Connecting to Bridges2 OnDemand at the Pittsburgh Supercomputing Center (PSC)

Plan for Enhancing Diverse Perspectives (PEDP)

hubmap@hubmapconsortium.org

Competency

- Become proficient in using Bridges2 OnDemand for training sessions, research or both.

Objectives

- Remotely connect to the Bridges2 OnDemand at the Carnegie Mellon University – Pittsburgh Supercomputing Center.

- Define the environment to work with Jupyter notebooks.

- Transfer files between the participant's local computer and the remote supercomputer for the training sessions.

Target Audience

- This training is addressed to beginners, highly motivated wanting to learn about the Bridges2 OnDemand supercomputer to perform Human Biomolecular Atlas Program (HuBMAP) data analysis on HuBMAP public datasets.
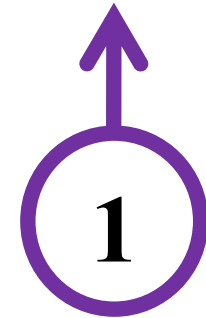
Connect to Bridges2 OnDemand [1]

Type **bridges2 ondemand** in your web browser.

bridges2 ondemand   **1**

Type bridges2 ondemand & hit the Enter key or activate the magnifier icon.

Log in to Bridges2   **2**   **Activate the Log in to Bridges2**

Navigation Logo. Logo. Log in to **Bridges2**. U wor

Pittsburgh Supercomputing Center (PSC)
https://www.psc.edu › resources › bridges-2 › user-guide   ⋮

Bridges-2 User Guide

Jan 31, 2024 — You can access **Bridges-2** through a web browser by using the **OnDemand** software. You will still need to understand **Bridges-2's** partition structure ...

XSEDE
https://software.xsede.org › bridges-open-ondemand-po...   ⋮

Bridges Open OnDemand Portal - Research Software Portal

Open **OnDemand** portal to the Pittsburgh Supercomputing Center (PSC) **Bridges2** HPC Resource. Vendor Component: Open **OnDemand**. Version: 1.6.22. Support Contact:.

People also ask   ⋮

What is the time limit for bridges2?   ⌄

6

Input your bridges2 access credentials.

Type your Username

1

lvazque2

2 **Type your Password**

3

Click in the Log in button

Log in

Activate **My Interactive Sessions.**

Bridges2 OnDemand Files▾ Jobs▾ Clusters▾ Interactive Apps▾ 🗗 My Interactive Sessions ◀━━━ **1** ❓Help▾ 👤 Logged in as lvazque2 ↦ Log Out
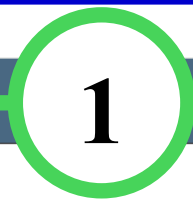
Activate the hyperlink
My Interactive
Sessions

OPEN

OnDemand

OnDemand provides an integrated, single access point f

Message of the Day

```
******************************** W A R N I N G ********************************
You have connected to vm003.bridges2.psc.edu, a virtual_machine node of Bridges 2.

This computing resource is the property of the Pittsburgh Supercomputing Center.
It is for authorized use only.  By using this system, all users acknowledge
notice of, and agree to comply with, PSC polices including the Resource Use
Policy, available at http://www.psc.edu/index.php/policies. Unauthorized or
improper use of this system may result in administrative disciplinary action,
civil charges/criminal penalties, and/or other sanctions as set forth in PSC
policies. By continuing to use this system you indicate your awareness of and
consent to these terms and conditions of use.

LOG OFF IMMEDIATELY if you do not agree to the conditions stated in this warning


******************************** W A R N I N G ********************************

For documentation on Bridges 2, please see www.psc.edu/resources/bridges-2/user-guide/
Please contact help@psc.edu with any comments/concerns
```

Activate **Jupyter Notebook.**

Bridges2 OnDemand   Files▾   Jobs▾   Clusters▾   Interactive Apps▾   🗗 My Interactive Sessions   ❓ Help▾   👤 Logged in as lvazque2   ➡ Log Out

Home / My Interactive Sessions

Interactive Apps

Servers

🗎 Jupyter Lab

🗎 Jupyter Notebook

🔵 RStudio Server

You have no active sessions.

1

Jupyter Notebook

Let's configure our **Jupyter Notebook** session.

Number of hours: 1

Number of nodes: 1

Account: hivepsc

Partition: RM-shared

Extra Slurm Args: -n 8 –meme=16000M

Launch

Interactive Apps

Servers

Jupyter Lab

Jupyter Notebook version: v1.0.1-3-g94d29b4

This app will launch one or more nodes.

Number of hours

1

Number of nodes

1

Account

hivepsc

Partition

RM-shared

For help please review the available Br...

Extra Slurm Args

-n 8 --mem=16000M

Extra Jupyter Args

☐ I would like to receive an email when the session starts

Launch

* The Jupyter Notebook session data for this session can be accessed under the data root

10

Let's connect to our Jupyter Notebook.

Bridges2 OnDemand   Files ▾   Jobs ▾   Clusters ▾   Interactive Apps ▾   🗗 My Interactive Sessions   ❓ Help ▾   👤 Logged in as lvazque2   ⮕ Log Out

Session was successfully created.   ✕

Home / My Interactive Sessions

Interactive Apps

Servers

🪐 Jupyter Lab

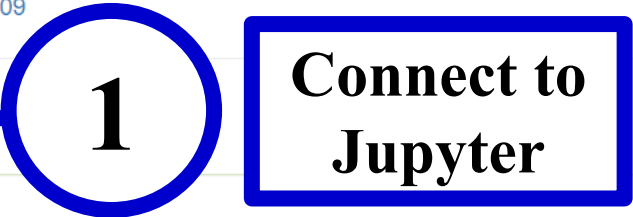🪐 Jupyter Notebook

⬢ RStudio Server

Jupyter Notebook (22784684)   1 node | 8 cores | Running

Host: ❯_r205.ib.bridges2.psc.edu   🗑 Delete

Created at: 2024-03-05 12:39:40 EST

Time Remaining: 59 minutes

Session ID: 79cdd951-99e4-407b-9d48-775cccd7ac09

👁 Connect to Jupyter   ←   **1**   **Connect to Jupyter**

powered by
OPEN OnDemand

OnDemand version: v1.8.20

Let's create a folder for each training session.

Let's rename our folder.

Rename

Let's rename our folder.

Type
hubmap_sc_rna_seq

1

2

Rename

Rules
All small caps, no spaces or special characters, and you can use the underscore to separate words.

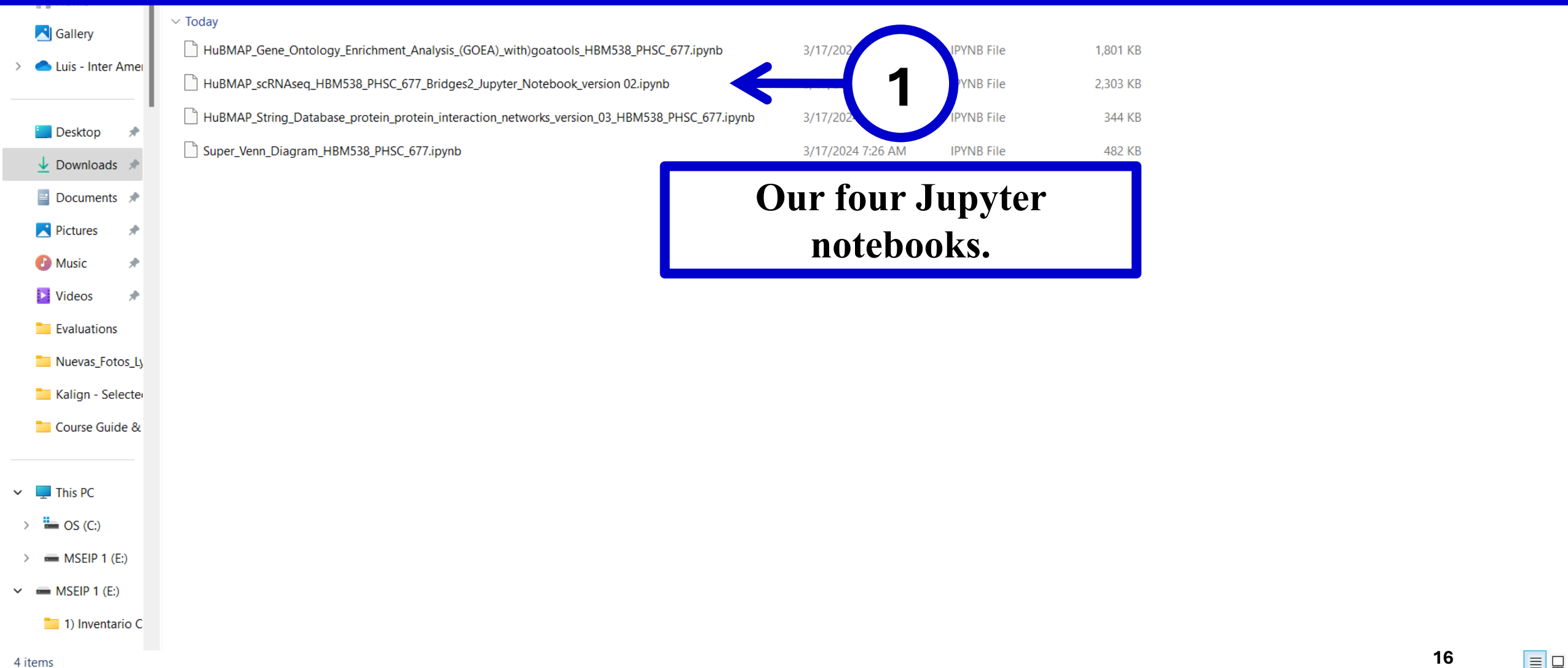# Let's create a folder for each training session.

Now let's create the following folders:
- **hubmap_venn_diagrams**
- **hubmap_string_db**
- **hubmap_goea**

Locate the Jupyter notebooks that on your computer's **Download** folder.

Gallery

Luis - Inter Amer

Desktop

Downloads

Documents

Pictures

Music

Videos

Evaluations

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Course Guide &

This PC

OS (C:)

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∨ Today

HuBMAP_Gene_Ontology_Enrichment_Analysis_(GOEA)_with)goatools_HBM538_PHSC_677.ipynb 3/17/202 IPYNB File 1,801 KB

HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Notebook_version 02.ipynb YNB File 2,303 KB

HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb 3/17/202 IPYNB File 344 KB

Super_Venn_Diagram_HBM538_PHSC_677.ipynb 3/17/2024 7:26 AM IPYNB File 482 KB

1

Our four Jupyter notebooks.

4 items

Activate the **hubmap_goea** folder to upload our Jupyter notebook.

Files   Running   Clusters

Select items to perform actions on them.

Upload | New ▾ | ↻

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☐	📁 previous		8 months ago	
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☐	📁 scRNAseq		4 months ago	
☐	📁 snATACseq		4 months ago	
☐	📁 string_db		4 months ago	
☐	📁 tmp_ondemand_ocean_hivepsc_symlink		10 months ago	

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Activate the **hubmap_goea** link with one click.

17

Upload the
HuBMAP_Gene_Ontology_Enrichment_Analysis_(GOEA)_with)goatools_HBM538_PHSC_677.ipynb
Jupyter notebook into our hubmap_goea folder.

jupyter

Quit   Logout

Files   Running   Clusters

Select items to perform actions on them.

1 → Upload   New ▾   ⟳

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Upload

The notebook list is empty.

Upload the
HuBMAP_Gene_Ontology_Enrichment_Analysis_(GOEA)_with)goatools_HBM538_PHSC_677.ipynb
Jupyter notebook into our hubmap_goea folder.

Organize ▾   New folder

- 🏠 Home
- 🖼️ Gallery
- ☁️ Luis - Inter Amer

- 🖥️ Desktop 📌
- ⬇️ Downloads 📌
- 📄 Documents 📌

Name	Date modified	Type	Size
⌄ Today			
Super_Venn_Diagram_HBM538_PHSC_677.ipynb	3/17/2024 7:26 AM	IPYNB File	482 KB
HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb	3/17/2024 7:26 AM	IPYNB File	344 KB
HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Notebook_version 02.ipynb	3/17/2024 7:26 AM	IPYNB File	2,303 KB
HuBMAP_Gene_Ontology_Enrichment_Analysis_(GOEA)_with)goatools_HBM538_PHSC_677.ipynb	3/17/2024 7:25 AM	IPYNB File	1,801 KB

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HuBMAP_Gene_Ontology_Enrichment_Analysis_(GOEA)_with)goatools_HBM538_PHSC_677.ipynb
Jupyter notebook.

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Open   **19**   Cancel
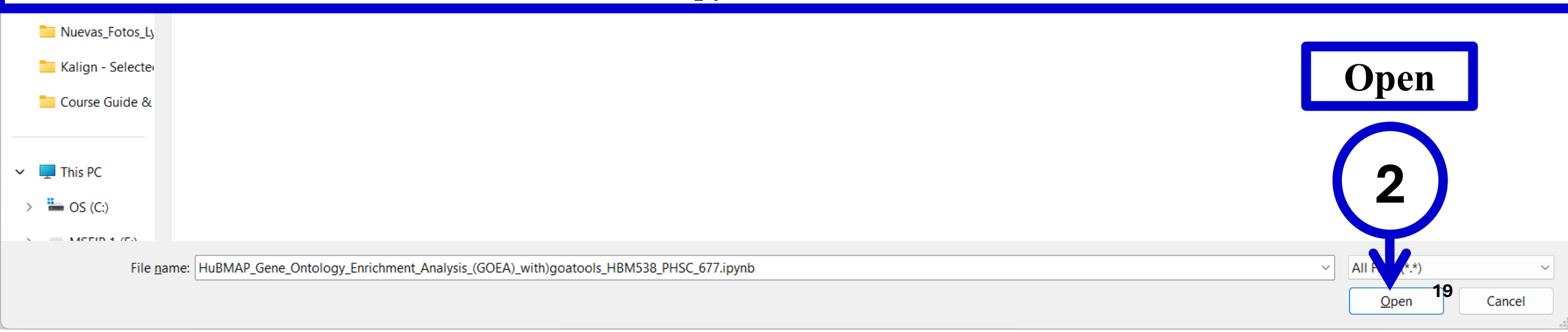
Upload the
HuBMAP_Gene_Ontology_Enrichment_Analysis_(GOEA)_with)goatools_HBM538_PHSC_677.ipynb
Jupyter notebook into our hubmap_goea folder.

Upload

Let's exit from our **hubmap_goea** folder.

Activate the **hubmap_sc_rna_seq** folder to upload our Jupyter notebook.

Files   Running   Clusters

Select items to perform actions on them.

Upload   New ▾   ⟳

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☐	📁 gene_ontology_enrichment_analysis			4 months ago	
☐	📁 hubmap_goea			seconds ago	
☐	📁 hubmap_sc_rna_seq			12 days ago	
☐	📁 hubmap_string_db			seconds ago	
☐	📁 hubmap_venn_diagrams			a minute ago	
☐	📁 ondemand			10 months ago	
☐	📁 previous			8 months ago	
☐	📁 scanpy_results			4 months ago	
☐	📁 scRNAseq			4 months ago	
☐	📁 snATACseq			4 months ago	
☐	📁 string_db			4 months ago	
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1 ← Activate the **hubmap_sc_rna_seq** link with one click.

Upload the HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Notebook_version 02.ipynb Jupyter notebook into our hubmap_sc_rna_seq folder.

Upload the HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Notebook_version 02.ipynb Jupyter notebook into our hubmap_sc_rna_seq folder.

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Jupyter

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Files   Running   Clusters

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**Upload the HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Notebook_version 02.ipynb
Jupyter notebook into our hubmap_sc_rna_seq folder.**

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1   ☐   ➔   ■ / **hubmap_sc_rna_seq**   Name ↓   Last Modified   File size
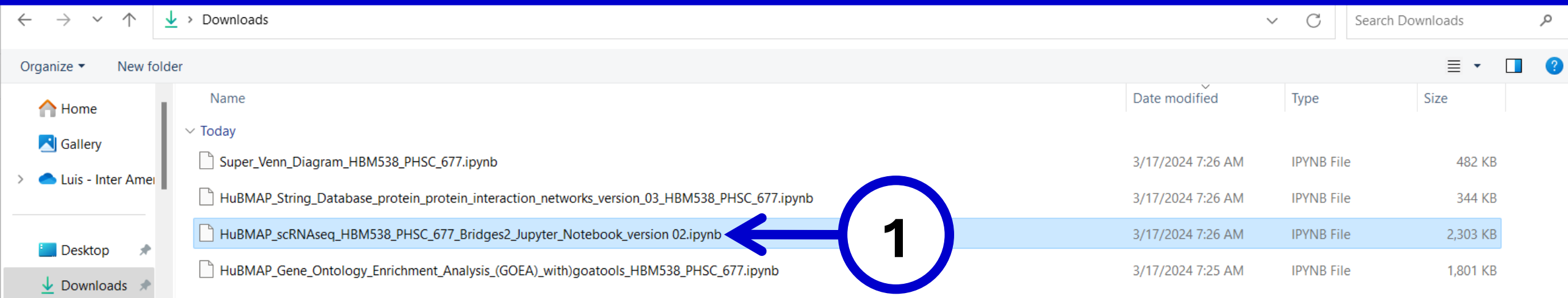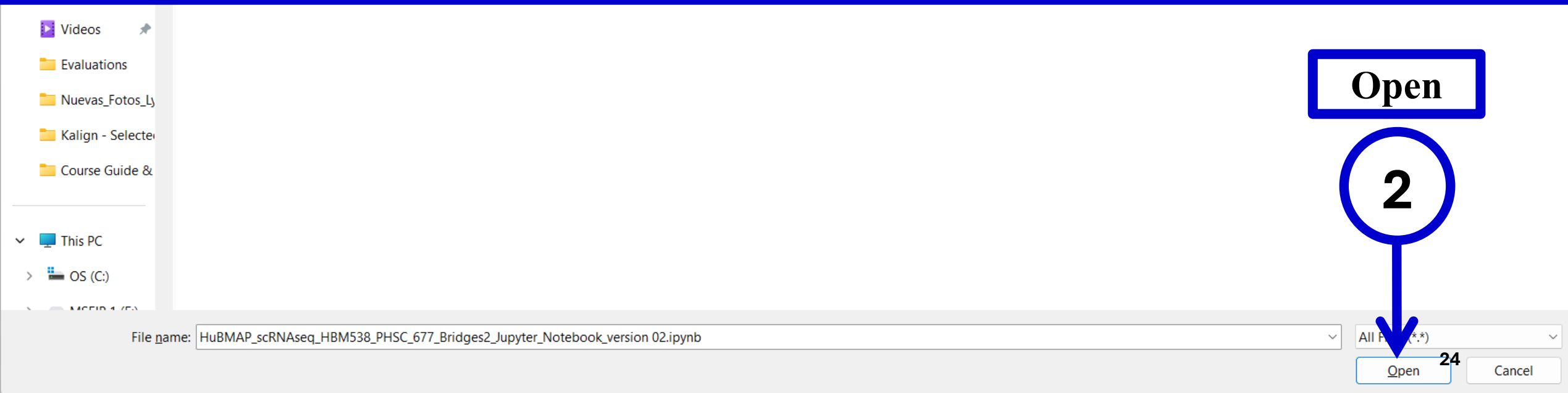
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**Click over
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folder.**

Activate the hubmap_string_db folder to upload our Jupyter notebook.

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☐ 📁 hubmap_string_db			seconds ago	
☐ 📁 hubmap_venn_diagrams			a minute ago	
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☐ 📁 snATACseq			4 months ago	
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Activate the hubmap_string_db link with one click.

Upload the
HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb
Jupyter notebook into our hubmap_string_db folder.

jupyter

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Files   Running   Clusters

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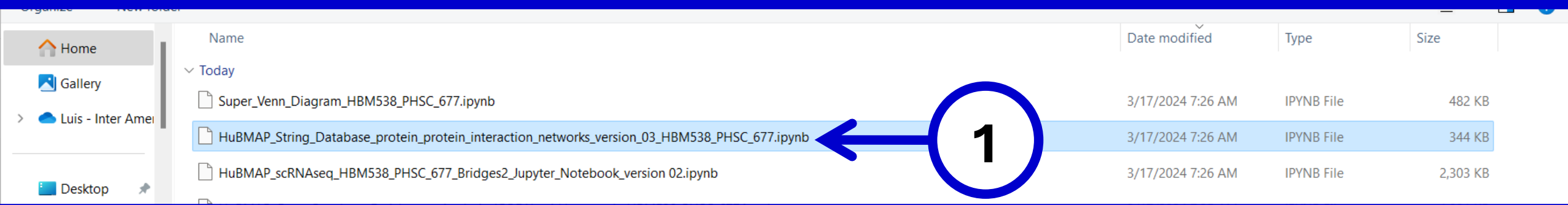
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HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb
Jupyter notebook into our hubmap_string_db folder.

Name	Date modified	Type	Size
⌄ Today			
🗎 Super_Venn_Diagram_HBM538_PHSC_677.ipynb	3/17/2024 7:26 AM	IPYNB File	482 KB
🗎 HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb	3/17/2024 7:26 AM	IPYNB File	344 KB
🗎 HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Notebook_version 02.ipynb	3/17/2024 7:26 AM	IPYNB File	2,303 KB

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Select the
HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb
Jupyter notebook.

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File name: HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb | All F... (*.*)
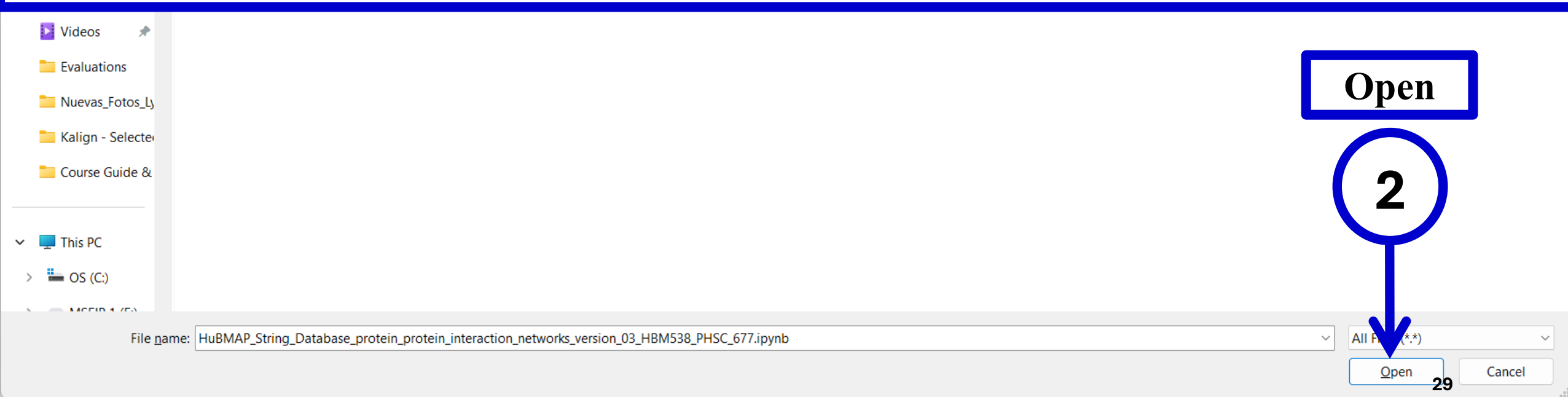
Open | Cancel

Upload the
HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb
Jupyter notebook into our hubmap_string_db folder.

Files   Running   Clusters

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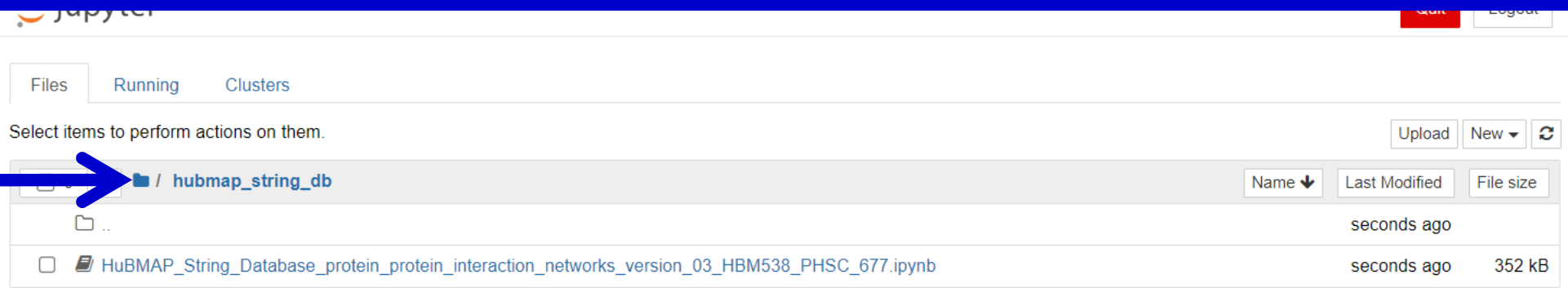▤ HuBMAP_String_Database_protein_pr   **1**   ➡   Upload   Cancel

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Upload the
HuBMAP_String_Database_protein_protein_interaction_networks_version_03_HBM538_PHSC_677.ipynb
Jupyter notebook into our hubmap_string_db folder.

Files   Running   Clusters

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Click over the folder icon to exit from the hubmap_string_db folder.

Activate the **hubmap_venn_diagrams** folder to upload our Jupyter notebook.

Files   Running   Clusters

Select items to perform actions on them.   Upload   New ▾   ⟳

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☐	📁 data		8 months ago	
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☐	📁 ondemand		10 months ago	
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1 ← Activate the **hubmap_venn_diagrams** link with one click.

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Organize ▾   New folder

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📄 Super_Venn_Diagram_HBM538_PHSC_677.ipynb ← **1**	3/17/2024 7:26 AM	IPYNB File	482 KB
📄 HuBMAP_String_Database_protein_protein_interaction_networks_versi...PHSC_677.ipynb	3/17/2024 7:26 AM	IPYNB File	344 KB

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Downloads

📄 Documents 📌

🖼 Pictures 📌

🎵 Music 📌

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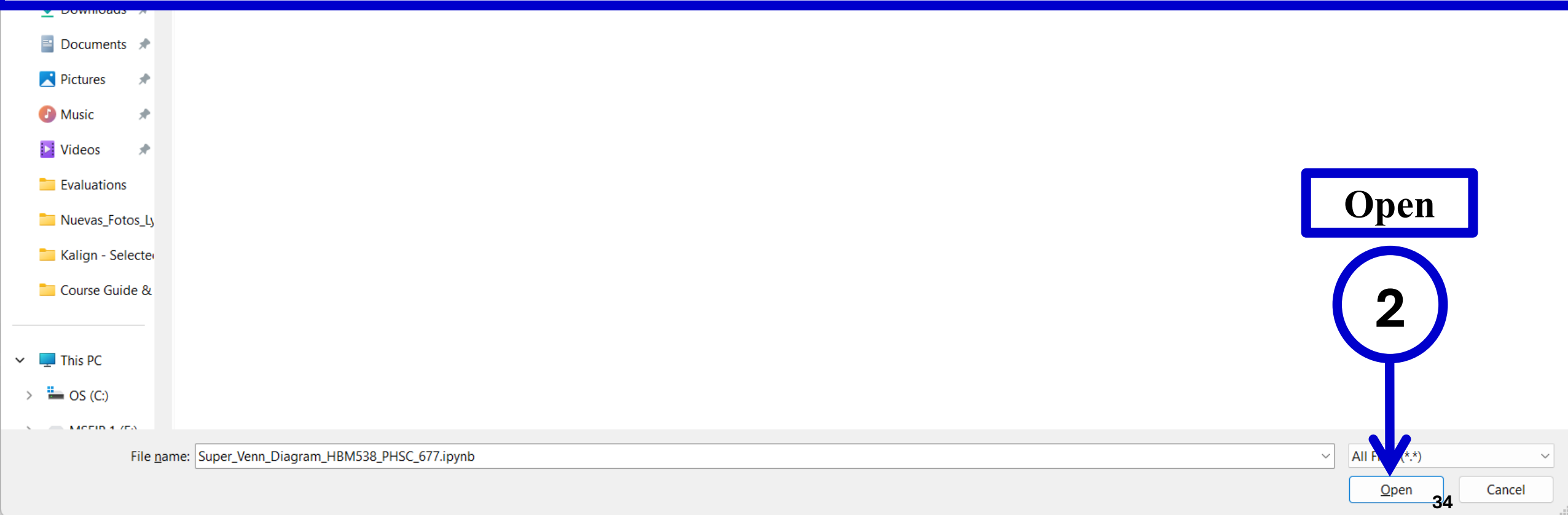**Upload the Super_Venn_Diagram_HBM538_PHSC_677.ipynb Jupyter notebook into our hubmap_venn_diagrams folder.**

Upload the Super_Venn_Diagram_HBM538_PHSC_677.ipynb Jupyter notebook into our hubmap_venn_diagrams folder.

![Jupyter logo] Jupyter

Quit   Logout

Files   Running   Clusters

Select items to perform actions on them.

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1 ➡ 📁 / **hubmap_venn_diagrams**

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Click over the folder icon to exit from the hubmap_venn_diagrams folder.

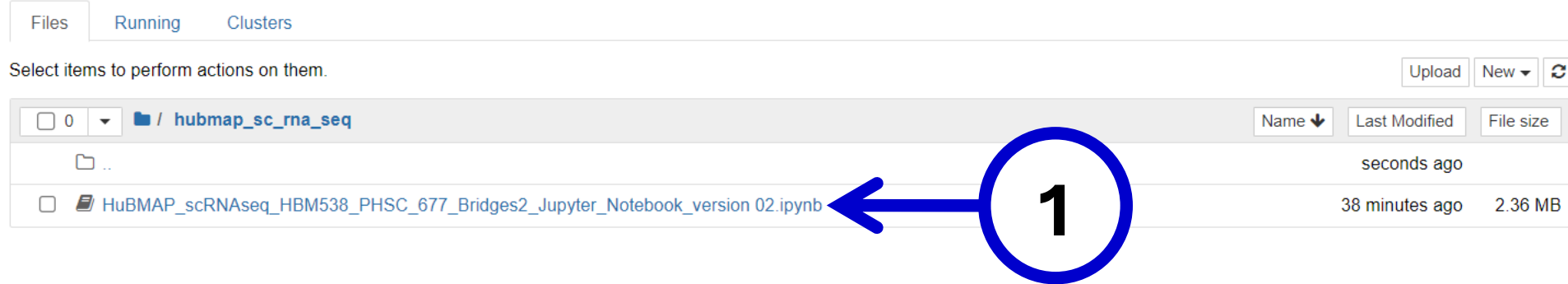# Now we are ready to start with the hubmap_sc_rna_seq data analysis.

Files   Running   Clusters

Select items to perform actions on them.   Upload   New ▾   ↻

☐ 0 ▾	▮ /	Name ↓	Last Modified	File size
☐	📁 data		8 months ago	
☐	📁 gene_ontology_enrichment_analysis		4 months ago	
☐	📁 hubmap_goea		seconds ago	
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Activate the hubmap_venn_diagrams link with one click.

37

Now we are ready to start with the hubmap_sc_rna_seq data analysis.

Activate the Jupyter notebook HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Notebook_version 02.ipynb link with one click.

jupyter HuBMAP_scRNAseq_HBM538_PHSC_677_Bridges2_Jupyter_Noteb... Last Checkpoint: 28 minutes ago (autosaved)   Logout

| File | Edit | View | Insert | Cell | Kernel | Widgets | Help | Trusted | Python 3 (ipykernel) ○

▶ Run ■ C ▶▶   Markdown ▾

Title: Introduction to Single-Cell RNA-Seq (scRNA-seq) Data Analysis

Competency

- Become proficient in single cell RNA-seq data analysis from HuBMAP.

Objectives

- Import HuBMAP preprocessed data into an anndata object with the Python library scanpy.

- Filter cell outliers based on the number of genes expressed for raw data.

- Normalize and log transform raw data.

- Generate clusters and visualize via UMAP dimensional reduction.

- Find cluster-specific marker genes with scanpy.

Install the required Python libraries to conduct the scRNA-seq analysis.

```
In [1]: #####################################################################
        # Install the required Python libraries to conduct the scRNA-seq analysis. #
        #####################################################################
```