTJZDQX-UYBVJOGSSA-N		Interactions Interactions & Density
TRP (Subject of Investigation/LOI) Query on TRP	F [auth A], H [auth B], J [auth C], L [auth D]	TRYPTOPHAN C ₁₁ H ₁₂ N ₂ O ₂ QIVBCDIJAJQPQS-VIFPVBQESA-N		Interactions Interactions & Density

open chemistry DB



<https://pubchem.ncbi.nlm.nih.gov/compound/643975>

Macromolecules

Find similar proteins by: Sequence (by identity cutoff) | 3D Structure

Entity ID: 1

Molecule	Chains	Sequence Length	Organism	Details	Image
AetF	A, B, C, D	663	Aetokthonos hydrillicola Thurmond2011	Mutation(s): 0 Gene Names: aetF	



<https://www.gbif.org/species/8198514>

Improve dataset with new metadata ?



ESRF
data repository

<https://doi.org/10.15151/ESRF-DC-1089735712>

Data Collection

Open access

Raw data (diffraction images) for PDB entry 8CJE "AETF, A SINGLE-COMPONENT FLAVIN-DEPENDENT TRYPTOPHAN HALOGENASE, IN COMPLEX WITH L-TRYPTOPHAN"

Simon Gäfe; Hartmut H. Niemann

Data set exhibiting non-merohedral twinning with high twin fraction of 0.4. The point group appears to be 422 but the space group is actually P212121. The publication describing the experiment can be accessed via the PDB entry.




User input required at sample or dataset creation

Metadata	
Identifier	
DOI	10.15151/ESRF-DC-1089735712
Proposals	Beamlines
MX-2393	ID30B
Public release year	
2023	
Publisher	
European Synchrotron Radiation Facility	
Licence (for files)	
Creative Commons Attribution 4.0	

PDB	8CJE
GBIF species PubChem	Aetokthonos hydrillicola FLAVIN-ADENINE DINUCLEOTIDE

ILL data example with chemical formula

 DOI > 10.5291/ILL-DATA.5-25-249

This proposal is publicly available since 06/24/2021

Title
2D - Lattice collapse in Lead di-acetate tri-hydrate on dehydration:Phase transitions, phase identification and decomposition behaviour

Abstract
Abstract is not yet public

Experimental Report
The experimental report is not available to download

Download Data
Please note that you will need to login with your ILL credentials to download the data.
[Download Data](#)

Data Citation
The recommended format for citing this dataset in a research publication is in the following format:
VISSER Dirk; GUTMANN Matthias and Thomas C. Hansen. (2016). 2D - Lattice collapse in Lead di-acetate tri-hydrate on dehydration:Phase transitions, phase identification and decomposition behaviour. Institut Laue-Langevin (ILL) doi:10.5291/ILL-DATA.5-25-249

Cited by
This data has not been cited by any articles.

Metadata

Identifier
DOI doi:10.5291/ILL-DATA.5-25-249

Authors
VISSER Dirk
GUTMANN Matthias
Thomas C. Hansen

Publisher
Institut Laue-Langevin

Publication year
2016

Cycles
20161 (19-05-2016 - 16-07-2016)

Instruments
D2B (high-resolution 2-axis diffractometer)

Proposal number
5-25-249

Experiment Parameters

Environment temperature
-40 - 450 oC

Experiment energy
1.9 - 2.4 A

Sample Parameters

Formula
Pb(CH3COO)2.3H2O
Pb(CD3COO)2.3H2O

ESRF sample management

USER PORTAL - DEMO Signed-in as bochot

My proposals Draft ID 120002 (missing title) Type: STD Role: PI

▲ Proposal ▲ Samples ▲ Description

Description Handling & Equipment Certify

All fields marked with an asterisk (*) are required.
All data are automatically saved as soon as you exit the field you were editing.

Sample form '[Not defined yet]'

Materials with similar composition should be grouped in one sample form.

Summary

A short name, reference or acronym to identify your sample in a list, e.g. Ni111a, Lyso3, ABC, Tom1...
It is prohibited to have several samples with the same name inside a single proposal.

Short Name* Used 0 of max 20 characters.

Select the categories of the sample

Select category* Biological > Select sub-category* Macromolecule > Select sub-category* Protein > Select sub-category* Toxin

Give name, empirical formula, sample function, gene annotation number and name in case of hypothetical protein or unknown substance.

Substance* Used 0 of max 500 characters.

Structural

Non-structural Used 0 of max 500 characters.

Toxin ✓ Used 0 of max 500 characters.

Hormone

Other

Description* Used 0 of max 500 characters.

Give an indication of sample size(s) and quantity.

Quantity and size of sample(s)* Used 0 of max 500 characters.

Describe any adduct or substrate or chemicals associated, including reference, solvent, gas, and give references

Adduct* Used 0 of max 500 characters.

Please click all the appropriate states, multiple choices are possible.*

Solid - stand alone Solid - dispersed Liquid Gas Aerosol Crystal Polycrystalline Powder Multilayer Gel Polymer Metallic Nanoparticles

Tissue Alloy Glass Composite Animal(s) Other

Please indicate if the sample presents one or several of the following risks*

Radioactive Explosive Flammable Toxic Corrosive CMR Pollutant Reactive/Unstable Oxidizing Biohazard Air sensitive Gas under pressure

Other None of the above

Please indicate if you will be working with specific compounds like heavy metals, lanthanides, antibiotics, D2O, chemicals, hormones, etc... or if the samples contain anomalous scatterers.

Will you be working with specific compounds or anomalous scatterers?* Yes No

Will the sample or/and equipment be exposed to or be irradiated by neutrons/protons before the experiment at ESRF?* Yes No

Biological

Give the source organism

Source organism* Used 0 of max 200 characters.

Select the class of risk

Class of risk*

Is the sample recombinant?* Yes No

Previously observed diffraction?* Yes No

Proposal & Dataset Citation

Proposal Id & Dataset DOI in publications

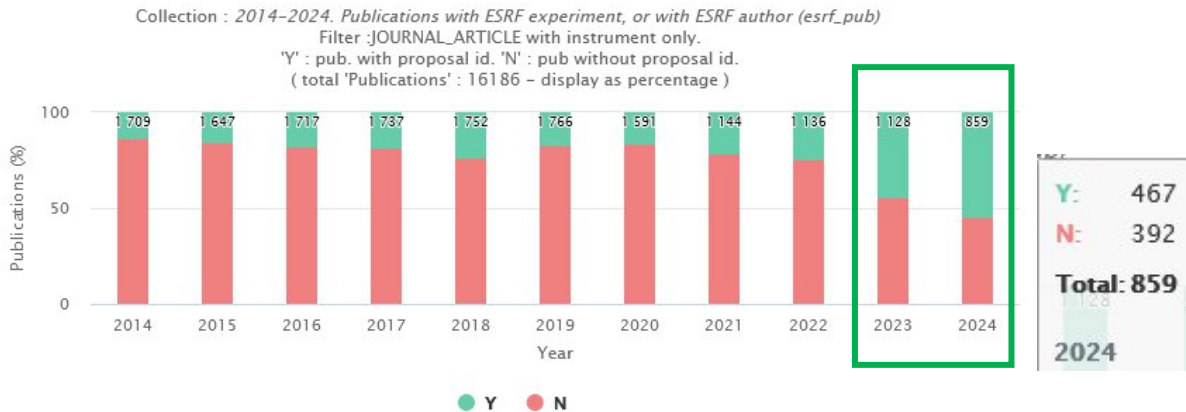
- Acknowledgment section. Ex: 10.1021/acs.chemmater.4c00555

Acknowledgments

Funding was received from the European Union (ERC AdG, UniEnMLD, No. 101097815). Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them. This work was also partly supported by the Finnish Cultural Foundation (THERMOF), Magnus Ehrnrooth Foundation, KU Leuven (GSFAH/22/001), Research Foundation Flanders (1263622N), JSPS KAKENHI (JP22H05143; Transformative Research Areas (A) “Supra-ceramics”), and Scandinavia-Japan Sasakawa Foundation. We acknowledge the European Synchrotron Radiation Facility (ESRF) for provision of synchrotron radiation facilities (beamline ID26) under the proposal number CH-6525 (DOI: 10.15151/ESRF-ES-894388406). We also acknowledge Diamond Light Source for time on Beamline I07 under proposal si29967 and thank Francesco Carlà, Jonathan Rawle, Jorid Smets, and Jesús Gándara-Loe. We also thank CSC – the Finnish IT Center for Science for computational resources. Anni Virta and Mikhail Kuklin are acknowledged for contributions to the USPEX crystal structure predictions. Olga Partanen is acknowledged for contributions to the thermal stability studies. Miwa Saito and Yusuke Asai are acknowledged for contributions to the in situ FTIR experiments.

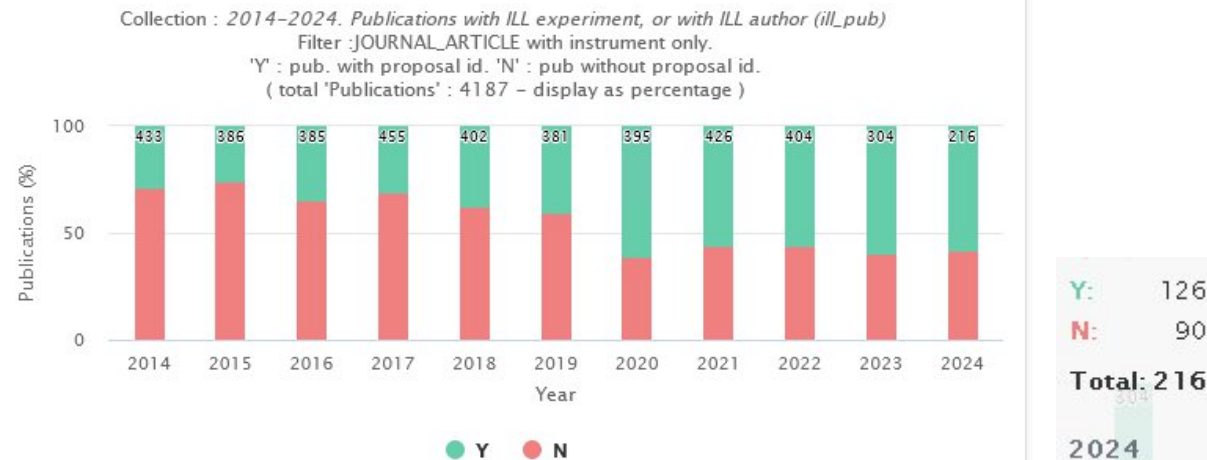
Publication – Proposal ID link

Pub citing ESRF proposal id, by year



Proposal id citation usually in 'acknowledgment' section. JOURNAL_ARTICLE and with instrument only.
 Source PUMA 2024/09/26 16:35. - PUMA_CORPUS_PUB_BY_YEAR_CIT_PROP_ID_STACKED

Pub citing ILL proposal id, by year



Proposal id citation usually in 'acknowledgment' section. JOURNAL_ARTICLE and with instrument only.
 Source PUMA 2024/09/18 20:51. - PUMA_CORPUS_PUB_BY_YEAR_CIT_PROP_ID_STACKED

ESRF

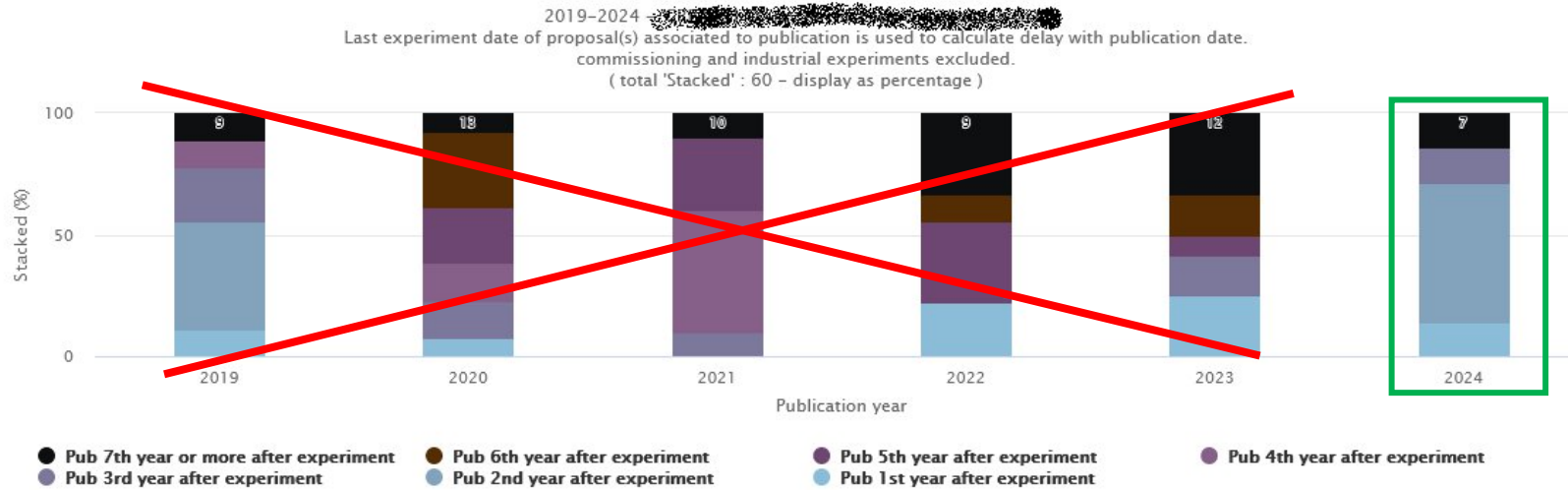
- Library email campaign : we now ask the users for missing proposal reference in publication ex: MX-12345. Flora **library** database is updated
- Email sent 08/2024 to publication corresponding authors (for 2023 and 2024 publications)
- Good user responses : we see impact on data quality for these years.
- First ESRF DOIs created in 2018 (source Datacite search api)

ILL

- Without email campaign
- Publication proposal link is better than ESRF
- First ILL DOIs created in 2013 (source Datacite search api)
- Email campaign planned by ILL library.

Time between experiment and publication

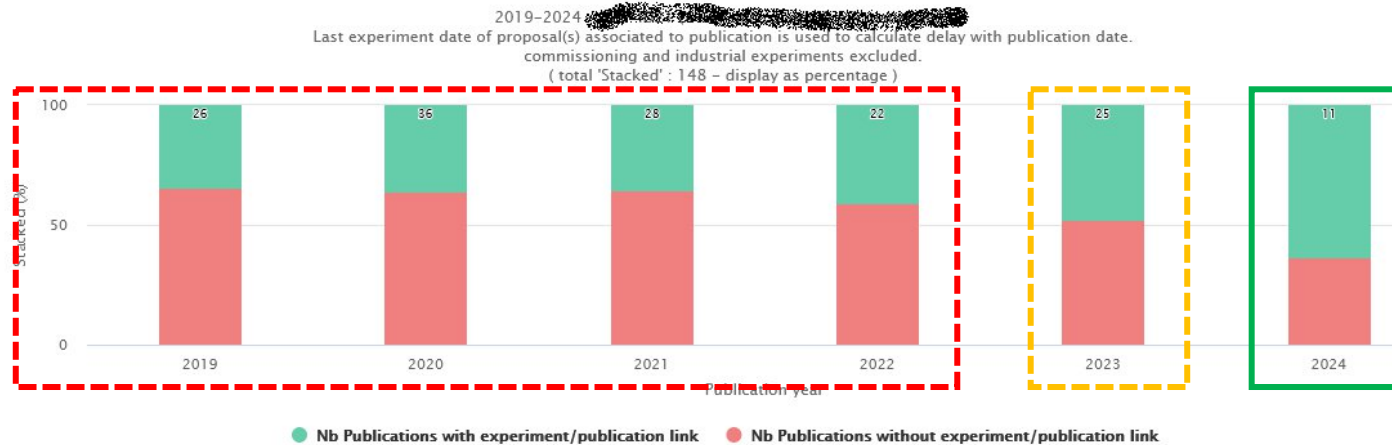
Time between publication and experiment



known limitations :


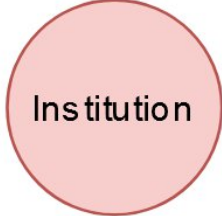


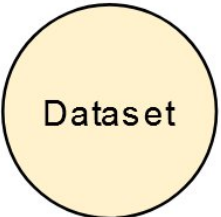



















Last experiment date of proposal(s) associated to publication is used to calculate delay with publication date. This may cause issues for proposals running over multiple years (BAG, LTP) : delay may be inaccurate (too short or even negative). BAG can involve multiple groups with same instruments associated to the same proposal. LTP can lead to multiple publications during proposal time.
 Source PUMA 2024/09/26 16:28. - PUMA_CORPUS_PUB_BY_YEAR_DELAY_EXP_PUB_STACKED

Percentage of publications with link to experiment



Conclusion

PIDs, Vocabularies, Ontologies...

	 <p>Institution</p>	 <p>ROR</p> <p>ESRF : https://ror.org/02550n020</p>		 <p>Dataset</p>	 <p>DataCite doi</p> <p>ESRF data doi : https://doi.org/10.1515/ESRF-DC-572196058</p>
	 <p>Person</p>	 <p>ORCID</p> <p>G. Bouchard : 0000-0003-0705-6026</p>		 <p>Grant/ Proposal</p>	 <p>Crossref doi</p>
	 <p>Publication</p>	 <p>Crossref doi</p> <p>https://doi.org/10.1038/s41592-021-01317-x</p>		 <p>Instrument</p>	 <p>DataCite doi</p>
	 <p>Journal</p>	 <p>ISSN</p> <p>Nature Communications : 2041-1723</p>		 <p>PaN Technique</p>	 <p>PaNET</p> <p>vocabulary/ontology Photon and Neutrons Experiment Techniques</p> <p>SAXS - Small Angle X-ray Scattering : http://purl.org/pan-science/PaNET/PaNET01188</p>

Wait... Could it work with bad metadata and a bit of AI/ML ?

Harvard dataset

<http://doi.org/10.7910/DVN/0JV5RU/U6LOAQ>



Add Data ▾ Search ▾ About User Guide

Ashley Rubinstein Dataverse

(UT Health McGovern Medical School)

Harvard Dataverse > Ashley Rubinstein Dataverse > Radiation-Induced Lung Toxicity in Mice Irradiated in a Strong Magnetic Field - Mouse 109 >

109_0166.dcm

This file is part of "Radiation-Induced Lung Toxicity in Mice Irradiated in a Strong Magnetic Field - Mouse 109".

Version 1.0

File Citation

Rubinstein, Ashley, 2018, "109_0166.dcm", *Radiation-Induced Lung Toxicity in Mice Irradiated in a Strong Magnetic Field - Mouse 109*, <https://doi.org/10.7910/DVN/0JV5RU/U6LOAQ>, Harvard Dataverse, V1

Cite Data File ▾

Learn about [Data Citation Standards](#).

Dataset Citation

Rubinstein, Ashley, 2018, "Radiation-Induced Lung Toxicity in Mice Irradiated in a Strong Magnetic Field - Mouse 109", <https://doi.org/10.7910/DVN/0JV5RU>, Harvard Dataverse, V1

Cite Dataset ▾

Learn about [Data Citation Standards](#).

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attributes:
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  suffix: "dvn/0jv5ru/u6loaq"
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  alternateIdentifiers: []
creators:
  0:
    name: "Rubinstein, Ashley"
    nameType: "Personal"
    givenName: "Ashley"
    familyName: "Rubinstein"
  affiliation:
    0: "(UT Health McGovern Medical School)"
    nameIdentifiers: []
titles:
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publisher: "Harvard Dataverse"
container: {}
publicationYear: 2018
subjects: []
contributors: []
dates: []
language: null
types: {}
relatedIdentifiers:
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relatedItems: []
sizes: []
formats: []
version: null
rightsList: []
descriptions:
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```

Radiation-Induced Lung Toxicity in Mice Irradiated in a Strong Magnetic Field - Mouse 109 109_0166.dcm

[HTML](#)[API](#)

Year: 2018

Type: dataset

Source: [Harvard Dataverse](#)

Author [Ashley Rubinstein](#)

Institution [The University of Texas Health Science Center at Houston](#)

Cites:

Cited by:

Related to: 10

Topic: [Biological Effects of Electromagnetic Fields](#)

Subfield: [Biophysics](#)

Field: [Biochemistry, Genetics and Molecular Biology](#)

Domain: [Life Sciences](#)

Open Access status: gold



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  0:  
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    author:  
      id: "https://openalex.org/A5061414245"  
      display_name: "Ashley Rubinstein"  
      orcid: "https://orcid.org/0000-0003-0221-4603"  
      institutions:  
        0:  
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```

<https://api.openalex.org/works/doi:10.7910/dvn/0jv5ru/u6loaq>

Next ?

- https://openalex.org/works?page=1&filter=type%3Atypes%2Fdataset,primary_location.source.id%3As4377196806
- <https://www.youtube.com/watch?v=cKUKXwxAlOM>



Webinar: Finding, tracking, and analyzing research datasets in OpenAlex





OpenAlex

[Article](#) [Talk](#)

From Wikipedia, the free encyclopedia

OpenAlex is a bibliographic catalogue of scientific papers, authors and institutions accessible in [open access](#) mode, named after the [Library of Alexandria](#). It started operating in January 2022 by [OurResearch](#) as a successor of the terminated [Microsoft Academic Graph](#). OpenAlex competes with commercial products such as [Clarivate's Web of Science](#) or [Elsevier's Scopus](#), and is complemented by [Bibliometrics](#) tools and an [API](#).^{[1][2]}

In 2024, the [French Ministry of Research and Higher Education](#) pledged to contribute financially to the project, considering it "as a crucial open science infrastructure".

Thanks :-)