

HW_2 (работа с NCBI)

```
In [61]: from Bio import Entrez
```

```
In [71]: Entrez.email = 'wwoskie@gmail.com'
```

```
In [72]: %load_ext rpy2.ipython
```

```
The rpy2.ipython extension is already loaded. To reload it, use:  
%reload_ext rpy2.ipython
```

```
In [73]: %%R  
if (!("reutils" %in% installed.packages()))  
  install.packages("reutils")  
library(reutils)
```

1. Найдем в PubMed статьи по интересному для нас запросу и возвратим абстракты этих статей;

```
In [74]: handle = Entrez.esearch(db = "pubmed", term = "cnv detection review")  
record = Entrez.read(handle)  
mshandle = Entrez.efetch(db="pubmed", id=record["IdList"][0:3],  
  rettype="abstract", retmode="text")  
with open("abstracts_py.txt", "w") as f:  
  for line in mshandle:  
    f.write(line)
```

```
In [20]: %%R  
ms <- esearch(db = "pubmed", term = "cnv detection review")[1:3]  
abstr <- efetch(ms, rettype = "abstract")  
abstr  
write(content(abstr), "abstracts_R.txt")
```

```
In [151... !esearch -email wwoskie@gmail.com -db pubmed -query "cnv detection  
review" | efetch -mode text -format abstract > abstracts_bash.txt
```

2. Найдем ID организма по названию в базе taxonomy;

```
In [77]: handle = Entrez.esearch(db = "taxonomy", term = "HIV-1")  
record = Entrez.read(handle)  
print(record['IdList'])  
handle = Entrez.esearch(db = "taxonomy", term = "HIV-2")  
record = Entrez.read(handle)  
print(record['IdList'])
```

```
['11676']  
['11709']
```

```
In [39]: %%R  
print(esearch(db = "taxonomy", term = "HIV-1"))  
print(esearch(db = "taxonomy", term = "HIV-2"))
```

```
Object of class 'esearch'
List of UUIDs from the 'taxonomy' database.
[1] "11676"
Object of class 'esearch'
List of UUIDs from the 'taxonomy' database.
[1] "11709"
```

```
In [135... !esearch -email wwoskie@gmail.com -db taxonomy -query "HIV-1" | esummary
| grep TaxId
!esearch -email wwoskie@gmail.com -db taxonomy -query "HIV-2" | esummary
| grep TaxId
```

```
<TaxId>11676</TaxId>
<AkaTaxId>0</AkaTaxId>
<TaxId>11709</TaxId>
<AkaTaxId>0</AkaTaxId>
```

3. Запросим в базе нуклеотидных последовательностей по названию гена, после чего вернем таблицу с UID (в XML это поле называется Id), accession number (в XML это поле называется Caption), длиной последовательности (Slen);

```
In [81]: handle = Entrez.esearch(db="nucleotide", term="gp120 AND HIV-1[orgn]")
record = Entrez.read(handle)
for rec in record["IdList"][0:10]:
    temphandle = Entrez.read(Entrez.esummary(db="nucleotide",
id=rec, retmode="text"))
    print(temphandle[0]['Id']+"\t"+temphandle[0]
['Caption']+"\t"+str(int(temphandle[0]['Length'])))#+"\n")
```

2557534022	LC722451	105
2557534020	LC722450	105
2557534018	LC722449	105
2557534016	LC722448	105
2557534014	LC722447	108
2557534012	LC722446	105
2557534010	LC722445	105
2557534008	LC722444	102
2557534006	LC722443	105
2557534004	LC722442	102

```
In [37]: %%R
request <- esearch(db = "nucleotide", term = "gp120 AND HIV-1[orgn]")
summary <- esummary(request)
content_summary <- content(summary, "parsed")
as.data.frame(content_summary[1:10,c("Id", "Caption", "Slen")])
```

	Id	Caption	Slen
1	2557534022	LC722451	105
2	2557534020	LC722450	105
3	2557534018	LC722449	105
4	2557534016	LC722448	105
5	2557534014	LC722447	108
6	2557534012	LC722446	105
7	2557534010	LC722445	105
8	2557534008	LC722444	102
9	2557534006	LC722443	105
10	2557534004	LC722442	102

```
In [139... !esearch -email wvoskie@gmail.com -db nucleotide -query "gp120 AND HIV-1[orgn]" | esummary -mode xml | xtract -pattern DocumentSummary -element Id Caption Slen | sed '11,$ d; s/"//g'
```

```
2557534022      LC722451      105
2557534020      LC722450      105
2557534018      LC722449      105
2557534016      LC722448      105
2557534014      LC722447      108
2557534012      LC722446      105
2557534010      LC722445      105
2557534008      LC722444      102
2557534006      LC722443      105
2557534004      LC722442      102
^C
```

4. Дадим в базу нуклеотидных или белковых последовательностей текстовый запрос, а затем вернем последовательности в формате fasta и запишем их в файл;

```
In [91]: handle = Entrez.esearch(db="nucleotide", term="gp120 AND HIV-1[orgn]")
record = Entrez.read(handle)

with open("HIV-1_gp120_py.fa", "w") as outf:
    for rec in record["IdList"][0:10]:
        lne = Entrez.efetch(db="nucleotide", id=rec, retmode="text",
        rettype="fasta").read()
        outf.write(lne+"\n")
```

```
In [140... %%R
request <- esearch(db = "nucleotide", term = "gp120 AND HIV-1[orgn]")
fasta_nuc <- efetch(uid = request[1:10], db = "nucleotide", rettype =
"fasta", retmode = "text")
write(content(fasta_nuc), "HIV-1_gp120_R.fa")
```

```
In [145... !esearch -email wvoskie@gmail.com -db nucleotide -query "gp120 AND HIV-1[orgn][1:10]" | efetch -format fasta -mode text > HIV-1_gp120_bash.fa
```

```
^C
```

5. Скачаем белок, соответствующий известному UID нуклеотида;

```
In [126... lhandle = Entrez.elink(dbfrom="nucleotide", id="2557534022",
linkname='nuccore_protein') # без linkname не работало
lrecord = Entrez.read(lhandle)
prothandle = lrecord[0]["LinkSetDb"][0]['Link'][0]['Id']
rrecord = Entrez.efetch(db="protein", id=prothandle, rettype="fasta",
retmode="text")
print(rrecord.read())
```

```
>BDQ05264.1 envelope glycoprotein, partial [Human immunodeficiency virus 1]
CTRPNNNTRXXIXXGPGQXXXATGXIIGBIRXAXC
```

```
In [51]: %%R
nuc_to_prot <- elink(uid = content_summary$Id[1], dbFrom = "nucleotide",
dbTo = "protein")
efetch(nuc_to_prot, rettype = "fasta", retmode = "text")
```

```
Object of class 'efetch'
>BDQ05264.1 envelope glycoprotein, partial [Human immunodeficiency virus 1]
CTRPNNNTRXXIXXGPGQXXXATGXIIGBIRXAXC

...
EFetch query using the 'protein' database.
Query url: 'https://eutils.ncbi.nlm.nih.gov/entrez/eutils/efetch.fcgi?ef
e...'
Retrieval type: 'fasta', retrieval mode: 'text'
```

```
In [148.. !elink -id 2557534022 -db nuccore -target protein | efetch -format fasta
-mode text
```

```
>BDQ05264.1 envelope glycoprotein, partial [Human immunodeficiency virus 1]
CTRPNNNTRXXIXXGPGQXXXATGXIIGBIRXAXC
```

6. Скачаем все последовательности из работы с PMID 22124968 и запишем их в файл fasta.

```
In [127.. lhandle = Entrez.elink(dbfrom="pubmed", db="nucleotide", id="22124968")
lrecord = Entrez.read(lhandle)
ids = []
for el in lrecord[0]["LinkSetDb"][0]["Link"]:
    ids.append(el['Id'])
rrecord = Entrez.efetch(db="nucleotide", id=ids[:4], rettype="fasta",
retmode="text")
with open ("human_receptors_py.fa", "w") as ouf:
    ouf.write(rrecord.read()+"\n")
```

```
In [60]: %%R
lnk <- elink("22124968", dbFrom = "pubmed", dbTo = "nuccore")
print(lnk) # take first entry type only to avoid batching
f2 <- efetch(lnk[1], rettype = "fasta", retmode = "text")
write(content(f2), "human_receptors_R.fa")
```

```
Object of class 'elink'
ELink query from database 'pubmed' to destination database 'nuccore'.
Query UUIDs:
[1] "22124968"
Summary of LinkSet:
      DbTo      LinkName LinkCount
1 nuccore pubmed_nuccore_refseq      20
2 nuccore pubmed_nuccore_weighted 8242
```

```
In [150... !elink -db pubmed -target nucleotide -id 22124968 | efetch -format fasta  
-mode text > human_receptors_bash.fa
```

```
In [ ]:
```