PhUSE CSS

Linked Data for Clinical Trials

An Interactive Hands-on Workshop

EXERCISES

Version 3.0

04 March 2018

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# Introduction

Instructions in this document are specific to the PhUSE cloud server environment, Graph Editor application and workshop methods. The exercises represent one of many possible approaches to the material and make no claim to be best or recommended method. The instructor will complete the exercises during the session, along with the attendees.

Your feedback is welcomed and encouraged. Please send your comments to: **tim.williams@PhUSE.eu**

**Materials**

* Laptop with Remote Desktop capability
* Printed copies of the following will be supplied by the instructor:
  + Exercises (this document)
  + Info Sheet
  + Graph Editor Reference

**Symbols**

|  |  |
| --- | --- |
|  | Stop and wait. Do not proceed to the next section until instructed. |
| **!** | Cautions and warnings. Failure to follow these steps may lead to unanticipated results and problems. |
|  | The instructor presents important material at this point. |
| IdeaIcon_clean_20mm | Helpful tips and advice. |
| Image result for information icon | Additional information. |

# Server Login

Login to the cloud server using Remote Desktop. Instructions assume Windows 10 operating system.

1. In the search box on the taskbar on your laptop, type **remote desk,** then select **Remote Desktop Connection** from the Programs section.﻿
2. Click **Show Options** if needed to show the fields for **Computer:** and **User name:**

The instructor will provide the password and an IP Address for the Computer: field.

**Computer:** \_\_\_\_\_\_\_\_\_\_\_\_\_\_

(See Info Sheet)

**User name:** phuseldw

**Password:** \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

(Provided by Instructor)

1. Entering values in the **Computer:** and **User name:** fields, then click **Connect**.
2. When prompted, enter the password supplied by the instructor and click **OK**.

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation follows |  |

# Exercises

# Create a Study Graph

The PhUSE Cloud Server environment is used for all exercises.

# Open the Graph Editor

1. Open Google Chrome.
2. Click on "GraphEditor" on the shortcuts bar. 
3. The Graph Editor opens and shows two IRI nodes: One for **Drug1** and one for the drug's name, **Serum114.**



Ask for assistance if you do not see these nodes.

|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | If the Graph Editor does not load, click Cancel "x" and reload the page. Ask for assistance if the graph editor still fails to load. |

# Add a Study, Study Phase, and Treatment Arms

|  |  |
| --- | --- |
| **!** | Refer to the **Info Sheet** handout when instructions contain references to <Info Sheet:> . The sheet contains values unique to your graph. |

1. Create a **Study** node using the label value from your **Info Sheet**.

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | *<Info Sheet: Study>* | Image result for information icon*See Info Sheet for value* |

1. Create link ***from*** **Drug1** ***to*** the **Study** node:

Link values:

|  |  |
| --- | --- |
| **Prefix:** | ncit |
| **Label:** | study |

1. Create a Study **Phase** node. You may choose any of these phases: **Phase2**, **Phase3**, **Phase4.**

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | ncit |  |
| **Type:** | IRI |  |
| **Label:** | *<Input a value: Phase2 or Phase3 or Phase4, etc.>* | Image result for information icon*You choose a value for phase:* **Phase2, Phase3, Phase4**  *NO SPACE in the name!* |

1. Link ***from*** the **Study** ***to*** the Study **Phase**.

Link values:

|  |  |
| --- | --- |
| **Prefix:** | ncit |
| **Label:** | phase |

1. Create two Treatment Arm nodes for the **Study** using values from your **Info Sheet**.

Node values:

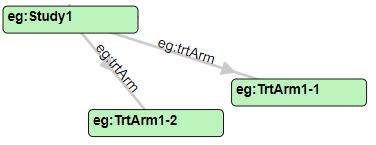
|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | *<Info Sheet: Treat Arm One>* | Image result for information icon*See Info Sheet for value.* |

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | *<Info Sheet: Treat Arm Two>* | Image result for information icon*See Info Sheet for value.* |

Ensure you have two Treatment Arm (**TrtArm***n-n*) nodes in your graph.

1. Link ***from*** the **Study** ***to*** each of the two Treatment Arm nodes. The relations have identical values.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | trtArm | Image result for information icon*Note lowercase 't' for relation label* |

There should now be one ***eg:trtArm*** link to each of the Treatment Arm nodes.

1. Create two Treatment Type nodes to represent **PlaceboArm** and **ActiveArm** treatments

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | PlaceboArm |  |

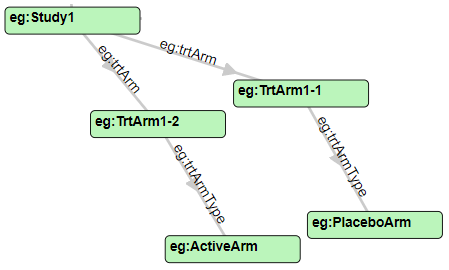
Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | ActiveArm |  |

1. Now join each Treatment Arm node (created in **Step 5**) to one of the Treatment Type nodes. It does not matter which is linked to the **PlaceboArm** or the **ActiveArm**. You will create two links, each with the same label:

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | trtArmType | Image result for information icon*Note lowercase 't' at start of label.* |



The Study and Treatment Arm portion of your graph should look similar to:

|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | Click  to create a copy in case anything goes wrong in the next steps. |

|  |  |
| --- | --- |
| Image result for information icon | In these steps you defined two Treatment Arms that are unique to your study, then assigned those arms to one of two Treatment Arm Types: PlaceboArm, ActiveArm. These "type of arm" nodes are identical across the studies in the workshop and allow identification of "all persons who received active treatment." In a real application, the Treatment Arm would be further extended to include dosage and administration information unique to that study. This graph would be too complex for the workshop. |

# Add Persons and Treatments

1. Add two **Person** nodes using values from your **Info Sheet**.

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | *<Info Sheet: Person One>* | Image result for information icon*See Info Sheet for values.* |

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | *<Info Sheet: Person Two>* | Image result for information icon*See Info Sheet for values.* |

1. Create ***participatesIn*** relations ***from*** each of the two Person nodes ***to*** the Study node.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | participatesIn | Image result for information icon*Note uppercase "I" .* |

1. Create a link ***from*** one of the Person nodes ***to*** one of the Treatment Arm (trtArm*n-n*) nodes using the ***randomizedTo*** relation.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | randomizedTo | Image result for information icon*Note uppercase "T" .* |

1. Create a link ***from*** the second Person node ***to*** the other Treatment Arm (trtArm*n-n*) node using the ***randomizedTo*** relation.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | randomizedTo | Image result for information icon *Note uppercase "T" .* |

Now the two Persons with ***participatesIn*** relations to the **Study** are also ***randomizedTo*** Treatment Arms.

# Add Demographics

1. Create a node for **Male** and a node for **Female .** Note that both use the **ncit** prefix.

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | ncit |  |
| **Type:** | IRI |  |
| **Label:** | Male |  |

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | ncit |  |
| **Type:** | IRI |  |
| **Label:** | Female |  |

1. Create links ***from***the two Person nodes ***to*** a Gender node using the ***gender*** relation. This relation also uses the ncit prefix.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | ncit |  |
| **Label:** | gender | Image result for information icon*Label is all lowercase.* |

1. Create one **Given Name** (First name) for each **Person** node in the graph. Note that these have Type: STRING because they are string literals.

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | *NOT APPLICABLE* | Image result for information iconPrefix is not applicable to literals. You may ignore this field. |
| **Type:** | STRING |  |
| **Label:** | *<Any name you want>* |  |

1. Link ***from*** each **Person** node ***to*** their **Given Name** using the ***givenName*** relation. Note the use of the schema prefix.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | schema |  |
| **Label:** | givenName |  |

1. Create **Age** nodes for each Person as INT (integer) literals:

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | *NOT APPLICABLE* | Image result for information iconPrefix is not applicable to literals. |
| **Type:** | INT |  |
| **Label:** | *<Any integer age value you want>* |  |

1. Link ***from***a Person ***to*** an age using the ***age*** relation.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg | Image result for information icon The eg: prefix is used because age calculation may be specific to this graph. |
| **Label:** | age |  |

# Add another Person

1. Add another **Person** node to the graph:

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Type:** | IRI |  |
| **Label:** | *<Info Sheet: Person Three>* | Image result for information icon*See Info Sheet for values.* |

***This node will represent you and your role in this study!***

1. Create a new node for your **Given Name** as a string literal.

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | NOT APPLICABLE | Image result for information iconPrefix is not applicable to literals. You may ignore this field. |
| **Type:** | STRING |  |
| **Label:** | *<Your given (first) name>* |  |

1. Link ***from*** your new **Person** node ***to*** your **Given Name** using the ***givenName*** relation. Remember to use the **schema** prefix.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | schema |  |
| **Label:** | givenName |  |

1. Create a ***gender*** link ***from*** your Person node ***to*** your gender.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | ncit |  |
| **Label:** | gender | Image result for information icon*Label is all lowercase.* |

*The polite instructor will not ask you to create an age node and link. :)*

1. Your role in this study is Linked Data Expert. Create the ***LDExpert*** relation ***from*** your **Person** node ***to*** the **Study** node.

Link values:

|  |  |  |  |
| --- | --- | --- | --- |
| **Prefix:** | | eg |  |
| **Label:** | | LDExpert |  |
| IdeaIcon_clean_20mm | | Congratulate yourself for becoming a Linked Data Expert, then Click  to save a copy of your graph. | | | |

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  As for the instructor or assistant to review your graph prior to taking the next steps. This will help prevent errors in later steps. |  |

# Export to TTL

1. Click on  to export the graph to TTL format.
2. The graph will be saved to your downloads folder as **WhiteBoardTriples.TTL :**

**C:\Users\phuseldw\downloads\WhiteBoardTriples.TTL**

|  |  |
| --- | --- |
| **!** | Leave the graph open in Chrome. You will refer to it in the next section when creating queries. Ask for assistance if you accidentally close or refresh the Graph Editor window. |
| Image result for information icon | If you click Create TTL more than once, you will create new files that include a number in their name:  WhiteBoardTriples(1).TTL  WhiteBoardTriples(2).TTL  etc.  Make sure to use the highest numbered file in the next steps. |

1. Use Windows explorer to navigate to the TTL file.
2. Double click on the .TTL file to open it.
3. Follow along with the instructor's explanation of the TTL file content.
4. Find the various ***nodes*** and ***links*** you created in your graph.

# Validate the Data

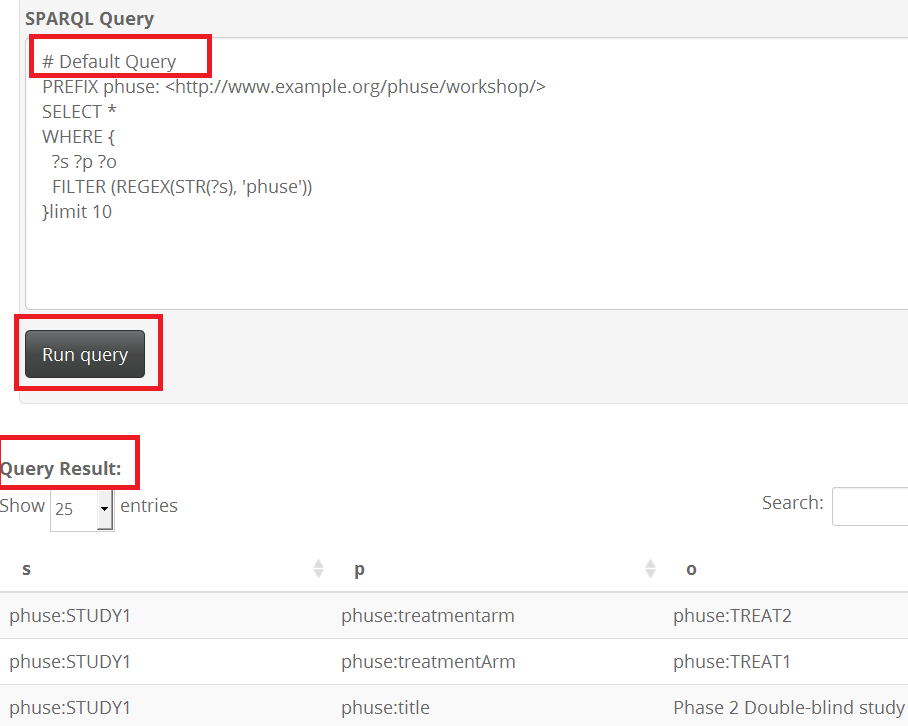
1. Double-click on this file to open it into RStudio:

..../scripts/R/**TTLValidation.R**

1. Run the code by clicking the Run App icon 
2. Load your TTL file in the application by clicking **Browse...** under **.TTL File** and navigate to the file C:\LinkedDataWorkshop\data\**RDFModel.TTL** . Double-click the file to load it into the app.

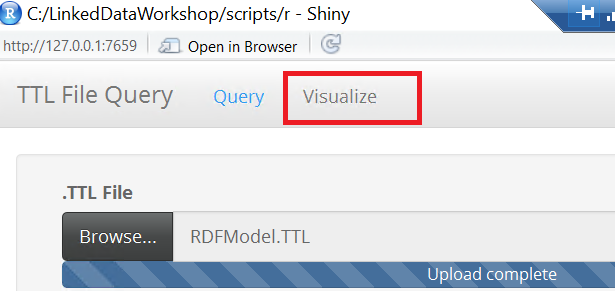
|  |  |
| --- | --- |
| **!** | Remember to load the most recent version of your TTL file, which may have a number in the name : WhiteBoardTriples(1).TTL, WhiteBoardTriples(2).TTL , etc. If in doubt, ask for assistance. |

1. A default query is already available within the app. Click **Run query** to execute the query and view the result in the **Query Result:** area.



1. Review the Subject, Predicate, Object values in the **Query Result** and compare them to your graph.
2. Click on the  tab and review the results for the Nodes and Relations checks. Both should read "All QC checks passed." If not:
   1. Review the values listed and compare them to your graph. Do the values or their prefixes need to change to match the values given in the exercises?
   2. If the problem is not obvious, ask for assistance.

|  |  |
| --- | --- |
| **!** | Do not proceed past this step if both results do not show "All QC checks passed" , unless advised to proceed by the instructor. Failure to validate at this step may cause errors in later exercises. |

1. Click on the **Visualize** tab at the top of the app to view a network graph of the query result.
2. Use your mouse or touchpad to pan and zoom the graph.
3. Explore your graph by clicking on nodes. Mouse-over the links to show the relationship labels. You may also use the drop-down selections for highlighting node categories and groups.

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor. |  |

# Upload to Database

1. Open a new window in Google Chrome, **keeping your graph editor window open.**
2. Click the **Stardog** shortcut on the bookmarks bar.
3. If you are prompted for a username and password:
   1. On the login screen, enter the Username: **phuseldw**
   2. You can leave the Password field blank. Click **Sign in**.
4. In the Stardog application window, click **Databases** on the top menu.
5. Under Databases, double-click the row for **LDWStudy.**
6. In the upper left, click 



1. Select **Data | Add** from the Stardog menu:
2. Click **Browse** and navigate to, then select your WhiteBoard.TTL file:

C:\Users\phuseldw\Downloads\**WhiteBoardTriples.TTL**

1. Click **Upload**.
2. You should see the message: ***Success! Data added successfully.***

# Query Graph Data

Update the query scripts by following these steps:

1. Using Windows Explorer, right click on the folder C:\\_github\LinkedDataWorkshop
2. Select **Git Sync** from the menu.



1. Click **Pull**
2. Click **Close** when the command completes. You have updated all content to the latest version as needed for the following exercises.

# Show all triples

Return to the Stardog menu in Chrome.

Find all Subject-Predicate-Object relations in your graph.

1. If the "Query Panel" is not displayed, click on the >\_Query menu item at the top of the Stardog display.
2. Select the Open Folder icon  in the Query Panel.
3. Navigate to the file C:\\_gitHub\LinkedDataWorkshop\CSS2018\scripts\SPARQL**\210-AllTriples.rq** and double-click on it to load it into the query window.
4. With the query loaded in to the window, click the  button. Scroll down to review the results.
5. Compare this view to what you expected after viewing the TTL file.

# How many people *participateIn* the study?

Find the number persons participating in your study by counting the number of ***participatesIn***relationships.

1. Load the SPARQL query **220-CountParticipants.rq**.
2. Examine the query while the instructor explains how it relates to your graph.
3. Execute the query.
4. Is this this result you expected?
5. Note how the ***LDExpert*** is not included in the count.

# Find the names of people who participate in the study.

In this example you want to select the **givenName** of the Persons who participate in the study. Refer back to the your graph in the Graph Editor while creating the query.

Try modifying the query from **Exercise 2.2** using the next steps as a guide. If you are new to SPARQL you can skip down to the SOLUTION at the end of this section.

1. Return the person's name (givenName) in the SELECT statement:

SELECT ?person\_name

1. In the WHERE statement, identify Person nodes that have the ***participatesIn*** relation:

?person eg:participatesIn ?study ;

1. Then follow from that same Person node using the ***givenName*** relation to find their name.

?person eg:participatesIn ?study ;

schema:givenName ?person\_name .

1. Execute your query and view the results. If you have trouble writing the query, load and execute the SOLUTION file:

SOLUTION: **230-NameParticipants.rq**

# List the names of the people randomized to each treatment type.

1. Modify the SELECT statement from **Exercise 2.3** to select treatment type in addition to person name variables.

SELECT ?trt\_type ?person\_name

1. Change the relation in the first line of the WHERE statement to use the ***eg:randomizedTo*** relation, as follows:

?person eg:randomizedTo ?trt\_arm ;

schema:givenName ?person\_name .

1. Refer to your graph in the Graph editor. You want to follow the path from **?trt\_arm** along the **eg:trtArmType** relation to the type of treatment ( **?trt\_type** ) .

?person eg:randomizedTo ?trt\_arm ;

schema:givenName ?person\_name .

?trt\_arm eg:trtArmType ?trt\_type .

1. You may wish to add an ORDER BY statement after the WHERE :

ORDER BY ?trt\_type ?person\_name

SOLUTION: **240-NamesInTreatmentType.rq**

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation on Ontologies and Reasoning |  |

# Ontology and Inference

In this section you will add an ontology to the data and employ a reasoner on your data.

# Review the Ontology

1. Double-click on the file C:\\_gitHub\LinkedDataWorkshop\CSS2018\data\**StudyOntology.TTL** to open into a text editor.
2. Follow along with the instructor's explanation of the file.

# Add the Ontology to the LDWStudy database

1. Select **Data | Add** from the Stardog menu.
2. Click **Browse** and select the file:

C:\\_gitHub\LinkedDataWorkshop\CSS2018\**data\StudyOntology.TTL**

1. Click **Upload**.
2. You should see the message: **Success! Data added successfully.**

# Explore the data

1. Ensure reasoning is turned **OFF**.
2. Select **Explore | Class Hierarchy**
3. A SPARQL query appears in the window.
4. **Execute** the query and view the results.
5. Note the **types** and **supertypes** added to your data.



1. Turn on the reasoner by clicking the **Reasoning** button.
2. **Execute** the query again and view the results.
3. Scroll through the results to find where **HumanStudySubject** and **LinkedDataExpert** both types of **Person**. These are not part of your original study data but can now be used in queries to find these "types of things!"

# Find the names of HumanStudySubjects in your study.

*Remember: Your original data contained no definition of a HumanStudySubject.*

1. Review the ontology file for how a HumanStudySubject is *inferred* using the ontology.

|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | In SPARQL the predicate **rdf:type** can be shorted to **a** and interpreted as "*is a*".  Example:  You read: eg:Person11 rdf:type eg:HumanStudySubject  as: "Person11 ***is a*** HumanStudySubject." |

Instead of querying on the **participatesIn** predicate, as in:

?person eg:participatesIn ?study ;

You can now query using the *inferred* entity **eg:HumanStudySubject**.

?person a eg:HumanStudySubject;

1. Open the query file **230-NameParticipants.rq** that you used in **Exercise 2.3** and modify the queryto find ?person "is a" Human Study Subject.
2. Ensure Reasoning is turned on, then execute the query.
3. Refer back to your graph in the Graph Editor and be amazed : there is no "Human Study Subject" defined in your graph.
4. What happens if you turn OFF the reasoner and execute the query? Don't forgot to turn the reasoner back ON!

SOLUTION: **340-NameHumanStudySubject.rq**

Bonus Question: How would you modify the query to select all Data Experts associated with the study?

Hint: What is the superclass of LinkedDataExpert?

SOLUTION: **341-NameDataExperts.rq**

# Write a reasoner-based query to find all types (classes) of People associated with the study (not just participants)

1. Write a query that uses the superclass of the HumanStudySubject and DataExpert classes.

CAUTION: The superclass prefix is not "eg" because the class you will use is not defined in the study ontology!

1. Return the following results: Person IRI, Given Name of the Person, and the Person Type

HINT: Use the "is a" relation: ?person a ?person\_type

SOLUTION: **350-NamesAllPeople.rq**

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation on Merging Data |  |

# Merge Studies

# Create the Data Pool

1. Click on Admin Console at the top of the Stardog application. 



1. Click on **Drug1Pool** in the Databases panel.
2. In the upper right, click 
3. Open the query **410-PoolAllStudies.rq** into the query window an execute it. A blue progress line will display briefly at the top of the application while the query is executing.

|  |  |
| --- | --- |
| **!** | Having all attendees create the pool may cause bandwidth and connection issues. This happens, follow the alternative instructions provided by the instructor using the query:  **411-AltPoolCreator.rq**. DO NOT run this query unless advised by the instructor! |

1. After the query has completed, execute the query **415-PoolTripleCount.rq**. Note the number of triples and compare them to the number provided by the instructor to ensure you have the correct data.

# List Drug1 studies by phase.

1. Load the query **420-StudiesByPhase.rq** .
2. Execute the query and locate your study in the results.

BONUS Question: How would you alter the query to obtain the number of studies in each phase?

Hint: a) In the **SELECT** statement: **?phase** (**COUNT**(**?phase**) **AS** **?count**)

b) Use a **GROUP BY** after the **WHERE**.

SOLUTION: **425-StudyCountByPhase.rq**

# How many HumanStudySubjects participated in all Drug1 studies?

1. Ensure the Reasoner is turned On.
2. Load the query **430-Drug1CountHSS.rq** and examine the query.
3. Execute the query.

|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | If the count is 0, you may need to turn ON the Reasoner. |

BONUS Question : Alter the query to count **all people** involved in Drug1 Studies (not just HumanStudySubjects).

HINT: a) What is the superclass of HumanStudySubject?

b) Ensure you are suing the correct prefix!

SOLUTION: **435-Drug1CountPeople.rq**

# How many women received active treatment (non placebo) across all Drug1 studies combined?

1. Use the graph of your study in the Graph Editor to determine the paths that need to be followed to obtain the solution.

HINT : follow the pattern: ?person -- gender -- **Female** ;

-- randomizedTo --- ?trt\_arm .

?trt\_arm -- treatmentArmType -- **ActiveArm**.

SOLUTION: **440-Drug1WomenActiveTreat.rq**

# List all Persons in the studies.

1. List all Person IRIs, their givenName, their assigned Study, and their role in that study (HumanStudySubject or Investigator).

*It is getting late so you may wish to skip directly to the Solution to see one way of solving this question.*

1. Review the results. Do you find anything surprising in the pooled results?

SOLUTION: **450-Drug1PersonsAllStudies.rq**

Congratulations! You've made to the

---- END OF THE EXERCISES ----

Before you leave, please Sign out from the server using **Windows | Person Icon | Sign out**.



|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation follows |  |

# Appendix 1: Course Resources

* [Introduction to Semantic Web](https://www-stage.cambridgesemantics.com/semantic-university/introduction-semantic-web)

https://www-stage.cambridgesemantics.com/semantic-university/introduction-semantic-web

* [What is Linked Data?](https://www-stage.cambridgesemantics.com/semantic-university/what-linked-data)

https://www-stage.cambridgesemantics.com/semantic-university/what-linked-data

* [Introduction to Linked data](https://www-stage.cambridgesemantics.com/semantic-university/introduction-linked-data)

https://www-stage.cambridgesemantics.com/semantic-university/introduction-linked-data

* [SPARQL in 11 minutes](https://www.youtube.com/watch?v=FvGndkpa4K0)

https://www.youtube.com/watch?v=FvGndkpa4K0

* [Learning SPARQL](http://www.learningsparql.com/)

http://www.learningsparql.com/

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[Hands-on Workshop Github Repository](https://github.com/phuse-org/LinkedDataWorkshop/tree/master/CSS2018)

Course content is available at:

https://github.com/phuse-org/LinkedDataWorkshop/tree/master/CSS2018