

Supplemental File 1:

SPARQL scripts developed for the ODNAE analyses used in the ODNAE manuscript:

Note: Six sets of SPARQL scripts (20 individual scripts in total) were generated for the ODNAE study. All the four sets of SPARQL scripts were stored in the ODNAE Github folder:

<https://github.com/odnae/odnae/tree/master/docs/SPARQL>

The contents of these six sets of 20 SPARQL scripts are provided below:

The content of SPARQL File 1:

Title: **query_G_protein_linked_receptor_interaction_drugs**

Script:

- **1.1.** SPARQL query for searching the ODNAE drugs annotated with G-Protein-linked Receptor Interactions [MoA] (N0000000152) and its subclasses.

The content of SPARQL File 2:

Title: **query_agonists_antagonists**

- **2.1.** drugs link to agonist
- **2.2.** The agonist that links to ODNAE drugs
- **2.3.** drugs and agonist pair:
- **2.4.** drugs link to antagonist
- **2.5.** The antagonist that links to ODNAE drugs
- **2.6.** Antagonist and drugs pair
- **2.7.** drug link to both a kind of agonist and antagonist
- **2.8.** query drugs that have a specific role, e.g., Serotonin Agonists [MoA]. (used for Fig. 6)

The content of SPARQL File 3:

Title: **query_all_drug_with_MoAs**

- **3.1.** SPARQL query for searching all ODNAE drugs link to MoAs : subclassOf http://purl.obolibrary.org/obo/ODNAE_0000002 (role in cellular and molecular interactions)

The content of SPARQL File 4:

Title: **query_neurotransmitters_interaction_drugs**

- **4.1.** SPARQL query for searching the ODNAE drugs annotated with Neurotransmitter Transporter Interactions [MoA] (N0000000105) and its subclasses.
- **4.2.** # SPARQL query for searching the ODNAE drugs annotated with Dopamine Transporter Interactions [MoA] (N0000000219) and its subclasses.
- **4.3.** SPARQL query for searching the ODNAE drugs annotated with Norepinephrine Transporter Interactions [MoA] (N0000000234) and its subclasses.
- **4.4.** SPARQL query for searching the ODNAE drugs annotated with Serotonin Transporter Interactions [MoA] (N0000000167) and its subclasses.

The content of SPARQL File 5: (Note: The file to be generated)

Title: **link_chemicals_and_drugs**

- **5.1.** identify the drugs having proper part of chemical elements

- 5.2. identify all ancestor CHEBI terms of CHEBI_9667 (Triamcinolone)
- 5.3: get drugs for all child levels of a parent CHEBI term
- 5.4. Goal: get drugs for all levels of chebi terms --> #2 cleanup

SPARQL File 6: (Note: The file to be generated)

Title: link_drugs_Chebi_AEs

- 6.1: This is to find drugs vs AEs that are associated with these drugs.
- 6.2: This is to find AE and related drugs for the AE.
- 6.3: This is to identify chebi chemical terms for a specific AE. (Note: This is the script used to generate data for heatmap.)

The Content of SPARQL file 1:

Script file name: query_G_protein_linked_receptor_interaction_drugs

Content:

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SPARQL 1.1

SPARQL query for searching the ODNAE drugs annotated with G-Protein-linked Receptor Interactions [MoA] (<<http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000152>>) and its subclasses.

prefix rdf: <<http://www.w3.org/1999/02/22-rdf-syntax-ns#>>

prefix owl: <<http://www.w3.org/2002/07/owl#>>

prefix obo: <<http://purl.obolibrary.org/obo/>>

SELECT distinct ?s ?label

From <<http://purl.obolibrary.org/obo/merged/ODNAE>>

WHERE

{ ?s rdfs:subClassOf ?s1 .

?s rdfs:label ?label .

?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .

?s2 rdfs:subClassOf <<http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000152>> option (transitive).

}

Notes:

To count the total number (instead of providing the list):

- Change "distinct ?s ?label" TO: "count(distinct ?s)" in the script.

Related terms used in the script:

- http://purl.obolibrary.org/obo/RO_0000087 --> has role
- ODNAE: N0000000152: <http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000152> : <http://www.ontobee.org/ontology/ODNAE?iri=http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl%23N0000000152> → G-Protein-linked Receptor Interactions [MoA]

results: (run on <http://sparql.hegroup.org/sparql/>, at 8:40 CST 4/30/2015 by Asiyah Yu Lin)

20

s label

http://purl.obolibrary.org/obo/DRON_00020516	Amantadine Oral Tablet
http://purl.obolibrary.org/obo/DRON_00022309	Losartan Oral Tablet
.....	
http://purl.obolibrary.org/obo/DRON_00020955	Betaxolol Oral Tablet
--	

The Content of SPARQL File 2:

Script file name: **query_agonists_antagonists**

Content:

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SPARQL query for searching the ODNAE drugs are agonists and antagonists

SPARQL 2.1. drugs link to agonist

```

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
  ?s2 rdfs:label ?label2 .
  FILTER REGEX(str(?label2), "Agonist")
}

```

results in total 17 drugs: (run on <http://sparql.hegroup.org/sparql/>, at 9:56 CST 4/30/2015 by Asiyah Yu Lin)

s	label	
http://purl.obolibrary.org/obo/DRON_00013678		cevimeline
http://purl.obolibrary.org/obo/DRON_00022889		Pergolide Oral Tablet
.....		
http://purl.obolibrary.org/obo/DRON_00022385		Megestrol Oral Suspension

SPARQL 2.2. The agnoist that links to ODNAE drugs

```

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s2 ?label2
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .

```

```

?s rdfs:label ?label .
?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
?s2 rdfs:label ?label2 .
FILTER REGEX(str(?label2), "Agonist")
}

```

results in total 9 agonists: (run on <http://sparql.hegroup.org/sparql/>, at 9:14 CST 4/30/2015 by Asiyah Yu Lin)

```

s2      label2
http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000104  Cholinergic Muscarinic Agonists [MoA]
http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000117  Dopamine Agonists [MoA]
.....
http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000185  Progestational Hormone Receptor
Agonists [MoA]

```

SPARQL 2.3. drugs and agonist pair:

```

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?label ?label2
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
  ?s2 rdfs:label ?label2 .
  FILTER REGEX(str(?label2), "Agonist")
}

```

results in 17 drugs and agonist pair: (run on <http://sparql.hegroup.org/sparql/>, at 10:28 CST 4/30/2015 by Asiyah Yu Lin)

```

label      label2
cevimeline  Cholinergic Muscarinic Agonists [MoA]
Pergolide Oral Tablet  Dopamine Agonists [MoA]
.....
Megestrol Oral Suspension  Progestational Hormone Receptor Agonists [MoA]

```

SPARQL 2.4. drugs link to antagonist

```

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>

```

```

prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
  ?s2 rdfs:label ?label2 .
  FILTER REGEX(str(?label2), "Antagonist")
}

```

results in total 16 drugs: (run on <http://sparql.hegroup.org/sparql/>, at 10:00 CST 4/30/2015 by Asiyah Yu Lin)

```

s      label
http://purl.obolibrary.org/obo/DRON_00022309      Losartan Oral Tablet
http://purl.obolibrary.org/obo/DRON_00020523      Amiodarone Oral Tablet
.....
http://purl.obolibrary.org/obo/DRON_00020960      bicalutamide Oral Tablet

```

SPARQL 2.5. The antagonist that links to ODNAE drugs

```

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s2 ?label2
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
  ?s2 rdfs:label ?label2 .
  FILTER REGEX(str(?label2), "Antagonist")
}

```

results in total 17 antagonist: (run on <http://sparql.hegroup.org/sparql/>, at 10:01 CST 4/30/2015 by Asiyah Yu Lin)

```

s2      label2
http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000070      Angiotensin 2 Receptor Antagonists
[MoA]
http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000069      Calcium Channel Antagonists [MoA]
.....
http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000243      Androgen Receptor Antagonists [MoA]

```

SPARQL 2.6. Antagonist and drugs pair

```
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?label ?label2
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
  ?s2 rdfs:label ?label2 .
  FILTER REGEX(str(?label2), "Antagonist")
}
```

results in 21 drugs and agonist pair: (run on <http://sparql.hegroup.org/sparql/>, at 10:28 CST 4/30/2015 by Asiyah Yu Lin)

```
label    label2
Losartan Oral Tablet    Angiotensin 2 Receptor Antagonists [MoA]
Amiodarone Oral Tablet    Calcium Channel Antagonists [MoA]
.....
bicalutamide Oral Tablet    Androgen Receptor Antagonists [MoA]
```

SPARQL 2.7. drug link to both a kind of agonist and antagonist

```
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label ?label2 ?label4
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .

  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
  ?s2 rdfs:label ?label2 .
  FILTER REGEX(str(?label2), "Agonist")

  ?s rdfs:subClassOf ?s3 .
  ?s3 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s4 .
  ?s4 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
  ?s4 rdfs:label ?label4 .
  FILTER REGEX(str(?label4), "Antagonist")
}
```

results in 1 drug : (run on <http://sparql.hegroup.org/sparql/>, at 12:10 CST 4/30/2015 by Asiyah Yu Lin)
--

SPARQL 2.8. query drugs that have a specific role, e.g., Serotonin Agonists [MoA] (N0000000256).

Note: This is the SPARQL script for Figure 6.

Goal: Find drugs that has role (RO_0000087) of Serotonin Agonists [MoA] (N0000000256) from ODNAE

```
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
prefix ndfrt: <http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#>
```

```
SELECT distinct ?drug ?drug_label
FROM <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE {
  ?drug rdfs:subClassOf ?bnode .
  ?drug rdfs:label ?drug_label .
  ?bnode owl:onProperty obo:RO_0000087; owl:someValuesFrom ndfrt:N0000000256 .
}
```

The Content of SPARQL File 3:

Script file name: **query_all_drug_with_MoAs**

Content:

--

SPARQL 3.1. SPARQL query for searching all ODNAE drugs link to MoAs : subClassOf http://purl.obolibrary.org/obo/ODNAE_0000002 (role in cellular and molecular interactions)

```
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://purl.obolibrary.org/obo/ODNAE_0000002> option (transitive).
}
```

results in total 162 drugs: (run on <http://sparql.hegroup.org/sparql/>, at 10:03 CST 4/30/2015 by Asiyah Yu Lin)

```
s      label
http://purl.obolibrary.org/obo/DRON_00020539      anastrozole Oral Tablet
http://purl.obolibrary.org/obo/DRON_00022714      Nitrofurantoin Oral Tablet
.....
http://purl.obolibrary.org/obo/DRON_00020960      bicalutamide Oral Tablet
```

--

The Content of SPARQL 4:

Script file name: **query_neurotransmitters_interaction_drugs**

Content:

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SPARQL 4.1. SPARQL query for searching the ODNAE drugs annotated with Neurotransmitter Transporter Interactions [MoA] (<<http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000105>>) and its subclasses.

```
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000105> option
(transitive).
}
```

results in total 12 drugs: (run on <http://sparql.hegroup.org/sparql/>, at 8:56 CST 4/30/2015 by Asiyah Yu Lin)

s	label	
http://purl.obolibrary.org/obo/DRON_00026665		Bupropion Oral Tablet
http://purl.obolibrary.org/obo/DRON_00020525		Amitriptyline Oral Tablet
.....		
http://purl.obolibrary.org/obo/DRON_00027059		Paroxetine Oral Tablet

SPARQL 4.2. # SPARQL query for searching the ODNAE drugs annotated with Dopamine Transporter Interactions [MoA] (<<http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000219>>) and its subclasses.

```
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
```



```
?s2 rdfs:subClassOf <http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000219> option
(transitive).
}
```

results in total 1 drug: (run on <http://sparql.hegroup.org/sparql/>, at 8:59 CST 4/30/2015 by Asiyah Yu Lin)

```
s      label
http://purl.obolibrary.org/obo/DRON_00026665      Bupropion Oral Tablet
```

SPARQL 4.3. SPARQL query for searching the ODNAE drugs annotated with Norepinephrine Transporter Interactions [MoA] (<<http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000234>>) and its subclasses.

```
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
  ?s rdfs:label ?label .
  ?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
  ?s2 rdfs:subClassOf <http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000234> option
(transitive).
}
```

results in total 10 drug: (run on <http://sparql.hegroup.org/sparql/>, at 8:59 CST 4/30/2015 by Asiyah Yu Lin)

```
s      label
http://purl.obolibrary.org/obo/DRON_00020525      Amitriptyline Oral Tablet
http://purl.obolibrary.org/obo/DRON_00020620      Imipramine Oral Tablet
.....
http://purl.obolibrary.org/obo/DRON_00026665      Bupropion Oral Tablet
```

SPARQL 4.4. SPARQL query for searching the ODNAE drugs annotated with Serotonin Transporter Interactions [MoA] (<<http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000167>>) and its subclasses.

```
prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>
SELECT distinct ?s ?label
From <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE
{ ?s rdfs:subClassOf ?s1 .
```

```

?s rdfs:label ?label .
?s1 owl:onProperty obo:RO_0000087; owl:someValuesFrom ?s2 .
?s2 rdfs:subClassOf <http://evs.nci.nih.gov/ftp1/NDF-RT/NDF-RT.owl#N0000000167> option
(transitive).
}

```

results in total 11 drug: (run on <http://sparql.hegroup.org/sparql/>, at 9:05 CST 4/30/2015 by Asiyah Yu Lin)

```

s      label
http://purl.obolibrary.org/obo/DRON_00020525      Amitriptyline Oral Tablet
http://purl.obolibrary.org/obo/DRON_00020620      Imipramine Oral Tablet
.....
http://purl.obolibrary.org/obo/DRON_00027059      Paroxetine Oral Tablet

```

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The Content of SPARQL File 5:

Script file name: **query_chemicals_and_drugs**

Content:

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SPARQL 5.1. identify the drugs having proper part of chemical elements

Note: http://www.obofoundry.org/ro/ro.owl#has_proper_part

prefix rdf: <<http://www.w3.org/1999/02/22-rdf-syntax-ns#>>

prefix owl: <<http://www.w3.org/2002/07/owl#>>

prefix obo: <<http://purl.obolibrary.org/obo/>>

```

SELECT ?d ?label1 ?c ?label2
FROM <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE {
  ?d rdfs:subClassOf ?s1 .
  ?d rdfs:label ?label1 .
  ?s1 owl:onProperty <http://www.obofoundry.org/ro/ro.owl#has_proper_part>;
  owl:someValuesFrom ?c .
  ?c rdfs:label ?label2 .
}

```

#Results:

#count (distinct ?d) → 213

Example:

d	label1	c	label2
http://purl.obolibrary.org/obo/DRON_00020336	Triamcinolone Oral Tablet	http://purl.obolibrary.org/obo/CHEBI_9667	Triamcinolone
http://purl.obolibrary.org/obo/DRON_00020337	Dexamethasone Ophthalmic Ointment	http://purl.obolibrary.org/obo/CHEBI_41879	dexamethasone

--

SPARQL 5.2. identify all ancestor CHEBI terms of CHEBI_9667 (Triamcinolone)

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>

```
SELECT distinct ?label_9667 ?s ?label
FROM <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE {
<http://purl.obolibrary.org/obo/CHEBI_9667> rdfs:label ?label_9667 .
<http://purl.obolibrary.org/obo/CHEBI_9667> rdfs:subClassOf ?s option (transitive) .
?s rdfs:label ?label .
FILTER REGEX(str(?s), "CHEBI") .
}
```

result
13

```
label_9667    s        label
Triamcinolone http://purl.obolibrary.org/obo/CHEBI_50830  fluorinated steroid
Triamcinolone http://purl.obolibrary.org/obo/CHEBI_35341  steroid
...
```

SPARQL 5.3: get drugs for all child levels of a parent CHEBI term:

CHEBI_22507: glycoside antibiotic

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>

```
SELECT distinct ?s ?d ?d2 ?label2
FROM <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE {
?s rdfs:subClassOf <http://purl.obolibrary.org/obo/CHEBI_22507> option (transitive) .
?d owl:onProperty <http://www.obofoundry.org/ro/ro.owl#has_proper_part>; owl:someValuesFrom ?s .

?d2 rdfs:subClassOf ?d .
?d2 rdfs:label ?label2 .
}
```

results: 2

s	d	d2	label2
http://purl.obolibrary.org/obo/CHEBI_17833	nodeID://b339944739	http://purl.obolibrary.org/obo/DRON_00022009	Gentamicin Sulfate (USP) Injectable Solution
http://purl.obolibrary.org/obo/CHEBI_17076	nodeID://b339944979	http://purl.obolibrary.org/obo/DRON_00030017	Streptomycin Oral Capsule

--

SPARQL 5.4. Goal: get drugs for all levels of chebi terms --> #2 cleanup

CHEBI_33582: carbon group molecular entities

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>

prefix owl: <http://www.w3.org/2002/07/owl#>

prefix obo: <http://purl.obolibrary.org/obo/>

SELECT distinct

<http://purl.obolibrary.org/obo/CHEBI_33582> ?label_targetchebi ?chebi_for_drug ?drug ?labeldrug

FROM <http://purl.obolibrary.org/obo/merged/ODNAE>

WHERE {

<http://purl.obolibrary.org/obo/CHEBI_33582> rdfs:label ?label_targetchebi .

?chebi_for_drug rdfs:subClassOf <http://purl.obolibrary.org/obo/CHEBI_33582> option (transitive) .

?d owl:onProperty <http://www.obofoundry.org/ro/ro.owl#has_proper_part>;

owl:someValuesFrom ?chebi_for_drug .

?drug rdfs:subClassOf ?d .

?drug rdfs:label ?labeldrug .

}

#part of results:

callret-0	label_targetchebi	chebi_for_drug	drug	labeldrug
http://purl.obolibrary.org/obo/CHEBI_33582	carbon group molecular entity	http://purl.obolibrary.org/obo/CHEBI_63581	http://purl.obolibrary.org/obo/DRON_00023447	Stavudine Oral Capsule
http://purl.obolibrary.org/obo/CHEBI_33582	carbon group molecular entity	http://purl.obolibrary.org/obo/CHEBI_127780	http://purl.obolibrary.org/obo/DRON_00025587	Foscarnet Injectable Solution
http://purl.obolibrary.org/obo/CHEBI_33582	carbon group molecular entity	http://purl.obolibrary.org/obo/CHEBI_44915	http://purl.obolibrary.org/obo/DRON_00026059	Propofol Injectable Suspension

Note: removed this line: ?chebi_for_drug rdfs:label ?label_chebi .

Why: because the label_chebi can have duplicate names for the same chebi.

The Content of SPARQL 6:

Script file name: **link_drugs_Chebi_AEs**

Content:

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SPARQL 6.1: This is to find drugs vs AEs that are associated with these drugs.

BFO_0000057: has_participant

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>

prefix owl: <http://www.w3.org/2002/07/owl#>

prefix obo: <http://purl.obolibrary.org/obo/>

```

SELECT ?p_dae ?labelp ?dae ?label1 ?drug ?labeldrug ?s1
FROM <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE {
  ?dae rdfs:subClassOf ?s1 .

  ?dae rdfs:subClassOf ?p_dae .
  ?p_dae a owl:Class .
  ?p_dae rdfs:label ?labelp .

  ?dae rdfs:label ?label1 .
  ?s1 owl:onProperty obo:BFO_0000057; owl:someValuesFrom ?drug .
  ?drug rdfs:label ?labeldrug .

FILTER REGEX(str(?p_dae), "OAE") .
}

```

#part of results:

p_dae	labelp	dae	label1	drug	labeldrug	s1
http://purl.obolibrary.org/obo/OAE_0000337	peripheral neuropathy AE	http://purl.obolibrary.org/obo/ODNAE_0000023	ciprofloxacin hydrochloride (Ciloxan, Cipro, Cetraxal)-associated peripheral neuropathy AE	http://purl.obolibrary.org/obo/DRON_00021347	Ciprofloxacin Oral Tablet	nodeID://b339945066
http://purl.obolibrary.org/obo/OAE_0001215	neurotoxicity AE	http://purl.obolibrary.org/obo/ODNAE_0000024	cefepime (Maxipime)-associated neurotoxicity AE	http://purl.obolibrary.org/obo/DRON_00024830	cefepime Injectable Solution	nodeID://b339945067
http://purl.obolibrary.org/obo/OAE_0000418	neuropathy AE	http://purl.obolibrary.org/obo/ODNAE_0000025	penicillin G benzathine (Bicillin L-A)-associated neuropathy AE	http://purl.obolibrary.org/obo/DRON_00034441	penicillin G benzathine 115 MG/ML Oral Solution	nodeID://b339945068

--

SPARQL 6.2: This is to find AE and related drugs for the AE.

#Note: an AE (e.g., ciprofloxacin hydrochloride (Ciloxan, Cipro, Cetraxal)-associated peripheral neuropathy AE or ODNAE_0000023) may have two superclasses, e.g., peripheral neuropathy AE, and drug-associated peripheral neuropathy adverse event. And this AE 'has participant' some 'Ciprofloxacin Oral Tablet'.

```

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>

```

```

SELECT ?p ?labelp ?d ?label1 ?c ?label2 ?s1
FROM <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE {
  ?d rdfs:subClassOf ?s1 .
  ?d rdfs:subClassOf ?p .

```

```

?p a owl:Class .
?p rdfs:label ?labelp .

?d rdfs:label ?label1 .
?s1 owl:onProperty obo:BFO_0000057; owl:someValuesFrom ?c .
?c rdfs:label ?label2 .

FILTER REGEX(str(?p), "OAE") .
}

```

#part of results:

p	labelp	d	label1	c	label2	s1
http://purl.obolibrary.org/obo/OAE_0000337	peripheral neuropathy AE	http://purl.obolibrary.org/obo/ODNAE_0000023	ciprofloxacin hydrochloride (Ciloxan, Cipro, Cetraxal)-associated peripheral neuropathy AE	http://purl.obolibrary.org/obo/DRON_00021347	Ciprofloxacin Oral Tablet	nodeID://b339945066
http://purl.obolibrary.org/obo/OAE_0001215	neurotoxicity AE	http://purl.obolibrary.org/obo/ODNAE_0000024	cefepime (Maxipime)-associated neurotoxicity AE	http://purl.obolibrary.org/obo/DRON_00024830	cefepime Injectable Solution	nodeID://b339945067
http://purl.obolibrary.org/obo/OAE_0000418	neuropathy AE	http://purl.obolibrary.org/obo/ODNAE_0000025	penicillin G benzathine (Bicillin L-A)-associated neuropathy AE	http://purl.obolibrary.org/obo/DRON_00034441	penicillin G benzathine 115 MG/ML Oral Solution	nodeID://b339945068

SPARQL 6.3: This is to identify chebi chemical terms for a specific AE.

#Note: Basically, this is to merge the above two scripts to map Chebi terms directly AE terms.

#Note: This is the script used to generate data for heatmap.

```

prefix rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
prefix owl: <http://www.w3.org/2002/07/owl#>
prefix obo: <http://purl.obolibrary.org/obo/>

SELECT distinct
<http://purl.obolibrary.org/obo/CHEBI_33582> ?label_targetchebi ?chebi_for_drug ?drug ?labeldrug ?p
?labelp
FROM <http://purl.obolibrary.org/obo/merged/ODNAE>
WHERE {
  <http://purl.obolibrary.org/obo/CHEBI_33582> rdfs:label ?label_targetchebi .
  ?chebi_for_drug rdfs:subClassOf <http://purl.obolibrary.org/obo/CHEBI_33582> option (transitive) .
  ?d owl:onProperty <http://www.obofoundry.org/ro/ro.owl#has_proper_part>;
  owl:someValuesFrom ?chebi_for_drug .

  ?drug rdfs:subClassOf ?d .
  ?drug rdfs:label ?labeldrug .

  ?dae rdfs:subClassOf ?s1 .
  ?dae rdfs:subClassOf ?p .
  ?p a owl:Class .
  ?p rdfs:label ?labelp .

```

?s1 owl:onProperty obo:BFO_0000057; owl:someValuesFrom ?drug .

FILTER REGEX(str(?p), "OAE") .

}

#part of results:

callret-0	label_target chebi	chebi_for_drug	drug	labeldrug	p	labelp
http://purl.obolibrary.org/obo/CHEBI_33582	carbon group molecular entity	http://purl.obolibrary.org/obo/CHEBI_63581	http://purl.obolibrary.org/obo/DRON_00023447	Stavudine Oral Capsule	http://purl.obolibrary.org/obo/OAE_0000337	peripheral neuropathy AE
http://purl.obolibrary.org/obo/CHEBI_33582	carbon group molecular entity	http://purl.obolibrary.org/obo/CHEBI_127780	http://purl.obolibrary.org/obo/DRON_00025587	Foscarnet Injectable Solution	http://purl.obolibrary.org/obo/OAE_0000418	neuropathy AE
http://purl.obolibrary.org/obo/CHEBI_33582	carbon group molecular entity	http://purl.obolibrary.org/obo/CHEBI_44915	http://purl.obolibrary.org/obo/DRON_00026059	Propofol Injectable Suspension	http://purl.obolibrary.org/obo/OAE_0000418	neuropathy AE

Notes:

- Some drugs are not associated with AEs. For example, DRON_00022253 -- Levodopa Oral Tablet are not associated with any AEs.
- Some drugs may have two AEs, for example, DRON_00022291 - lomefloxacin Oral Tablet