# Introduction to applied bioinformatics

PETRA MATOUŠKOVÁ

2023/2024

# Organization:

Each student 1 gene/protein

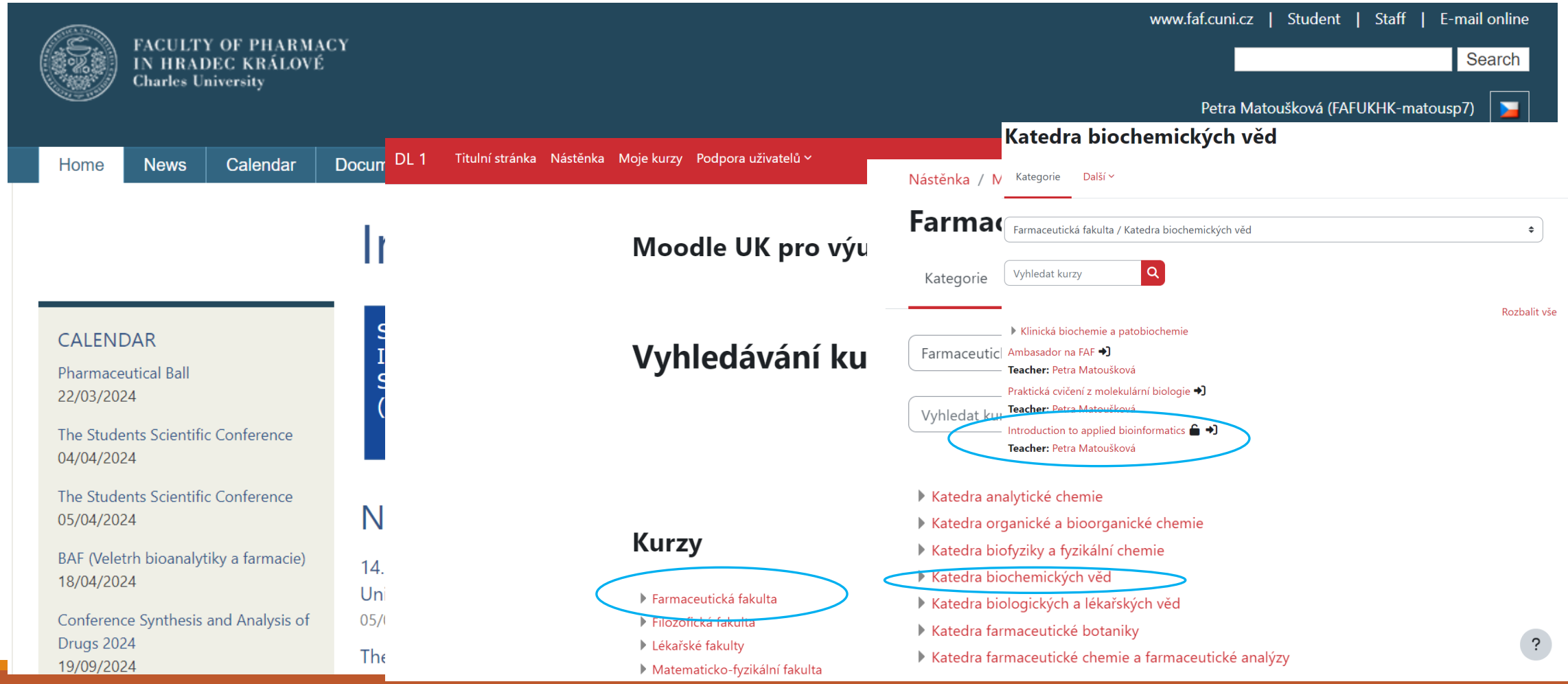
"**homeworks**": searching for informations about 1 gene/protein

(+ compulsory presence 8/10 lectures)

Exam: „written" by computer – selected exercises

| Týden | Datum | | Čas |
|---|---|---|---|
| *1* | *19.2.2024* | | *Po 8:00 - 9:30* |
| 1 | 20.2.2024 | 1 | Út 8:00 - 9:30 |
| 3 | 4.3.2024 | 2 | Po 8:00 - 9:30 |
| 3 | 5.3.2024 | 3 | Út 8:00 - 9:30 |
| *5* | *18.3.2024* | X | *Po 8:00 - 9:30* |
| *5* | *19.3.2024* | X | *Út 8:00 - 9:30* |
| *7* | *~~1.4.2024~~* | X | *Po 8:00 - 9:30* |
| 7 | 2.4.2024 | 4 | Út 8:00 - 9:30 |
| 9 | 15.4.2024 | 5 | Po 8:00 - 9:30 |
| 9 | 16.4.2024 | 6 | Út 8:00 - 9:30 |
| 10 | 23.4.2024 | 7 | Út 13:10 - 14:40 |
| 11 | 29.4.2024 | 8 | Po 8:00 - 9:30 |
| 11 | 30.4.2024 | 9 | Út 8:00 - 9:30 |
| 12 | 7.5.2024 | X | Út 13:10 - 14:40 |
| 13 | 13.5.2024 | 10 | Po 8:00 - 9:30 |
| *13* | *~~14.5.2024~~* | **exam?** | *Út 8:00 - 9:30* |

# Moodle (1)


FACULTY OF PHARMACY
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Petra Matoušková (FAFUKHK-matousp7)
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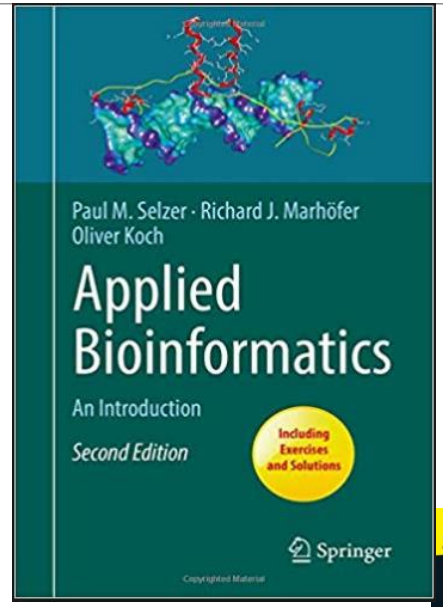
CALENDAR
Pharmaceutical Ball
22/03/2024
The Students Scientific Conference
04/04/2024
The Students Scientific Conference
05/04/2024
BAF (Veletrh bioanalytiky a farmacie)
18/04/2024
Conference Synthesis and Analysis of Drugs 2024
19/09/2024
Moodle UK pro výu
Vyhledávání ku
Kurzy
Farmaceutická fakulta
Filozofická fakulta
Lékařské fakulty
Matematicko-fyzikální fakulta
Katedra biochemických věd
Nástěnka / M
Kategorie
Další
Farmac
Farmaceutická fakulta / Katedra biochemických věd
Kategorie
Vyhledat kurzy
Rozbalit vše
Klinická biochemie a patobiochemie
Ambasador na FAF
Teacher: Petra Matoušková
Praktická cvičení z molekulární biologie
Teacher: Petra Matoušková
Introduction to applied bioinformatics
Teacher: Petra Matoušková
Katedra analytické chemie
Katedra organické a bioorganické chemie
Katedra biofyziky a fyzikální chemie
Katedra biochemických věd
Katedra biologických a lékařských věd
Katedra farmaceutické botaniky
Katedra farmaceutické chemie a farmaceutické analýzy

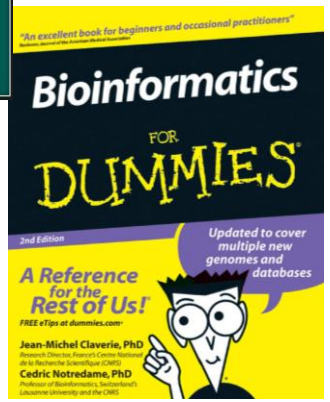
# Bioinformatics is about…

**= computational branch of molecular biology.**

- searching biological databases
- comparing sequences
- looking at protein structures
- …..asking biological and biomedical questions with a computer.

*„The bioinformatics can save you months of work in the lab at the minute cost of a few hours' work with your computer."*




-no installation
-web browser (+Java)

Retrieving DNA/protein sequences from databases

Computing nucleotide, amino-acids compositions, molecular weight, isoelectric point, and other parameters

Computing how hydrophobic or hydrophilic a protein is, predicting antigenic sites, locating membrane-spanning segments

Identifying restriction sites

Designing polymerase chain-reaction (PCR) primers

Identifying open reading frames (ORFs)

Predicting elements of DNA/RNA/protein secondary structure

Predicting 3-D structure and the domain organization of proteins

Finding all proteins that share a similar sequence and Classifying proteins into families

Finding evolutionary relationships between proteins, drawing proteins' family trees

Computing the optimal alignment between two or more DNA/protein sequences

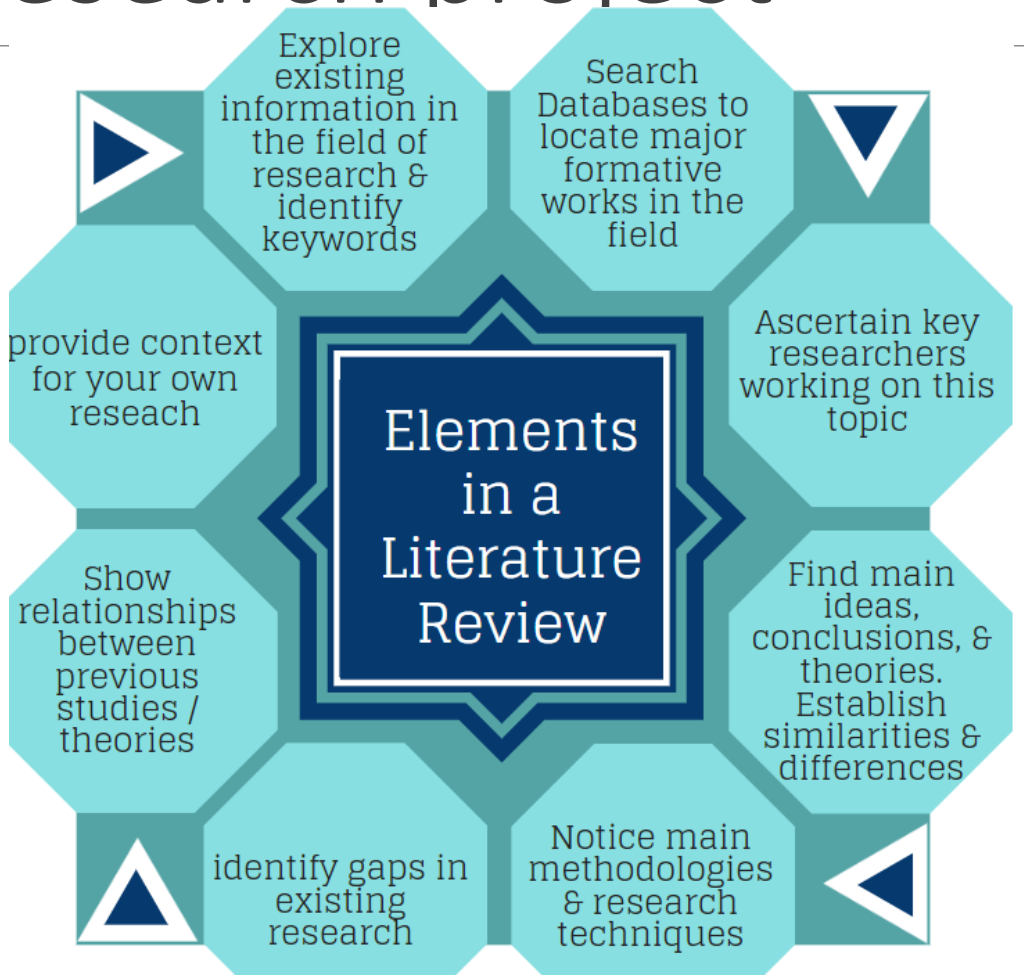
Finding polymorphic sites in genes (single nucleotide polymorphisms, SNPs)

Assembling sequence fragments

# Literature search / Research project

**The purpose of a literature review is to:**

- Provide a foundation of knowledge on a topic
- Identify areas of prior scholarship to prevent duplication and give credit to other researchers
- Identify inconstancies: gaps in research, conflicts in previous studies, open questions left from other research
- Identify the need for additional research (justifying your research)
- Identify the relationship of works in the context of their contribution to the topic and other works
- Place your own research within the context of existing literature, making a case for why further study is needed.



# Research Project: NQO1

Task : Find relevant information about your **gene of interest**

**(TYRP1, KAT7 √, SDHA √…)**

# Google … NQO1



## NAD(P)H dehydrogenase (quinone 1)

From Wikipedia, the free encyclopedia

**NAD(P)H dehydrogenase [quinone] 1** is an enzyme that in humans is encoded by the *NQO1* gene.[1]

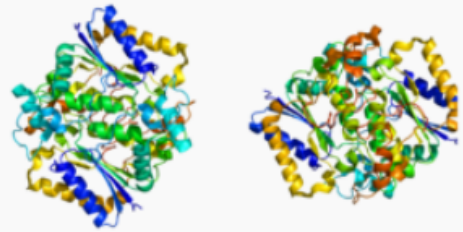
This gene is a member of the NAD(P)H dehydrogenase (quinone) family and encodes a cytoplasmic 2-electron reductase. This FAD-binding protein forms homodimers and reduces quinones to hydroquinones. This protein's enzymatic activity prevents the one electron reduction of quinones that results in the production of radical species. Mutations in this gene have been associated with tardive dyskinesia (TD), an increased risk of hematotoxicity after exposure to benzene, and susceptibility to various forms of cancer. Altered expression of this protein has been seen in many tumors and is also associated with Alzheimer's disease (AD). Alternate transcriptional splice variants, encoding different isoforms, have been characterized.[2] Recent pharmacological research suggests feasibility of genotype-directed redox chemotherapeutic intervention targeting NQO1*2 breast cancer, a common missense genotype encoding a functionally impaired NQO1 protein.[3]

### Interactions [edit]

NAD(P)H dehydrogenase (quinone 1) has been shown to interact with HSPA4.[4]

### References [edit]

**NAD(P)H dehydrogenase, quinone 1**

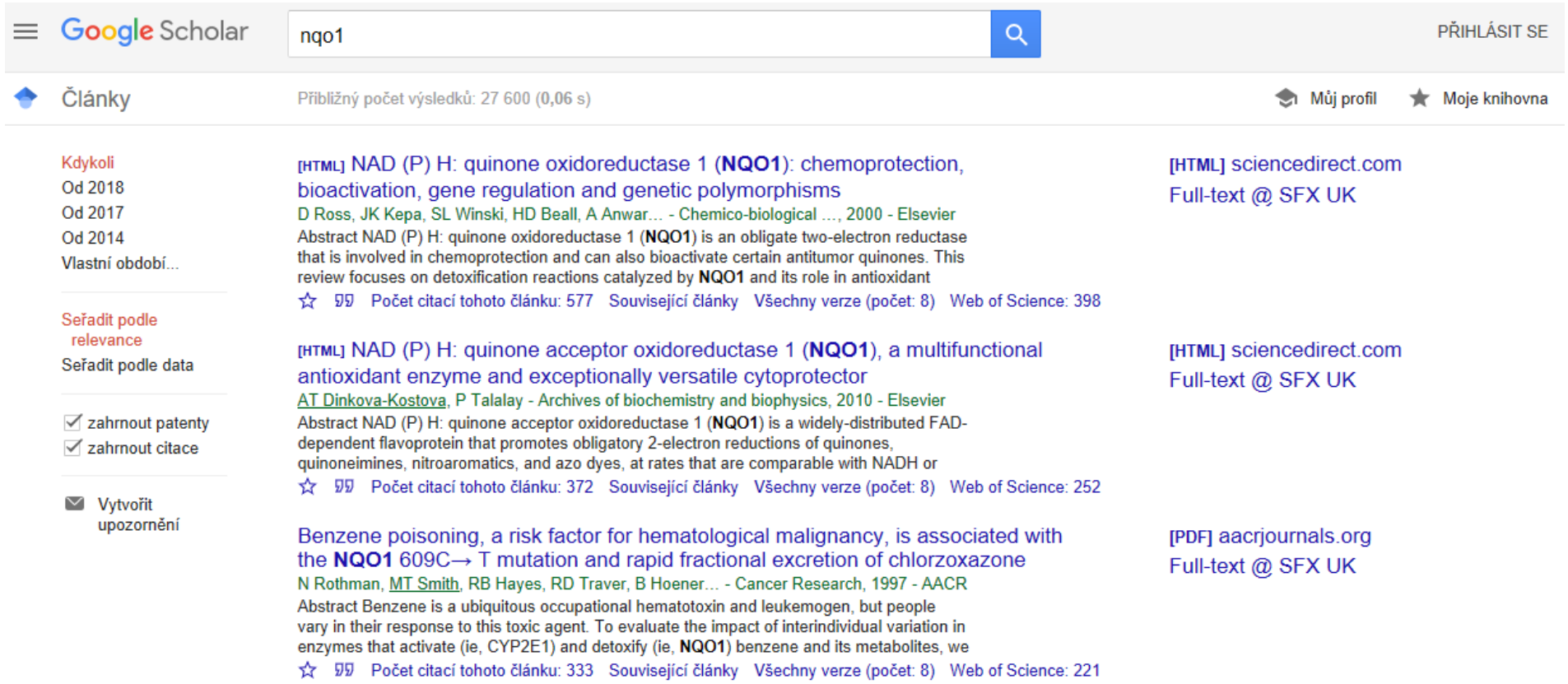


PDB rendering based on 1d4a.

| Available structures | |
|---|---|
| PDB | Ortholog search: PDBe, RCSB |
| List of PDB id codes | [show] |

| Identifiers | |
|---|---|
| Symbols | NQO1; DHQU; DIA4; DTD; NMOR1; NMORI; OR1 |

# Google scholar

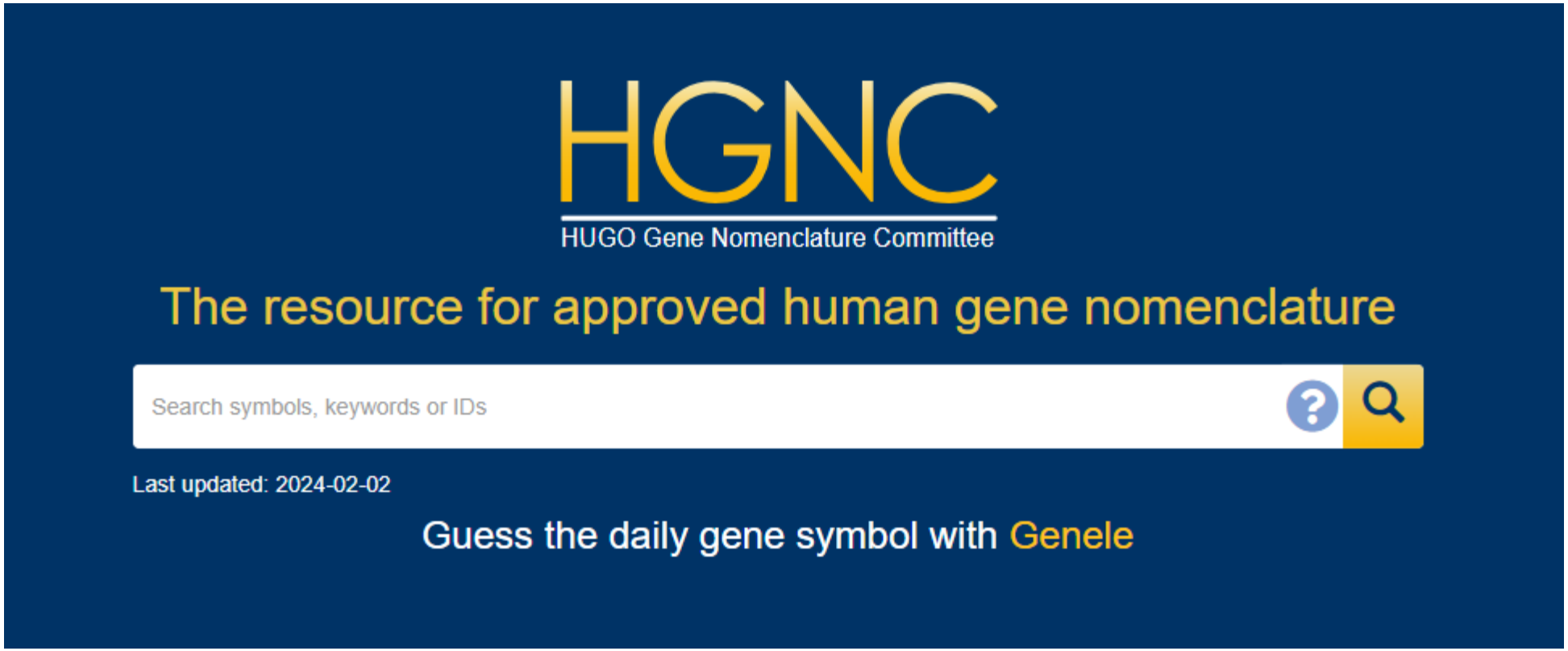


# Research Project: NQO1

**Quinone:NAD(P)H dehydrogenase 1**

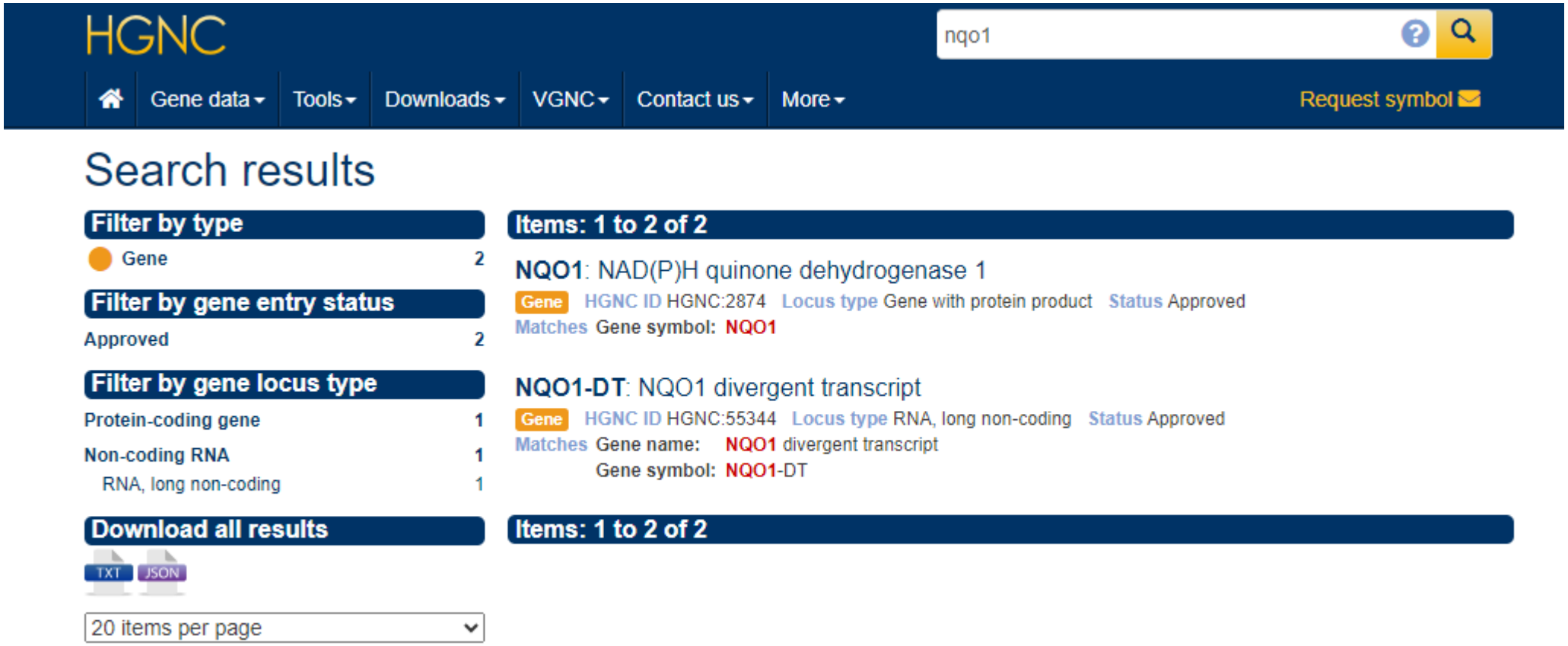
# Identify the gene symbol!

HUGO database

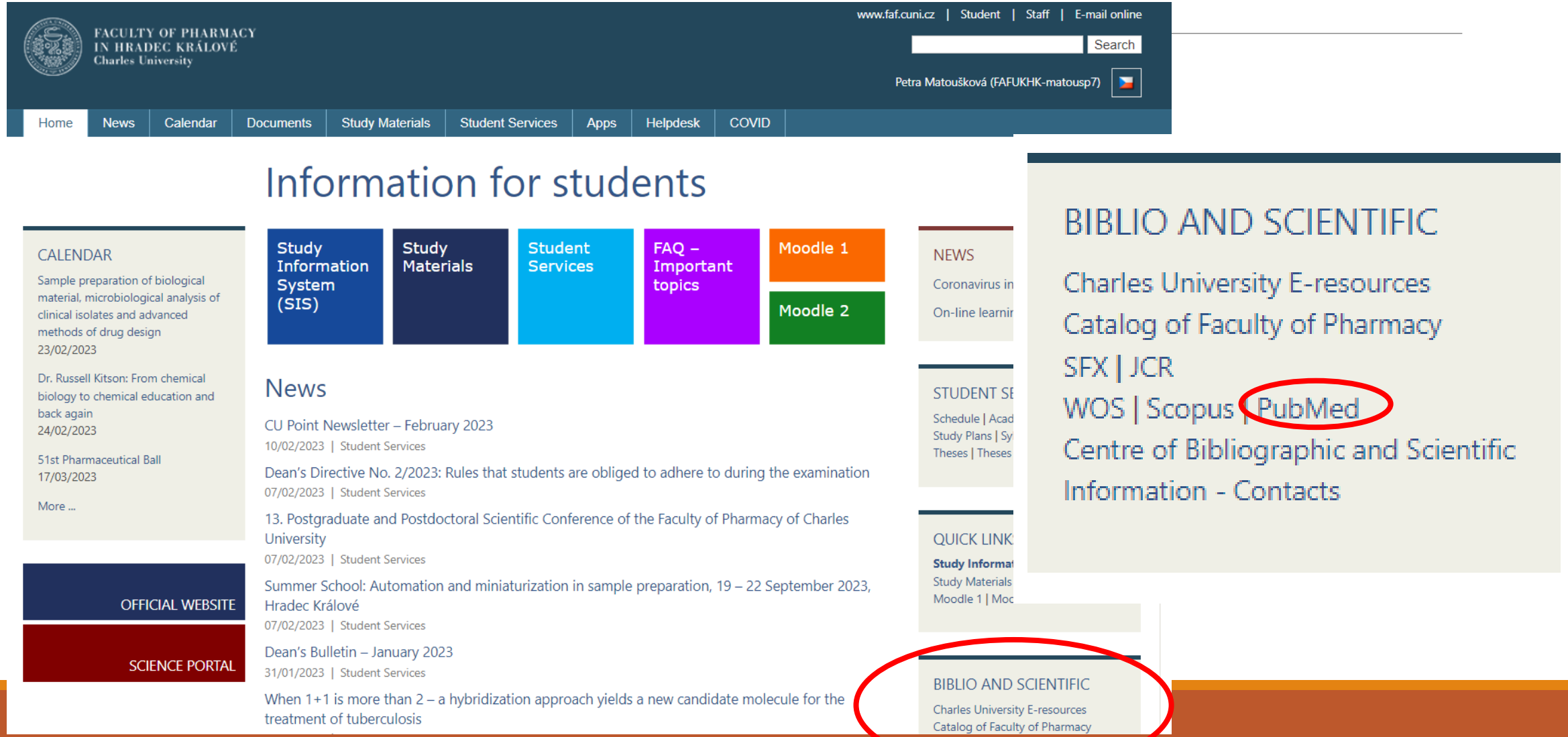


# Identify the gene symbol!

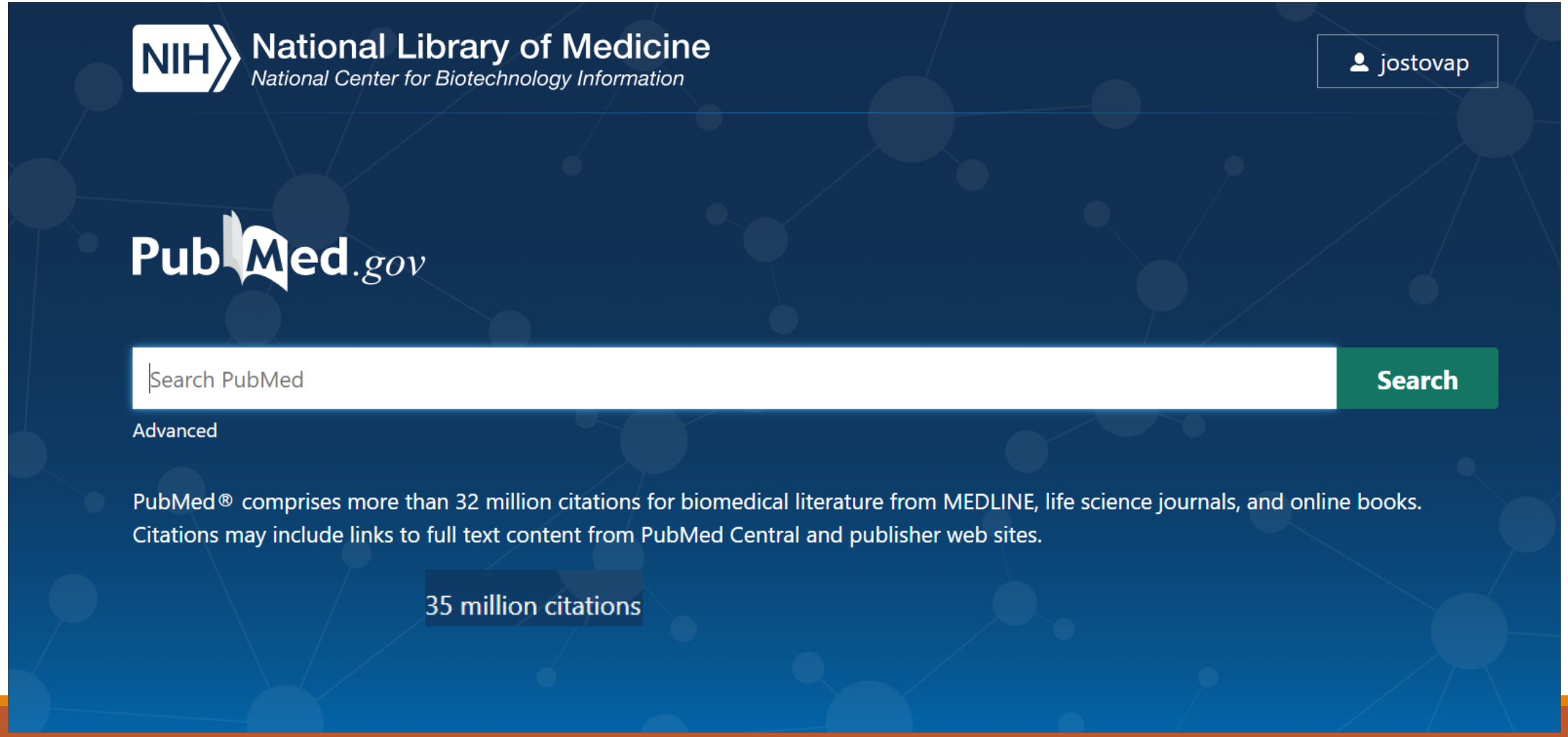
HUGO database



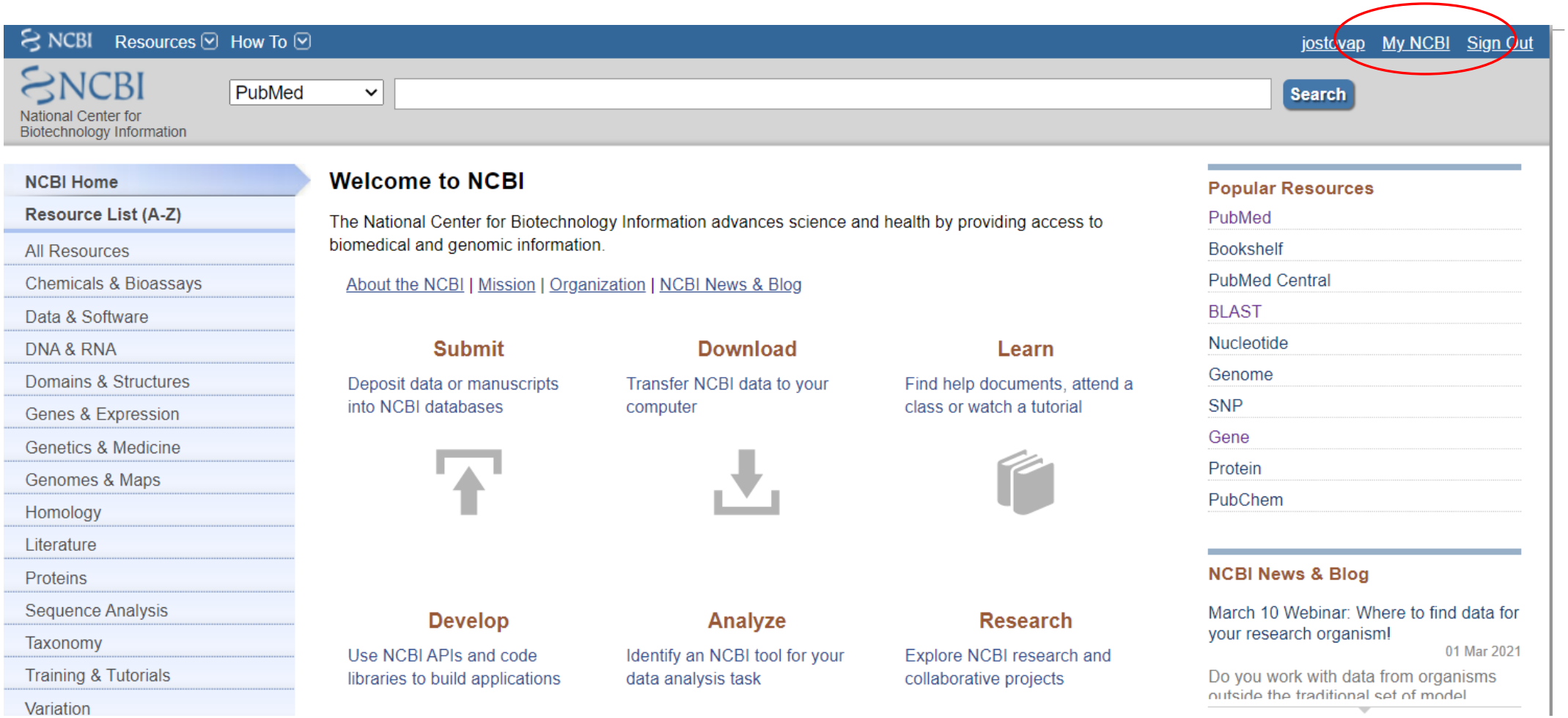
# Literature search



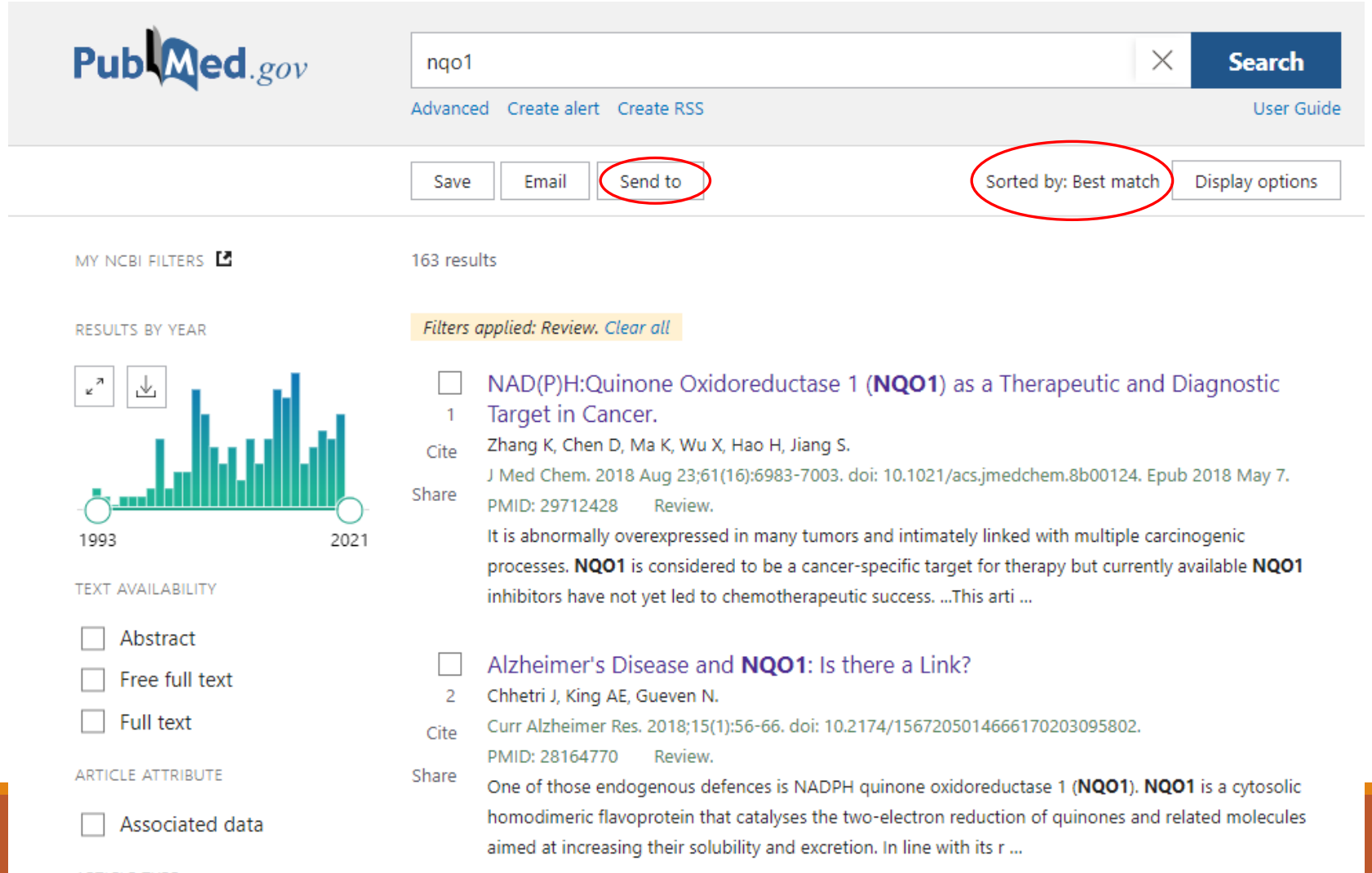
# Literature search **PubMed** http://www.ncbi.nlm.nih.gov/pubmed/



# Literature search **PubMed** http://www.ncbi.nlm.nih.gov/pubmed/

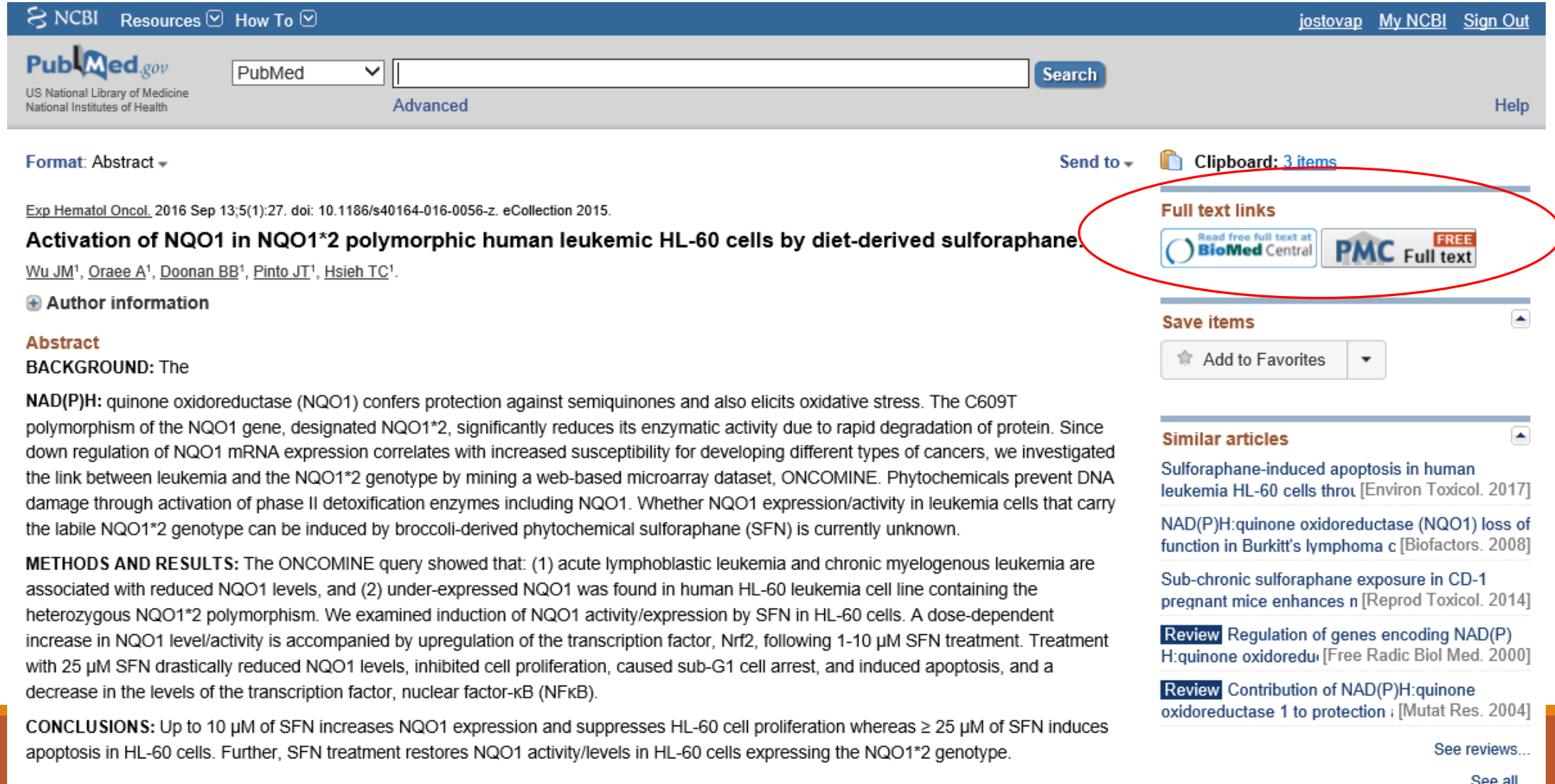


# Literature search **PubMed** http://www.ncbi.nlm.nih.gov/pubmed/



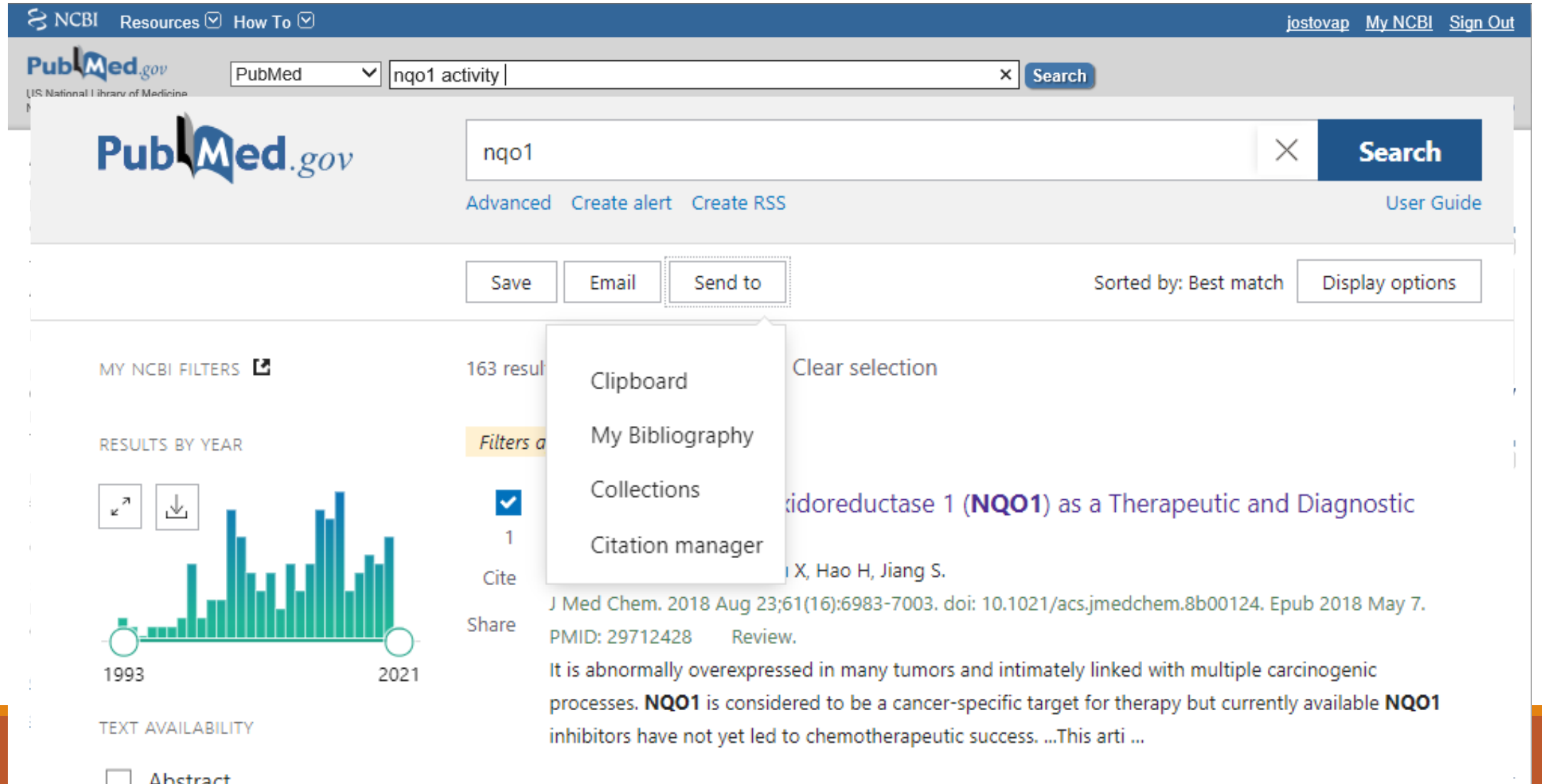
# Literature search

**PubMed** http://www.ncbi.nlm.nih.gov/pubmed/



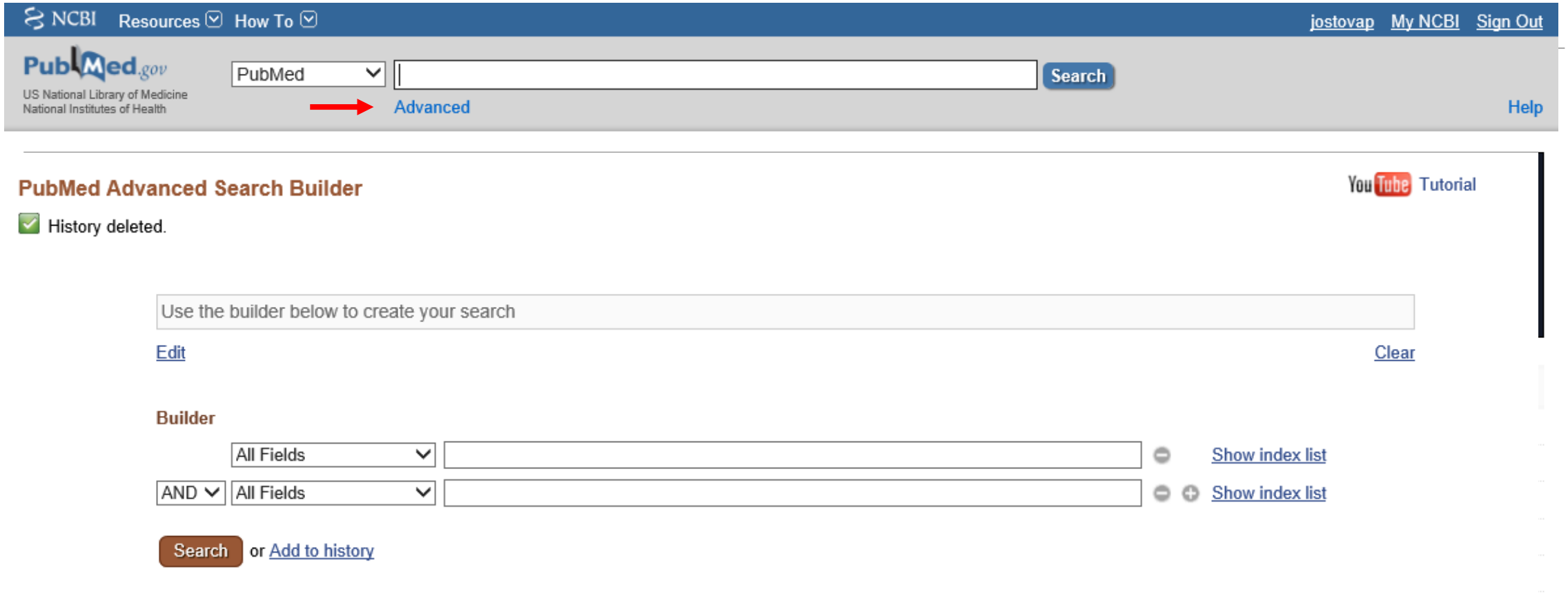
# Literature search

**PubMed** http://www.ncbi.nlm.nih.gov/pubmed/



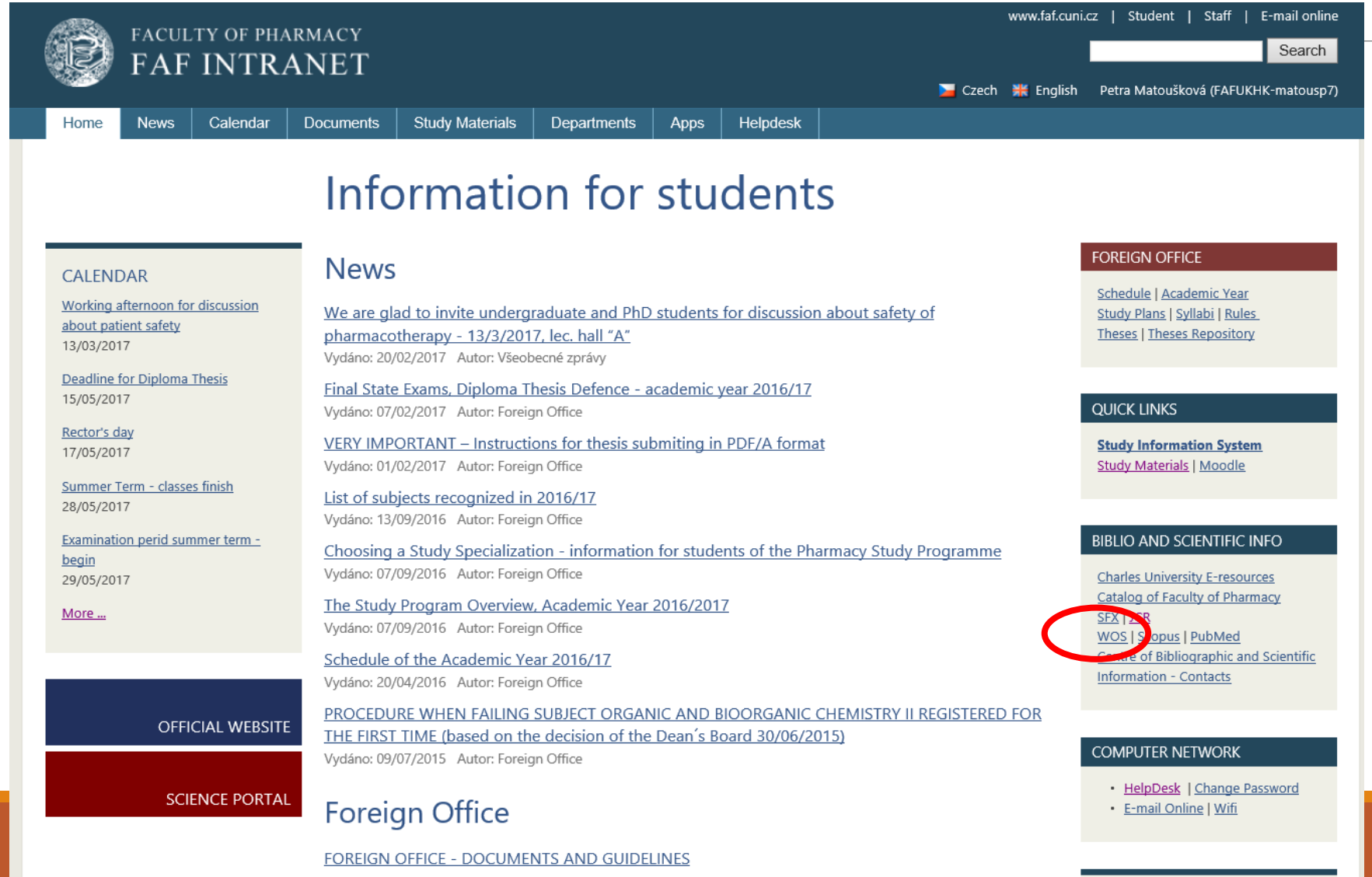
# Literature search

**PubMed** http://www.ncbi.nlm.nih.gov/pubmed/



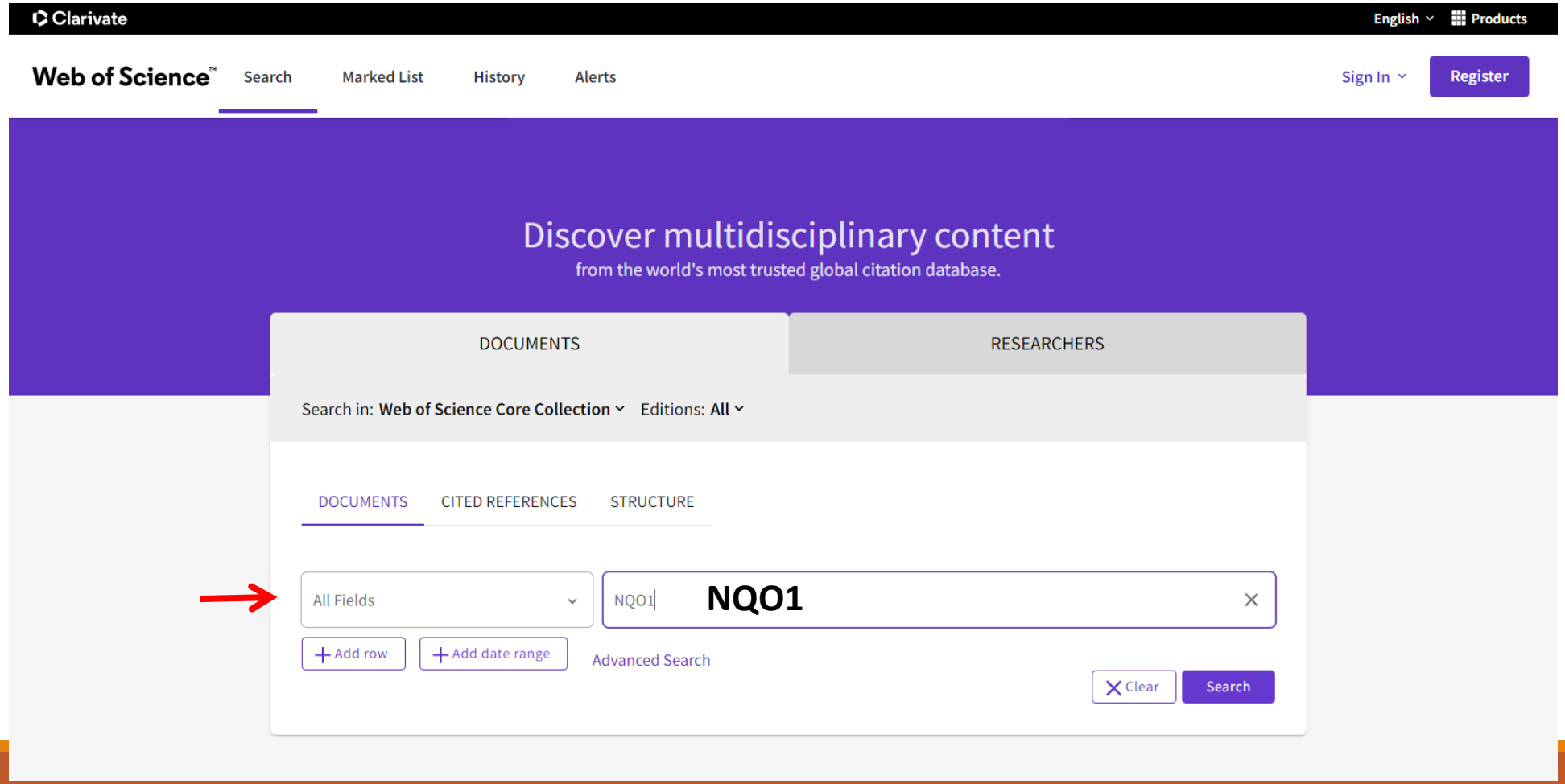
# Try PubMed !

# Literature search

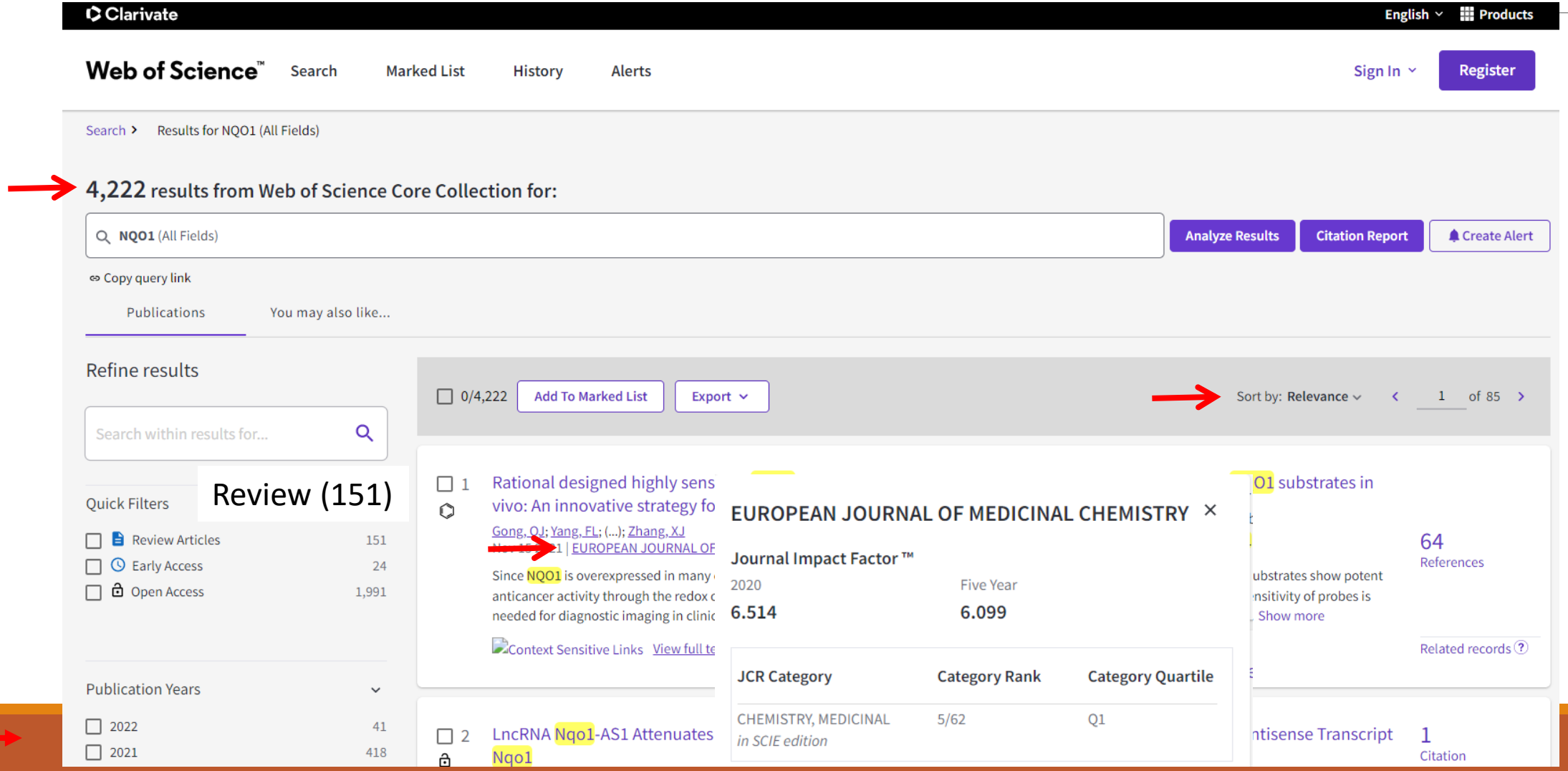


# Literature search

WOS http://apps.webofknowledge.com/



# Literature search



# impact factor

=scientometric index – reflects average number of citations of articles published in the last two years in the journal

~relative **importance of the journal** within its field

# Literature search

# Literature search

EBSCOhost

Searching: Business Source Ultimate | Choose Databases

AN 120068408

Search

Basic Search Advanced Search Search History

Lekarska fakulta UK v Hradci Kralove

Detailed Record

PDF Full Text (6.7MB)

SFX

Find author's articles in Web of Science

Find Similar Results using SmartText Searching.

Result List | Refine Search 1 of 1

Lipopolysaccharide derived from the digestive tract provokes oxidative stress in the liver of dairy cows fed a high-grain diet.

Authors: Abaker, J. A.[1]
Xu, T. L.[1]
Jin, D.[1]
Chang, G. J.[1]
Zhang, K.[1]
Shen, X. Z.[1] xzshen@njau.edu.cn

Source: Journal of Dairy Science. Jan2017, Vol. 100 Issue 1, p666-678. 13p.

Document Type: Article

Subject Terms: Lipopolysaccharides
Oxidative stress
Lactation
Rumen (Ruminants)
Blood plasma
Parameters (Statistics)

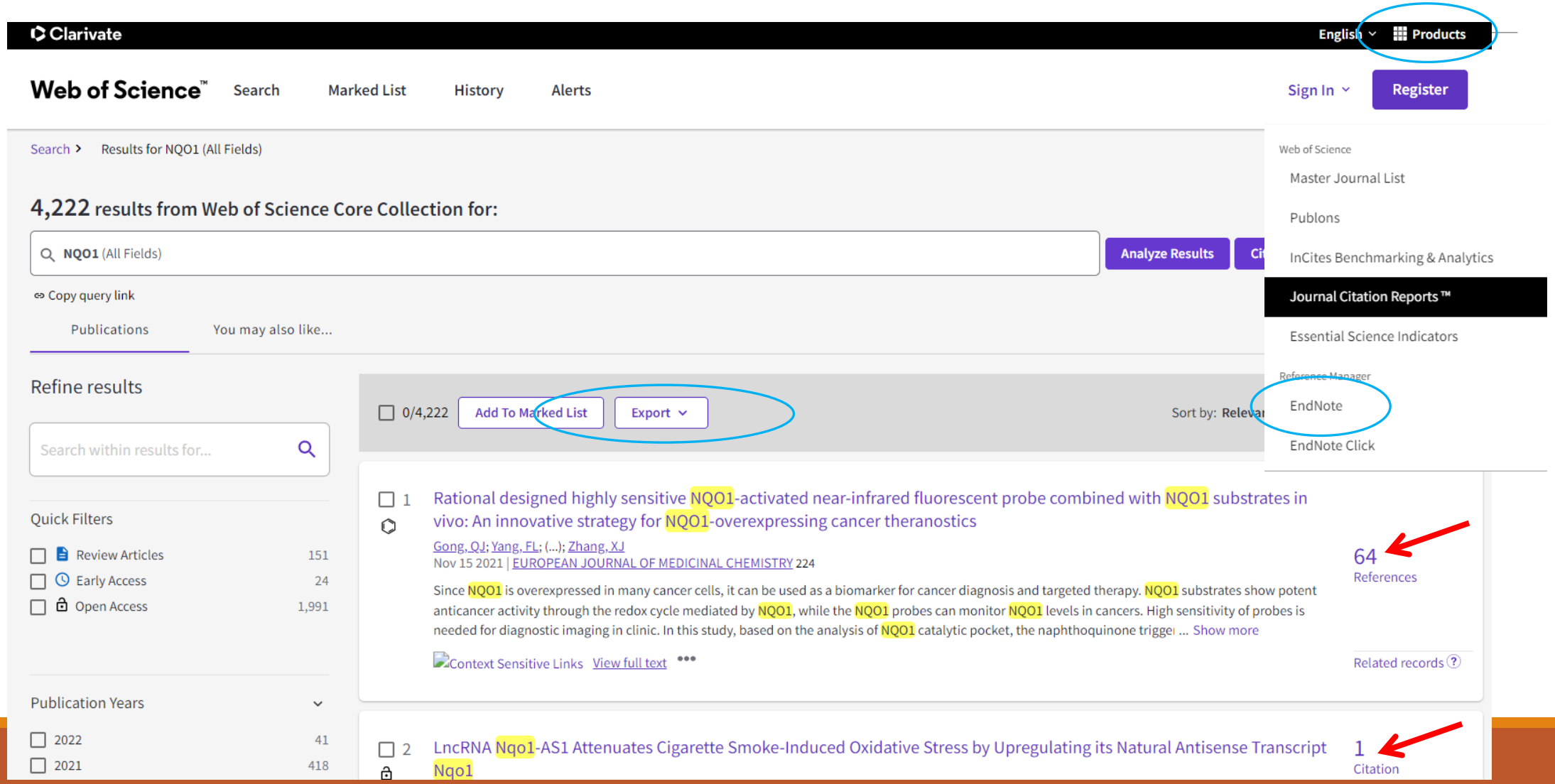
Author-Supplied Keywords: high-grain diet
lipopolysaccharide
liver
oxidative stress

NAICS/Industry Codes: 414510 Pharmaceuticals and pharmacy supplies merchant wholesalers

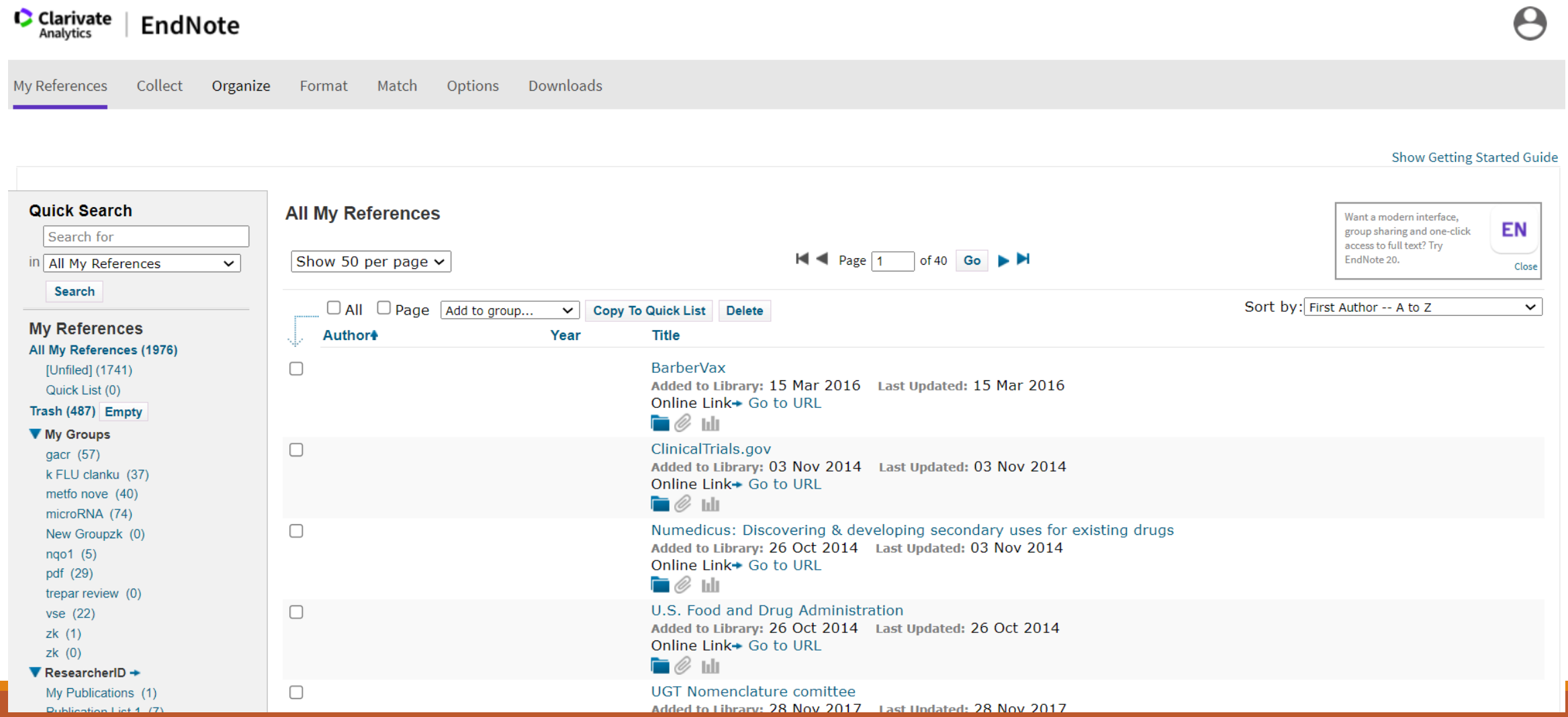
Abstract: The aims of this study were to measure oxidative stress parameters and to investigate the molecular mechanism triggered by grain-induced subacute ruminal acidosis in mid-lactation cows. Twelve Holstein-Friesian cows with an average weight of 455 ± 28 kg were divided into 2 groups and subjected to 2 diets over 18 wk: either a low-grain (forage-to-concentrate ratio = 6:4) or a high-grain (forage-to-concentrate ratio = 4:6) diet based on dry matter. Being fed a long-term highgrain diet resulted in a significant decrease in rumen pH and a significant increase in ruminal lipopolysaccharide (LPS) at 4 h postfeeding in the morning. The increase was also observed in LPS concentrations in the portal vein, hepatic vein, and jugular vein blood plasma as well as reduced milk yield in a high-grain diet. Cows fed a high-grain diet had lower levels of catalase and glutathione peroxidase (GPx) activity and total antioxidant capacity than cows fed a low-grain diet; however, super oxide dismutase (SOD) activity and malondialdehyde (MDA) levels were higher in both the liver and the plasma of high-grain than in low-grain cows. Positive correlations were observed between plasma LPS versus hepatic MDA, plasma MDA, and hepatic SOD activity, whereas hepatic GPx and plasma GPx were negatively correlated with plasma LPS. The relative mRNA abundances of GPX1 and CAT were significantly lower in the liver of cows fed a high-grain diet than those fed a low-grain diet, whereas SOD1 was significantly higher in cows fed a high-grain diet than cows fed a low-grain diet. The expression levels of Nrf2, NQO1, MT1E, UGT1A1, MGST3, and MT1A were downregulated, whereas NF-kB was upregulated, in cows fed a high-grain diet. Furthermore, nuclear factor E2-related factor 2 (Nrf2) total protein and mRNA levels were significantly lower than in low-grains. Our results demonstrate the relationship between the translocated LPS and the suppression of cellular antioxidant defense capacity, which lead to increased oxidative stress and suggests that the Nrf2-dependent antioxidant response may be affected by higher levels of LPS translocated to the bloodstream. [ABSTRACT FROM AUTHOR]

Tools
Add to folder
Print
E-mail
Save
Cite
Export
Create Note
Permalink
Share

# Literature search– citations (EndNote)



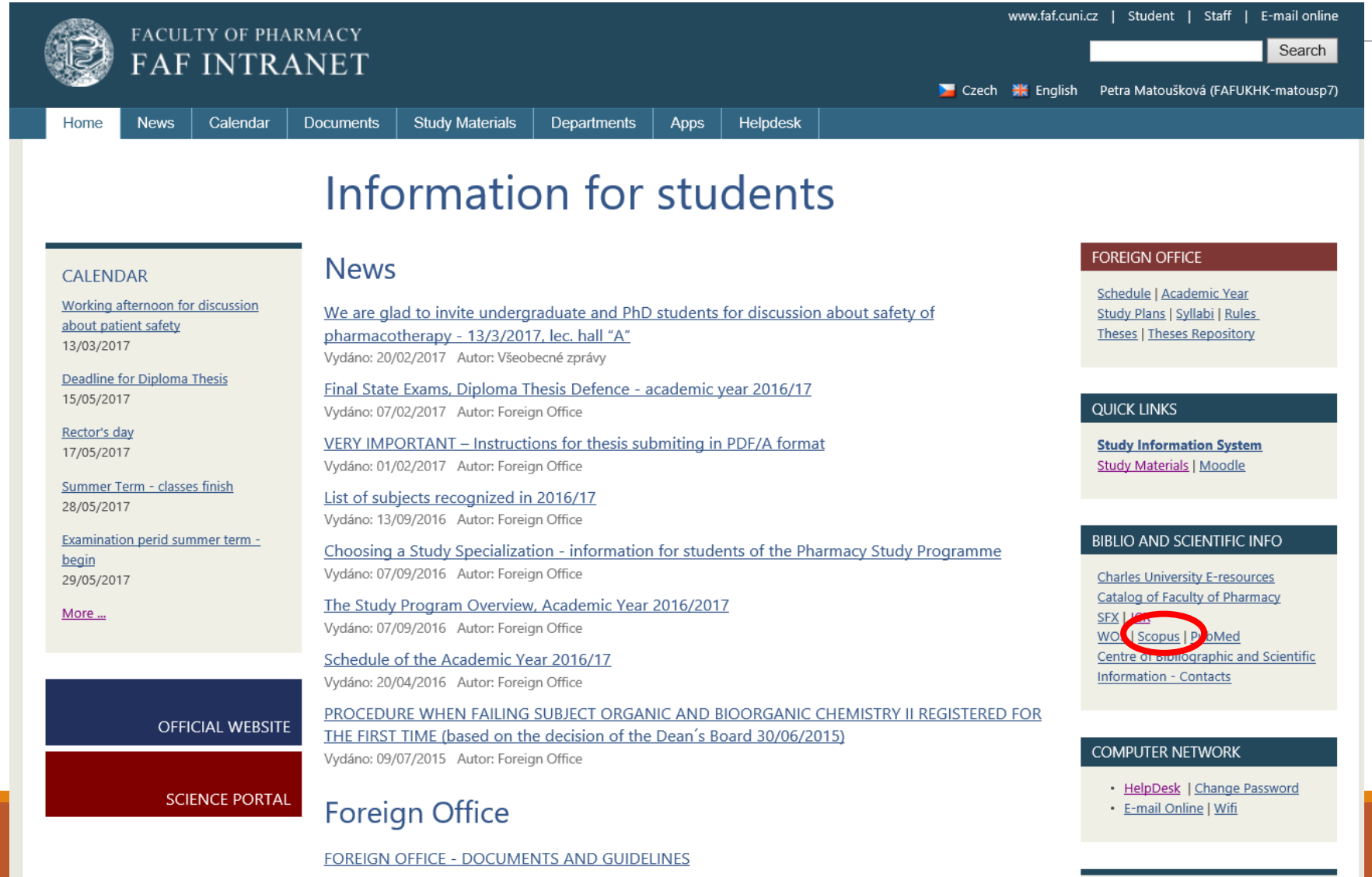
# Literature search



Try WOS !

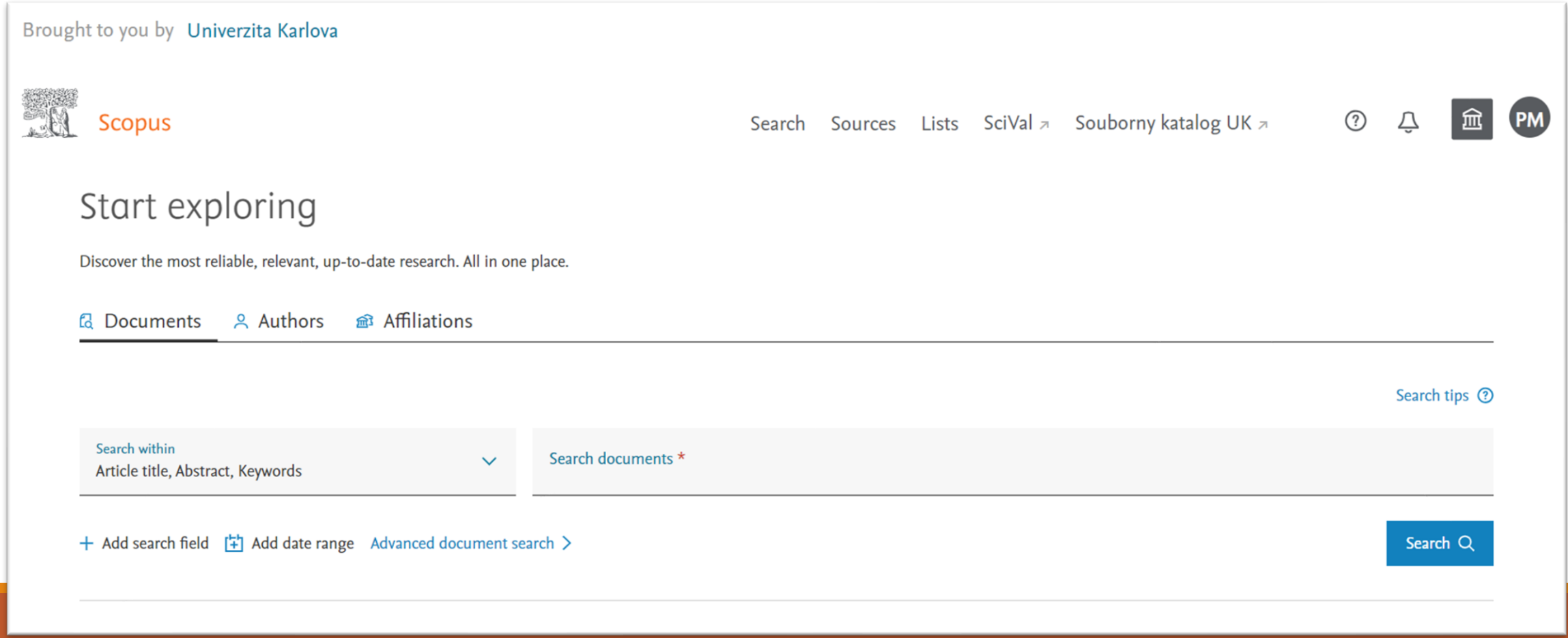
Register-Login into WebEndnote!

# Literature search



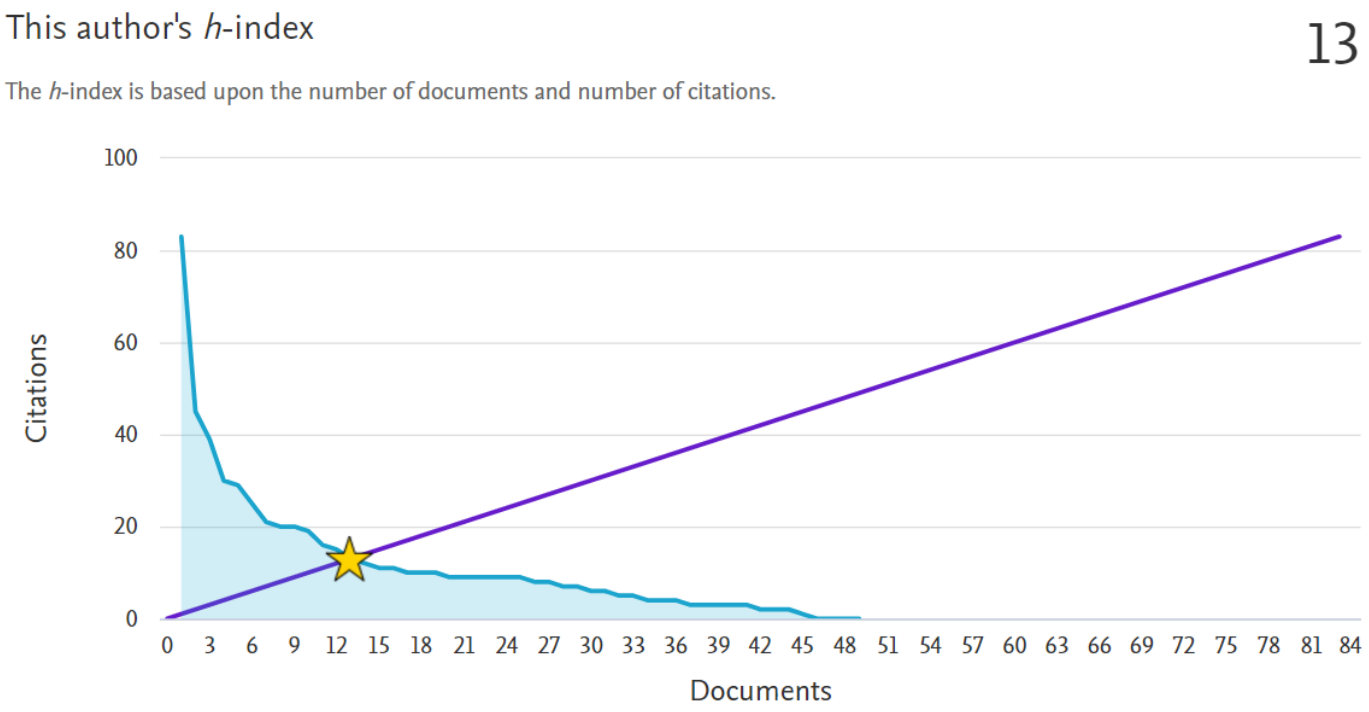
# Literature search / H-index

http://www.scopus.com



# H-index

= an **author-level metric** that measures both the productivity and citation impact of the publications of a scientist



# Literature search / Homework 1

1) find full name of your gene

2) find 5 relevant literature

   - at least one review

   - at least one publication from 2022-23

   - 1 older publication than 2000

3) log into WEB Endnote account a import your selected citations into „My references“

4) select one interesting fact about your gene

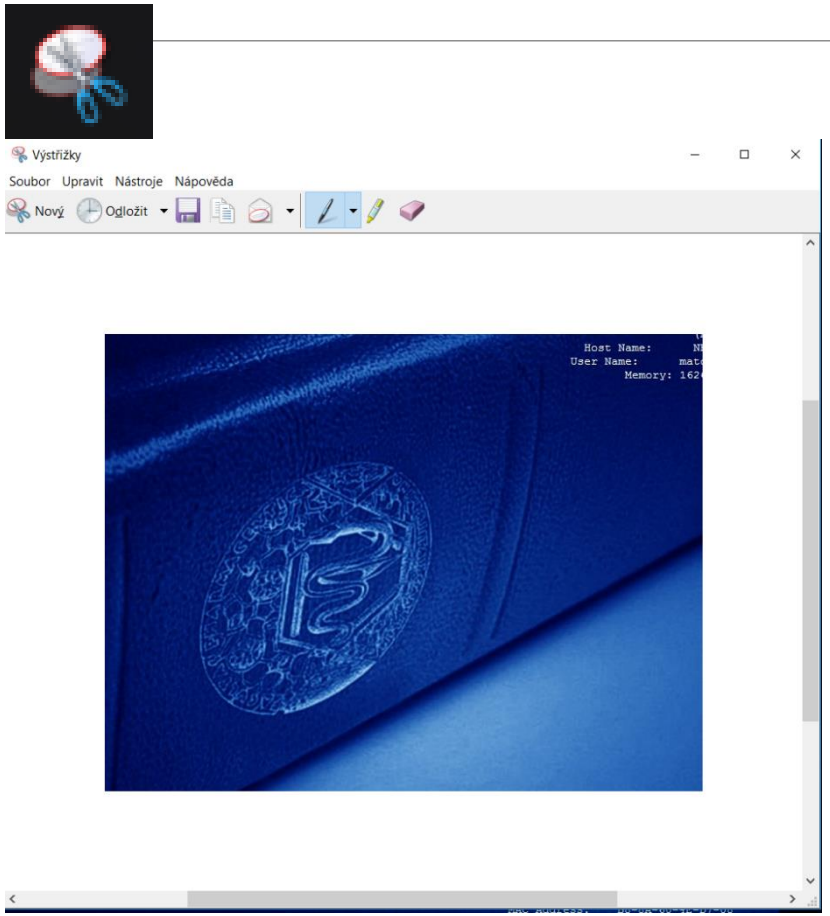
5) find the H-index of your favorite FaF teacher

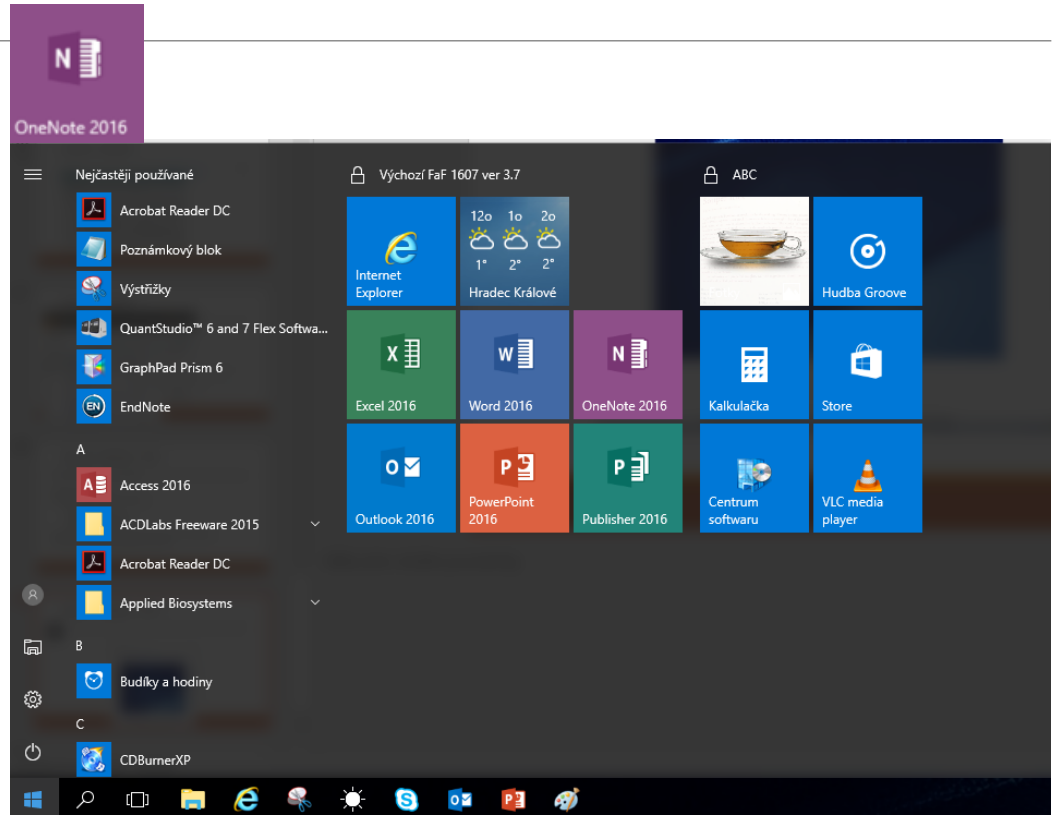
- E.g use „výstřižky“

- Compile in Word, pdf, one note…
- Submit in Moodle

„snipping tool“

# Literature search / Homework 1



# Literature search / Homework 1 - example