

## Chapter 4. Side Effect and Human Phenotype Ontology

### --Incorporate with drug repurposing

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## Outline

- ❑ Database searching by a novice or by an expert
- ❑ **SIDER (Drug- Side Effect)**
- ❑ **HPO (Drug-phenotype)** (夏野峰, 谢勇军)
- ❑ **Drugbank (Drug- mechanism)**
- ❑ **Web page mining codes**
- ❑ **Case study: Find clues for drug repurposing cases.**

HPO disease-gene-phenotype cross reference file:

For example:

```
...
OMIM:609307 FGF14 2259 HP:0002354 Memory impairment
OMIM:608647 HYDIN 54768 HP:0011108 Recurrent sinusitis
OMIM:608647 HYDIN 54768 HP:0003593 Infantile onset
OMIM:608647 HYDIN 54768 HP:0002837 Recurrent bronchitis
...
```

78876 lines

**Downloaded from the course page**  
**Use it within the scope of the course.**

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## Using Rcurl to fetch webpage items

```
install.packages("rjson")
install.packages("stringr")
install.packages("RCurl")
require(RCurl)
require(rjson)
require(stringr)
require(XML)
url = https://www.drugbank.ca/drugs/DB00316
doc = getURL(url)

HTML_File_Name="tmp.html"
writeLines("", con = HTML_File_Name, sep = "\n",
useBytes = F)
cat(doc, file = HTML_File_Name, append = TRUE)
```

```

...
<th class="divider"
colspan="2">Pharmacology</th></tr><tr><th>Indication</th><td>For
temporary relief of fever, minor aches, and
pains.</td></tr><tr><th>Structured Indications <a tabindex="0"
role="button" data-toggle="popover" data-trigger="focus" data-
content="Drug indications covering every FDA and Health Canada approved
indication, extracted from FDA drug labels and scientific publications. The
commercial version includes a text description, severity, type of indication,
and associated ICD10 or MedDRA identifiers. &mdash; &lt;a
href=&#39;https://www.drugbankplus.com/data.html&#39;&gt;Learn
More&lt;/a&gt;" title="About Structured Indications" id="structured-
indication-info" href="javascript:void(0);">
...
176 lines

Use vim :/Indication

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```

```

file <- file(HTML_File_Name, "r")
line=readLines(file,n=1)
while( length(line) != 0 )
{ if( grepl("Indication", line) )
{
my=line
sentence=unlist(strsplit(my,"<th>"))
sentence=sentence[grepl("Indication</th>", sentence)]
sentence=sub("</th>", "", sentence)
sentence=sub("<td>", "", sentence)
sentence=sub("</td>", "", sentence)
sentence=sub("<tr>", "", sentence)
sentence=sub("</tr>", "", sentence)
sentence=sub("Indication", "Indication: ", sentence)
print(sentence)
}
}
line=readLines(file,n=1)
}
close(file)

```

	Drug name	Initial indication	Repurposed usage	Drug bank	NCT	Pub M	dgID B
1	<a href="#">Viagra</a> (伟哥)	<a href="#">erectile dysfunction</a>	severe erythema nodosum (结节性红斑) leprosum		348	5132	0
2	<a href="#">thalidomide</a> (沙利度胺)	Sedative, morning sickness pregnant	severe erythema nodosum (结节性红斑) leprosum		112 3	9728	23
3	<a href="#">buprenorphine</a> (丁丙诺啡, 叔丁啡)	Control of moderate pain	interruption and maintenance of <a href="#">heroin</a> and other <a href="#">opioid</a> addictions		420	5762	3
4	<a href="#">Requip</a> (力必平)	Parkinsonian	Restless Legs Syndrome, SSRI-induced sexual dysfunction		80	810	0
5	<a href="#">Colessevelam</a> (考来维仑)	Diet, reduce elevated LDL-cholesterol	Glycemic control for diabetes		47	267	0
6	<a href="#">gabapentin</a> (加巴喷丁)	Epilepsy	Anxiety disorder, neuropathic pain		310	5481	5
7	<a href="#">pregabalin</a> (普瑞巴林)	Epilepsy	Anxiety disorder, neuropathic pain		371	2572	1
8	<a href="#">Plerixafor</a> (普乐沙福)	HIV	Stem cell mobilizing		138	1013	3

### Assignment:

Currently, you know several database, along with particular item tracing codes.

For 8 selected repurposed drugs, find clues in these databases, and explain:

1. Can you reproduce the finding of the drug repurposing;
2. Molecular explanation of them.

Find something novel and prepare a 10 minutes talk in next class. Two members win the points.