

# ESS-DIVE Sample Identifiers and Metadata Reporting Format Tutorial

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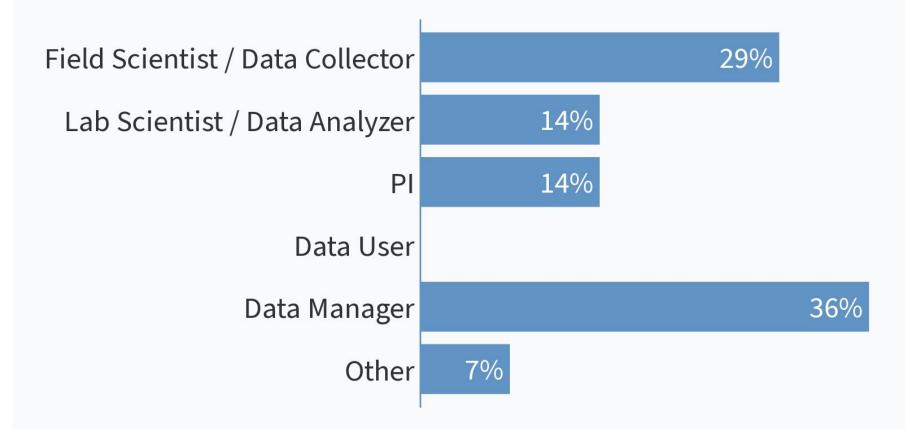








### What is your primary role in your research group?

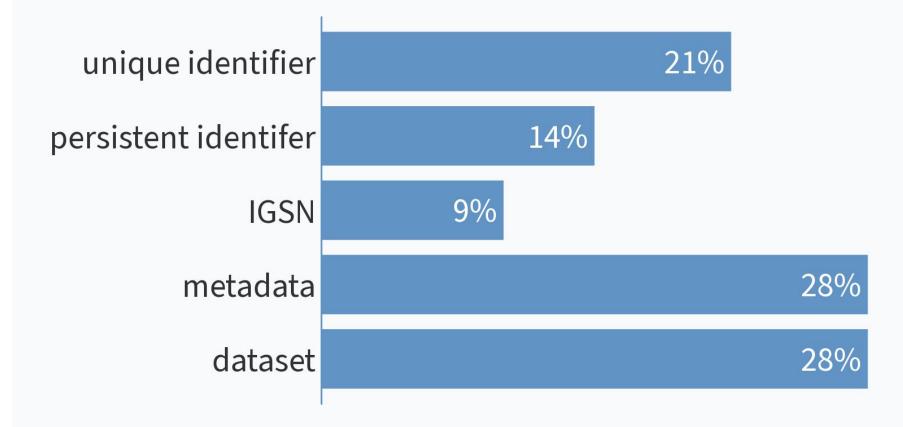


### What organization are you representing today?

- " University of Wisconsin-Madison"
- " NGEE Arctic "
- "LBNL"

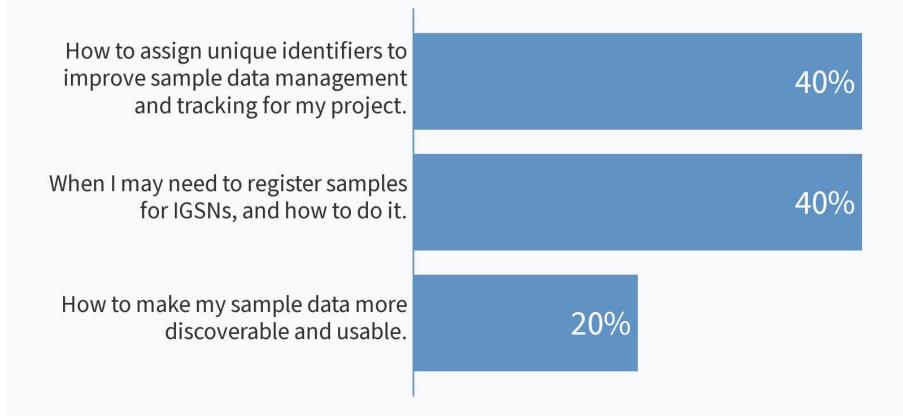
- " NGEEs/BNL "
- " University of Alaska Fairbanks"

### Which of the following terms are you familiar with?



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### What are you most interested in learning about today?



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### **Tutorial Overview**



- Sample identifiers and metadata
- ESS-DIVE sample ID and metadata guide/template
- Sample planning to publication workflow
- How and why to use International Geo/General Sample Numbers (IGSN)

https://bit.ly/ESSDIVE\_SampleTutorial

## Takeaways from this presentation



- Understand when to use unique and persistent IDs
- Standardize sample metadata using template
- Register samples for IGSNs
- Publish sample datasets in ESS-DIVE

ESS-DIVE guidance for sample identifiers and metadata will enable more effective sample planning, tracking, discovery, and reuse.

## Terminology Check: identifiers and metadata





## **Unique**<br/>**Identifier**

Provides a meaningful, project-specific unique ID to organize your data

### **Sample Name:**

RockCr001\_2021-05-25



### Metadata

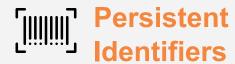
Descriptive information about data

**Sample Type:** Water

Feature: Stream

Location: Rock Creek,

Crested Butte, CO



Globally unique IDs with permanent link/landing page, associated metadata

**ORCiD:** People

**DOI:** Data, publications

IGSN: Samples IEWFS000U

## What is Sample Metadata?



### **Sample Collections Details**

- Collector/Chief Scientist\*
- Collection Date\*
- Collection Time
- Collection Method Description\*
- Sample Processing (MIxS)
- Field Program or Project Name\*

#### **Sample Access**

- Release Date\*
- Current Archive
- Current Archive Contact

#### Location

- Location Description
- Latitude\*
- Longitude\*
- Geolocation Instrument
- Elevation (start, end)
- Elevation Unit
- Country\*
- Minimum/Maximum Depth in Meters (DwC)
- Minimum/Maximum
   Distance above Surface in Meters (DwC)

#### **Environmental Context**

- Physiographic Feature\* (ENVO, MIxS)
- Biome (MlxS)

#### **Sample Description**

- IGSN-SESAR provides
- Sample Name\*
- Object Type\* (BCO)
- Material\* (ENVO, PO)
- Classification
- Sample Description
- Purpose
- · Size, Size Unit
- Filter Size (MlxS)
- Scientific Name (DwC)
- Sample Remarks

#### **Related Identifiers**

- Parent IGSN
- Collection ID (DwC)
- Event ID (DwC)
- Location ID (DwC)



# Using IGSNs for Sample Tracking and Linking

## When do you need persistent IDs for samples?



1.) Multiple datasets, journal publications

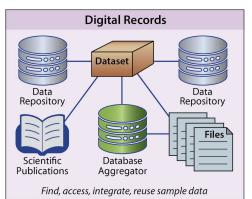
2.) Collaborators work on same samples

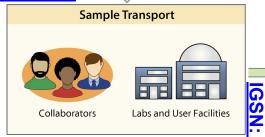
3.) Multiple labs for analyses

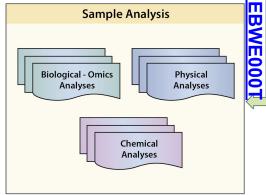
4.) Sample-related data in different repositories

5.) Archived, and used for multiple purposes over time









**IGSN: IEBWE000T** 

## Persistent IDs: Landing Pages



#### IGSN: IEWFS0001

Soil Sample Landing Page



Description

IGSN: IEWF50001 Sample Name: 115 Other Name(s):

Sample Type: Core Section Parent IGSN: Not Provided

Material: Soil

Classification: Not Provided Field Name: Not Provided

Soil cores that were collected seasonally during autumn, winter, snowmelt, and spring

at a high altitude field site which is predominately montane meadow

Age (min): Not Provided
Age (max): Not Provided

Collection Method: Manual>Hammer

Collection Method Description: Soil cores were collected using soil bulk density corer attached to a slide hammer

Size: Not Provided
Geological Age: Not Provided
Coological Hote

 Geological Unit:
 Not Provided

 Comment:
 Not Provided

 Purpose:
 Not Provided

Geolocation

Latitude (WGS84): 38.917216053 Longitude (WGS84): -106.955994698

#### Relevant Links:

- http://identifiers.org/gold:Gp0321263: Soil microbial communities from the East River watershed near Crested Buttle, Colorado, United States – Metgenomes (Genomes Online Database, GOLD)
- http://identifiers.org/gold:Gp0396393: Soil microbial communities from the East River watershed near Crested Butte, Colorado, United States – Metatranscriptomes (Genomes Online Database, GOLD)
- https://doi.org/10.15485/1577267: Dataset: Soil Nitrogen, Water Content, Microbial Biomass, and Archaeal, Bacterial and Fungal Communities from the East River Watershed, Colorado collected in 2016-2017.
- https://doi.org/10.21952/WTR/1573029: Dataset for sample collection metadata

### https://app.geosamples.org/sample/igsn/IEWFS0001



Sample Metadata:Sorensen P; Brodie E; Beller H; Wang S; Bill M Metadata for Soil Cores from the East River Watershed, Colorado co doi:10.21952/WTR/1573029 ESS-DIVE Dataset: Soil Measurements

https://doi.org/10.15485/1577267

## Benefits of using IGSNs Across Facilities and Data Systems





## Persistent Identifier Benefits

- Link and expand access pathways
- 2. Avoid duplication of information across platforms
- 3. Interpretation and reuse

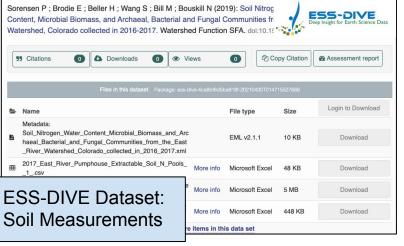
## Linking related interdisciplinary data



Landing Page

https://doi.org/10.21952/WTR

metadata



The synchronization of microbial and plant phenology in a mountainous watershed and its importance for nutrient retention under changing hydrologic regimes.

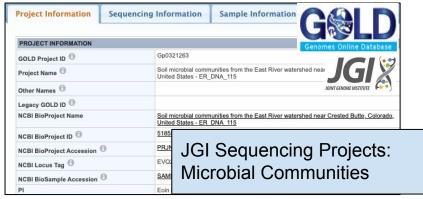
**Description** The goal of the study is to observe the activation of microbial metabolic potential beneath the snowpack during winter and during the snowmelt period, as well as advanced characterization of the chemistry of carbon and nutrient transformations and assimilation by microorganisms and vegetation in response to earlier snowmelt timing.

Metagenome: 48

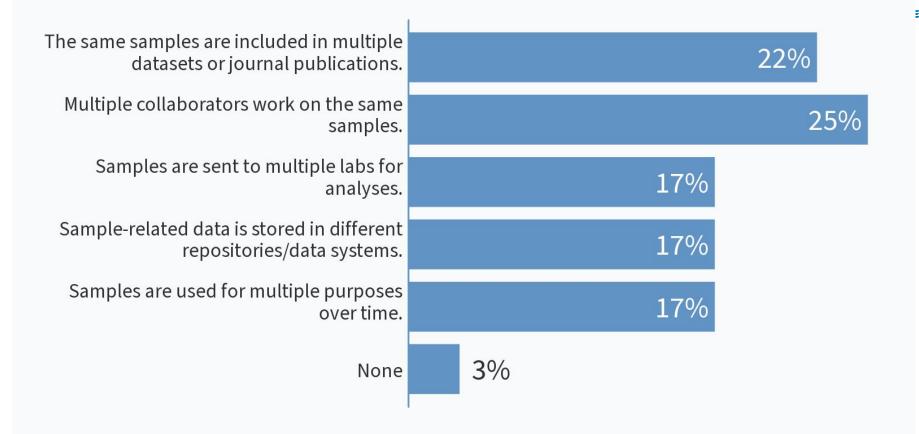


Metabolomics: 52 Metatranscriptome: 45

National Microbiome Data Collaborative: Study Page



### Which of the following apply for your project sample data?





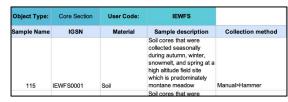
## Sampling Planning to Publication Workflow

## General Workflow - Sample IDs and Metadata Reporting Format



Step 1

Plan your sample campaign



Step 2

Standard sample metadata

Step 3

Register samples for IGSNs



### Step 4

Submit sample datasets to ESS-DIVE



## Step 1: Planning - consider file organization and IDs for your sampling campaign

Incorporate sample data management into planning your field campaign

### How to do it:

Assign project-specific unique identifiers (e.g. locations, samples, subsamples)

### Sample Collections File Collection ID (row label)

- Purpose
- Project Name\*
- Release Date\*
- Chief Scientist
- Country\*
- Biome
- Object Type\*

#### Methods File Method ID (row label)

 Collection Method Description\*

### Locations File Location ID (row label)

- Latitude\*
- Longitude\*
- Geolocation Instrument
- Location Description
- Physiographic Feature\*

### Sampling Events File

- Collection Date\*
  - Collector\*

### Samples File IGSN (row label)

- Sample Name\*
- · Material\*
- Sample Description
- Minimum Depth
- Maximum Depth
- Processing Details
- Collection ID
- Location ID
- Location it
- Event ID
- Method ID

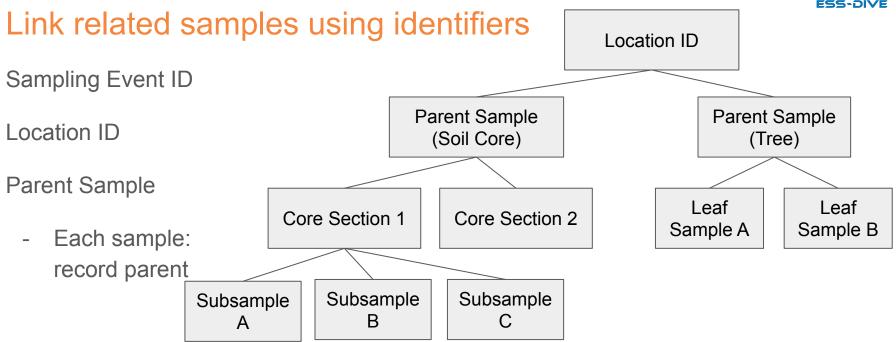
EESA20-060

Consistently using identifiers to manage and link related metadata across files

IocationID	Other name(s)			Description				Latit	ude	LOCATIONS F			<b>■</b>	
ER-GUM1	Gothic Upper Montane-1; GUM			Groundwater Monitoring We			38.95	8.9550494 -106		5.9923898				
ER-RCK1	Rock Creek; Rock			Groundwater Monitoring Wel			38.98	9816681 -107.0055887			887	E	SS-DIV	
ER-RUS1	Rustlers Gulch; Rustlers			Groundwater Monitoring Wel			1 38.9889397 -1		-10	07.007755				
ER-SHM1	Shumwa	ay Well; Shumw	ay	Grou	ındwater	Monitorin	g We	38.94	54058	-106	.98951	97		
ER-BRD1	Bradley Creek; Bradley			Water Quality-Discharge Sta			38.98	.9854093 -107.00484						
ER-CPR1 ER-EAQ1	Sa	ample Name	IGSN	lo	cationID	Collection date	on	Materi	ial	Field nan	ne (info	PARE SAME	:N I PLE FILI	E
ER-EBC0	GUM-1	_2021-03-10	IEWFS004C	EF	R-GUM1	2021-03-10	) L	iquid>aqu	ieous	groundw	ater [E	TU:OVN	001004]	
ER-TTL1			IEWFS004R		R-SHM1	2021-03-10				groundwater [l				
	Tuttle_2021-03-10 IEWFS0045			<b>1</b>		2021-03-10 Lie				:Ti			001004]	
	EAQ_2021-03-03 IEWFS004T									surface water [ENVO:0000				
	Rustlers_2021-03-03 IEWFS004U					3 L			surface water [ENVO:0000					
			IEWFS004V	NFS004V ER-E		R-BRD1 2021-03-03		Liquid>aqueous		surface water [ENVO:0		1VO:000	SUBSA	MDII
	Rock_2 Copper EBC_2	Sample	e Name		Parer	nt IGSN	Ю	GSN	loca	ationID	Colle	ction dat		
	2	EAQ 2021-03-0	03 DO		IEWFS0	04T	IEWF	S001I	ER-E	AQ1	2021-0	03-03	Liquid>a	aqueous
		EAQ_2021-03-03_CA			IEWFS0	04T	IT IEWF				2021-0	03-03	03 Liquid>aqueous	
	EAQ_2021-03-03_AM			IEWFS00 IEWFS00		04T	IEWF	S001K			2021-0	03-03		
	EAQ_2021-03-03_AN Rustlers_2021-03-03_DO		04T			IEWF		ER-E	AQ1	2021-0	03-03			
			04U IEW			S001M	001M ER-F		JS1 2021-03-0		Liquid>a	aqueous		
		Rustlers_2021-	03-03_CA		IEWFS0	04U	IEWF	S001N	ER-R	US1	2021-0	03-03	Liquid>a	aqueous
		Rustlers 2021-	03-03 AM		IEWFS0	04U	IEWE	S0010	ED D	1191	2021-0	03-03	Liquid>a	aqueous

### Time to Practice!





https://bit.ly/SampleRelationshipsActivity

# ESS-DIVE

## Time to Practice! Access the ESS-DIVE guide and template

- 1) ESS-DIVE documentation for samples https://ess-dive.gitbook.io/sample-id-and-metadata/
- 2) <u>Instructions</u> download sample metadata template
- 3) Access metadata quide
- 4) Shared vocabularies (e.g. Material)
- 5) Citation / References →







Characterize samples and collection details

### How to do it:

### **Download** and complete sample metadata template

\*Tip: use metadata guide for definitions and shared terms

Object Type:	Core Section	User Code:	IEWFS						
Sample Name	IGSN	Material	Sample description	Collection method	Collection method description	Latitude	Longitude	Location description	Field program/cruise
115	IEWF\$0001	Soil	Soil cores that were collected seasonally during autumn, winter, snowmelt, and spring at a high altitude field site which is predominately montane meadow	Manual>Hammer	Soil cores were collected using soil bulk density corer attached to a slide hammer	38.917216053	-106.9559947	Colorado The East River is a snow-dominated, headwater basin of the Upper Colorado River Basin located in the western United States.	Watershed Function SFA
116	IEWF\$0002	Soil	Soil cores that were collected seasonally during autumn, winter, snowmelt, and spring at a high altitude field site which is predominately montane meadow	Manual>Hammer	Soil cores were collected using soil bulk density corer attached to a slide hammer	38.917216053	-106.955994698	East River Watershed, Colorado The East River is a snow-dominated, headwater basin of the Upper Colorado River 3 Basin located in the	Watershed Function SFA
117	IEWFS0003	Soil	Soil cores that were collected seasonally during autumn, winter, snowmelt, and spring at a high altitude field site which is predominately montane meadow	Manual>Hammer	Soil cores were collected using soil bulk density corer attached to a slide hammer	38.917216053	-106.955994698	East River Watershed, Colorado The East River is a snow-dominated, headwater basin of the Upper Colorado River Basin located in the	Watershed Function SFA



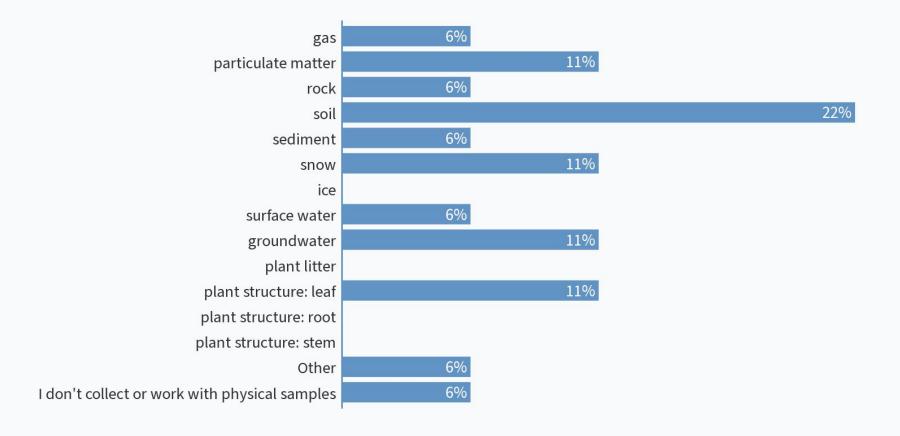
## Time to Practice!

### Characterize your sample material

Think of 1-2 of your samples types, and use the material vocabularies to characterize them. Links to shared vocabularies are listed in the guide.

### Link to material terms

### What sample type material do you most often work with?



## Step 3: Register samples for IGSNs



### How to do it:

- 1.) Choose a three character user code
  - Individual or project-specific (e.g. BWE)
    - Example IGSN: <u>IEBWE0094</u>
- 2.) Batch upload sample metadata file
- 3.) Update metadata as needed
  - Add links to related data
- 4.) Option to print labels

\*Demo Link to SESAR:

https://www.geosamples.org/







### How to do it:

- Include sample-related files: Sample metadata, location metadata, sample data
   a.) Files have sample names and IGSNs
- 2.) Include IGSNs as related identifiers
- After publication: update your SESAR IGSN sample metadata with related urls (dataset DOI, url type, url description)





## Sample Tracking Feedback - Poll Questions <a href="https://pollev.com/essdive">https://pollev.com/essdive</a>

Where is your sample data stored or published? Examples: paper only; personal files; personal or public databases; published dataset(s)

This poll question was skipped

What would other future researchers need to do to be able to compile and link the related sample data from your project?

This poll question was skipped

### Conclusions



### Sample Data Management

- Plan file organization and unique identifiers
- Standardize metadata (template)
- Register, manage, label samples IGSNs

Use IGSNs to enable tracking samples and exchanging related information:

- Over time
- Across data systems, publications, collaborators



## Questions?

Follow ESS-DIVE on Twitter! @ESSDIVE

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Contact us at <a href="mailto:ess-dive-support@lbl.gov">ess-dive-support@lbl.gov</a>