Introduction to applied bioinformatics

PETRA MATOUŠKOVÁ

2024/2025

Organization:

Each student 1 gene/protein

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

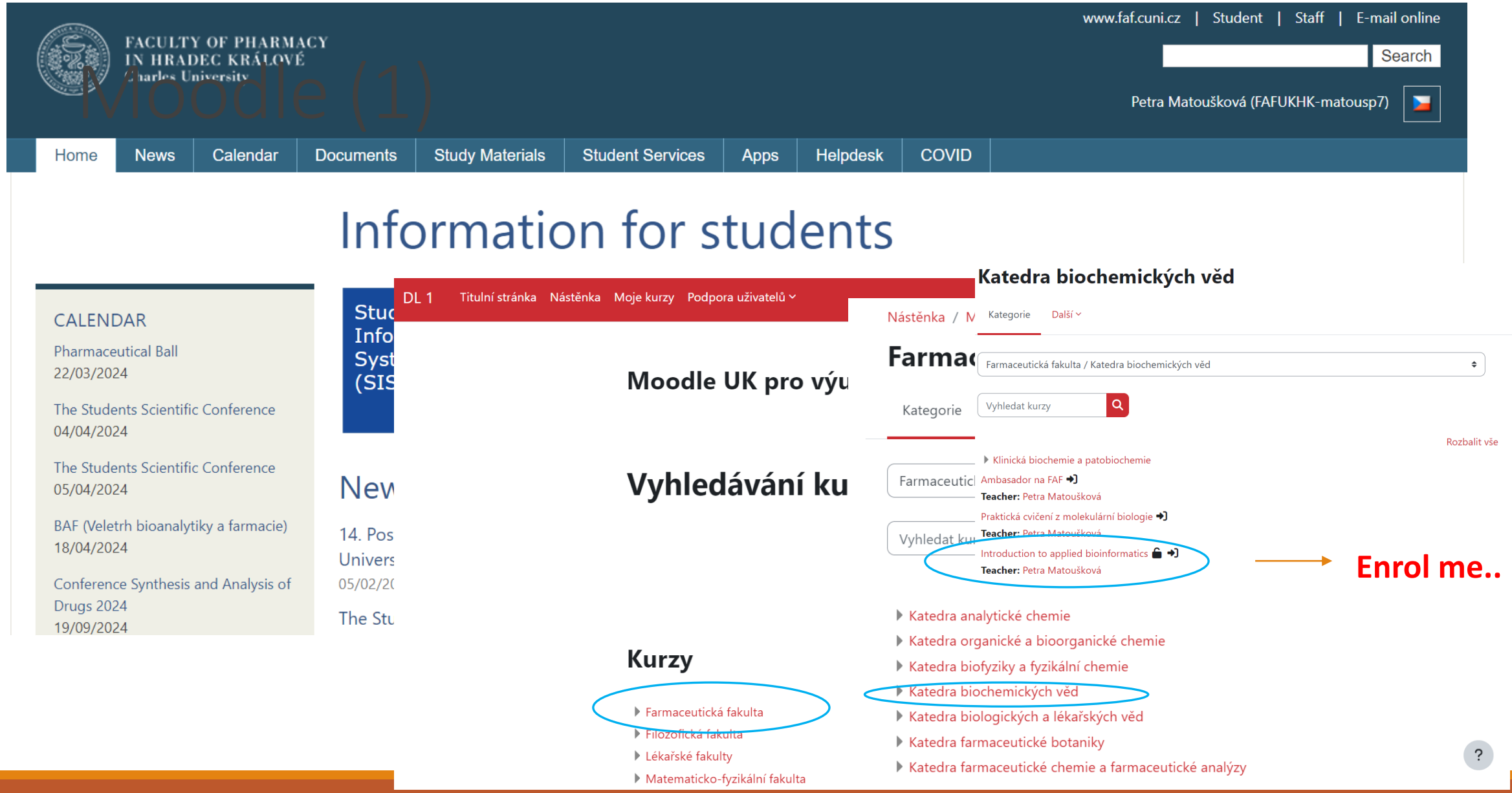
(+ compulsory presence 8/10 lectures)

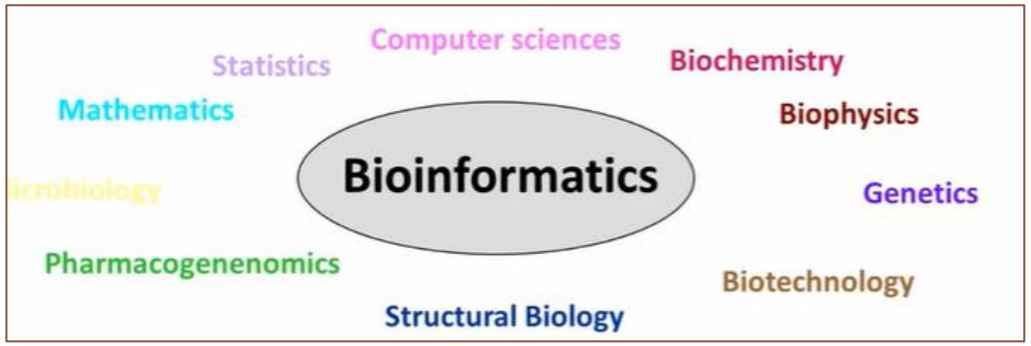
↓

Exam: „written" by computer – selected exercises

Týden	Datum		Čas
2	25.2.2025	1	Út 13:10 - 14:40
5	17.3.2025	2	Po 8:00 - 9:30
6	25.3.2025	3	Út 13:10 - 14:40
7	31.3.2025	4	Po 8:00 - 9:30
7	1.4.2025	5	Út 8:00 - 9:30
8	8.4.2025	6	Út 13:10 - 14:40
9	14.4.2025	7	Po 8:00 - 9:30
9	15.4.2025	~~?~~	Út 8:00 - 9:30
10	22.4.2025	8	Út 13:10 - 14:40
11	28.4.2025	9	Po 8:00 - 9:30
11	29.4.2025	~~10~~	Út 8:00 - 9:30
12	6.5.2025	**exam?**	Út 13:10 - 14:40
13	12.5.2025	**(Exam)**	Po 8:00 - 9:30
13	*~~13.5.2025~~*		*Út 8:00 - 9:30*

Moodle (1)


FACULTY OF PHARMACY
IN HRADEC KRÁLOVÉ
Charles University
www.faf.cuni.cz | Student | Staff | E-mail online
Search
Petra Matoušková (FAFUKHK-matousp7)
Home
News
Calendar
Documents
Study Materials
Student Services
Apps
Helpdesk
COVID
Information for students
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
DL 1
Titulní stránka
Nástěnka
Moje kurzy
Podpora uživatelů
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
Enrol me..
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

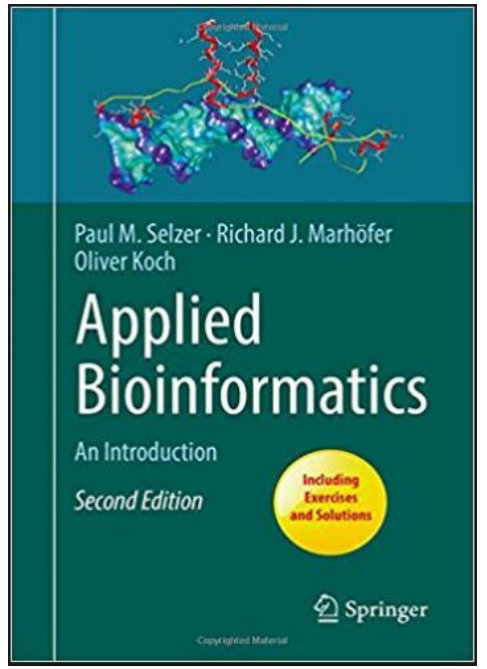


Bioinformatics is about…

= 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 need: be able to script and programme
need: knowledge of basic principles of molecular biology

DNA

Sequence analysis

Mutations and pleomorphism studies

Identification of regulatory regions

Gene finding

Genome annotations

Comparative genomics

RNA

RNA sequencing

Splice variants

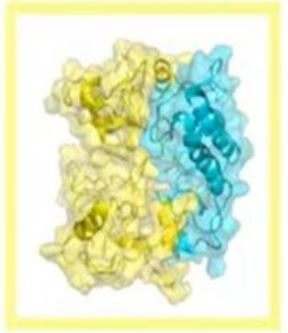
Tissue expression levels

MicoArray

Single gene analysis

Sequence contigs

Protein



Homology modeling

Structure-function prediction

Ligand docking

Protein-protein interactions

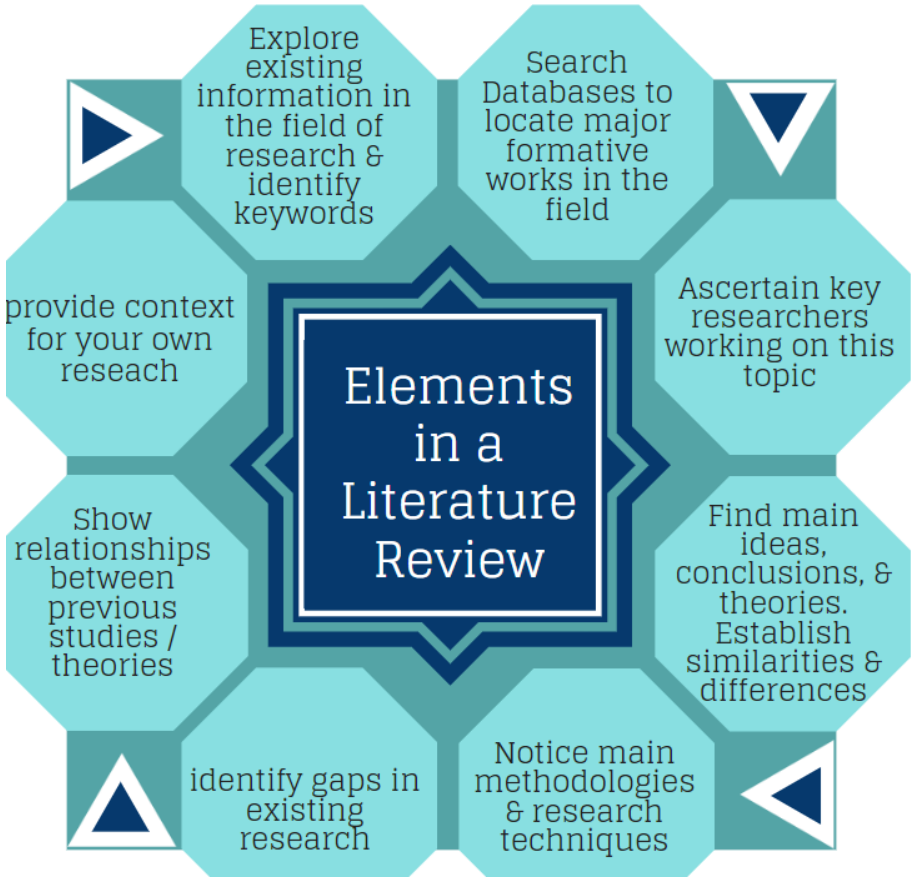
Protein expression

Phylogenetic analysis

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

Create account Log in

Article Talk Read Edit View history Search

WIKIPEDIA
The Free Encyclopedia

Main page
Contents
Featured content
Current events
Random article
Donate to Wikipedia

Interaction
Help
About Wikipedia
Community portal
Recent changes
Contact page

Tools

Print/export

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]

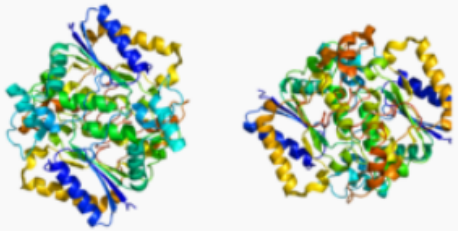
This gene is a member of the NAD(P)H dehydrogenase (quinone) family and encodes a cytoplasmic 2-electron reductase. This FAD-binding protein forms homodimers and reduces quinones to hydroquinones. This protein's enzymatic activity prevents the one electron reduction of quinones that results in the production 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

ChatGPT

what is NQO1?

NQO1 (**NAD(P)H:quinone oxidoreductase 1**) is an enzyme that plays a crucial role in cellular redox balance and detoxification. It is a flavoprotein that catalyzes the two-electron reduction of quinones to hydroquinones using NADH or NADPH as an electron donor. This process helps protect cells from oxidative stress and prevents the formation of reactive oxygen species (ROS).

Functions of NQO1:

1. **Detoxification** – Reduces quinones to less reactive and less toxic hydroquinones, preventing the formation of semiquinone radicals.
2. **Antioxidant Defense** – Contributes to cellular antioxidant mechanisms by maintaining reduced forms of coenzymes such as Coenzyme Q10 and vitamin E.
3. **Cancer Protection & Tumor Suppression** – NQO1 is often upregulated in response to oxidative stress and is associated with the protection of p53, a key tumor suppressor protein.
4. **Drug Metabolism** – Plays a role in activating or detoxifying certain drugs and environmental toxins.

Clinical Relevance:

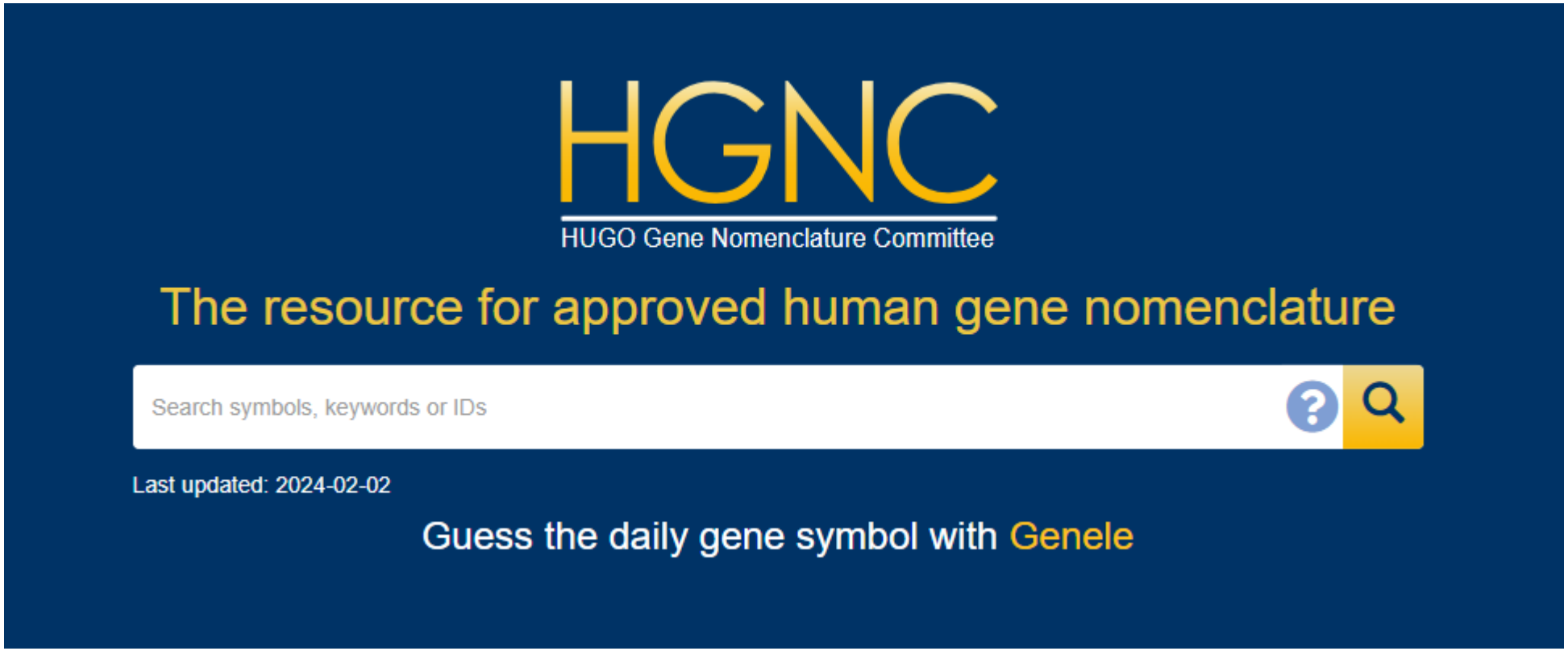
- **Cancer**: NQO1 is overexpressed in many cancers, making it a potential target for cancer therapy. Some anticancer drugs are designed to exploit this overexpression.

Research Project: NQO1

Quinone:NAD(P)H dehydrogenase 1

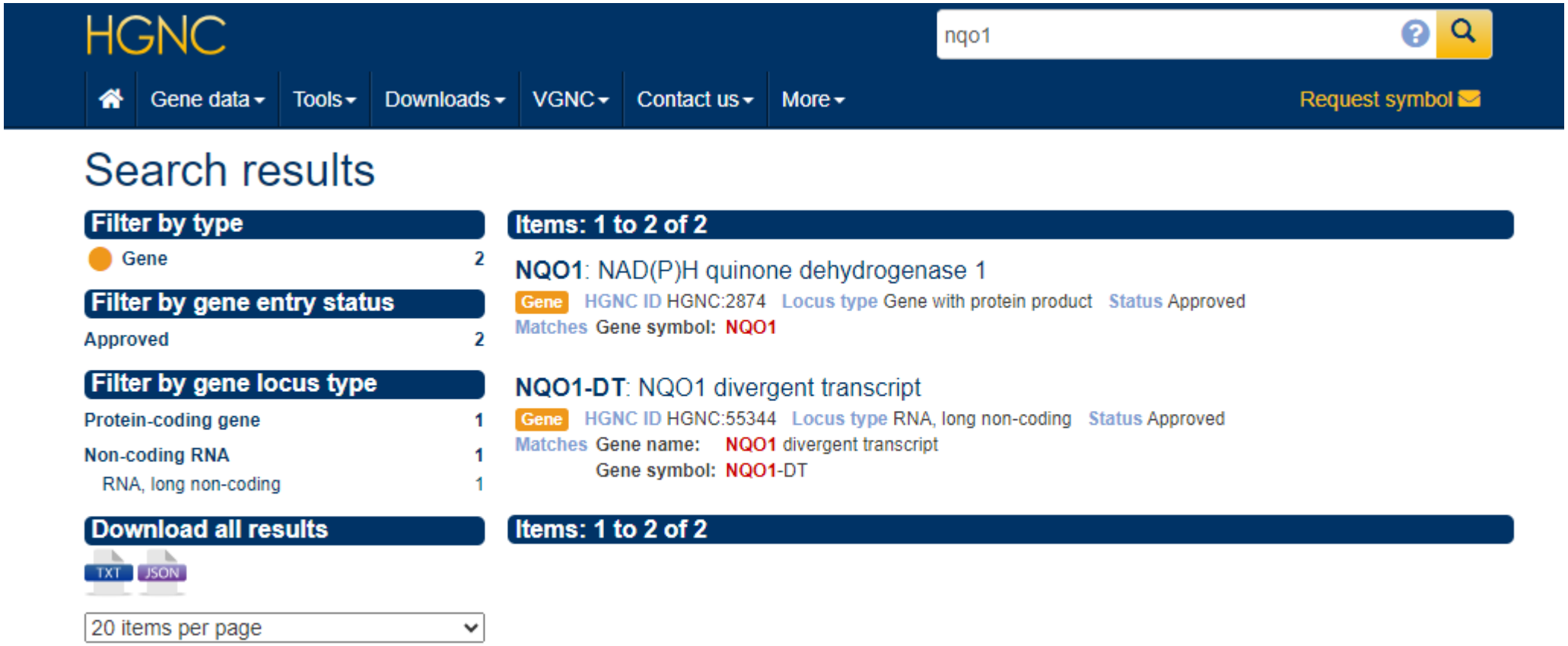
Identify the gene symbol!

HUGO database

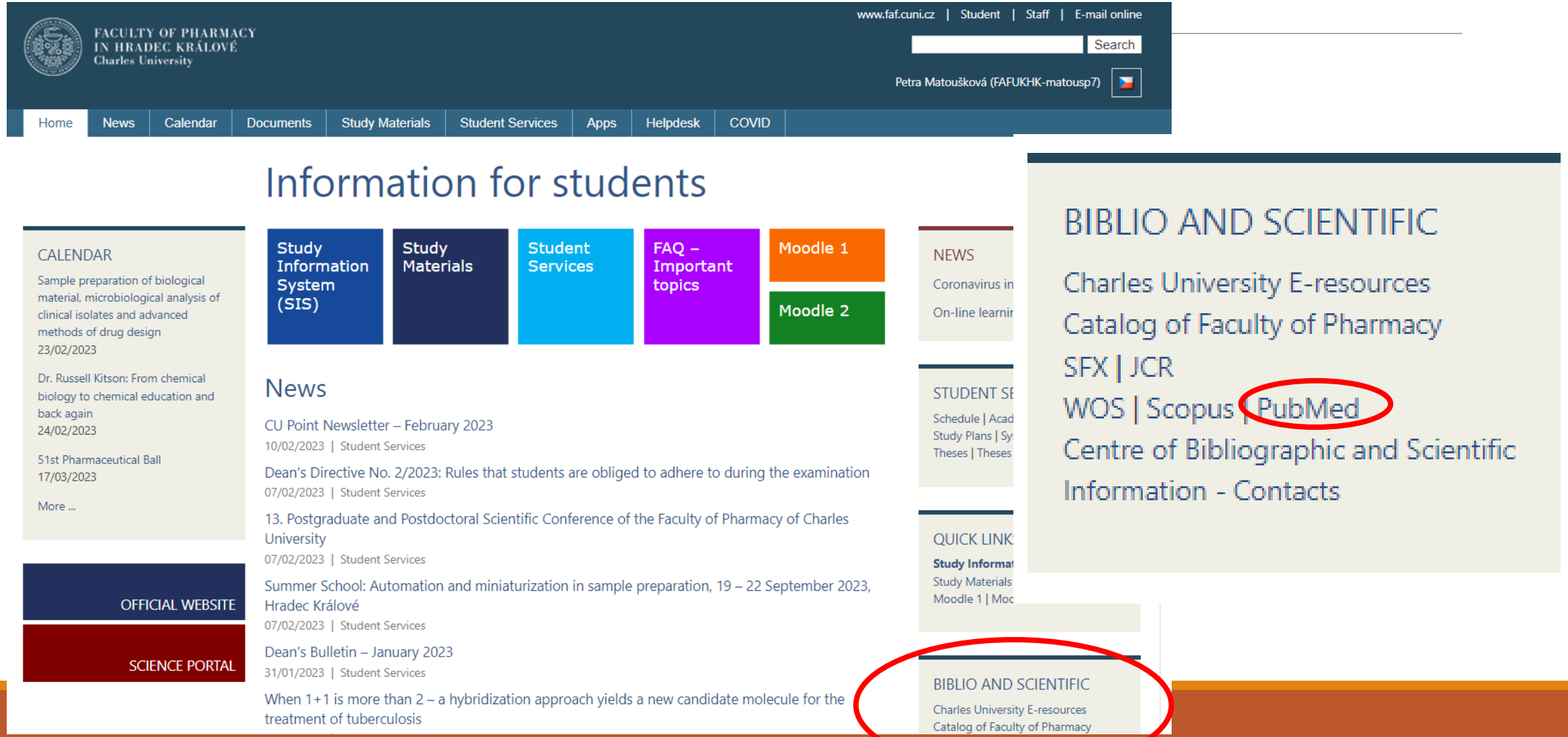


Identify the gene symbol!

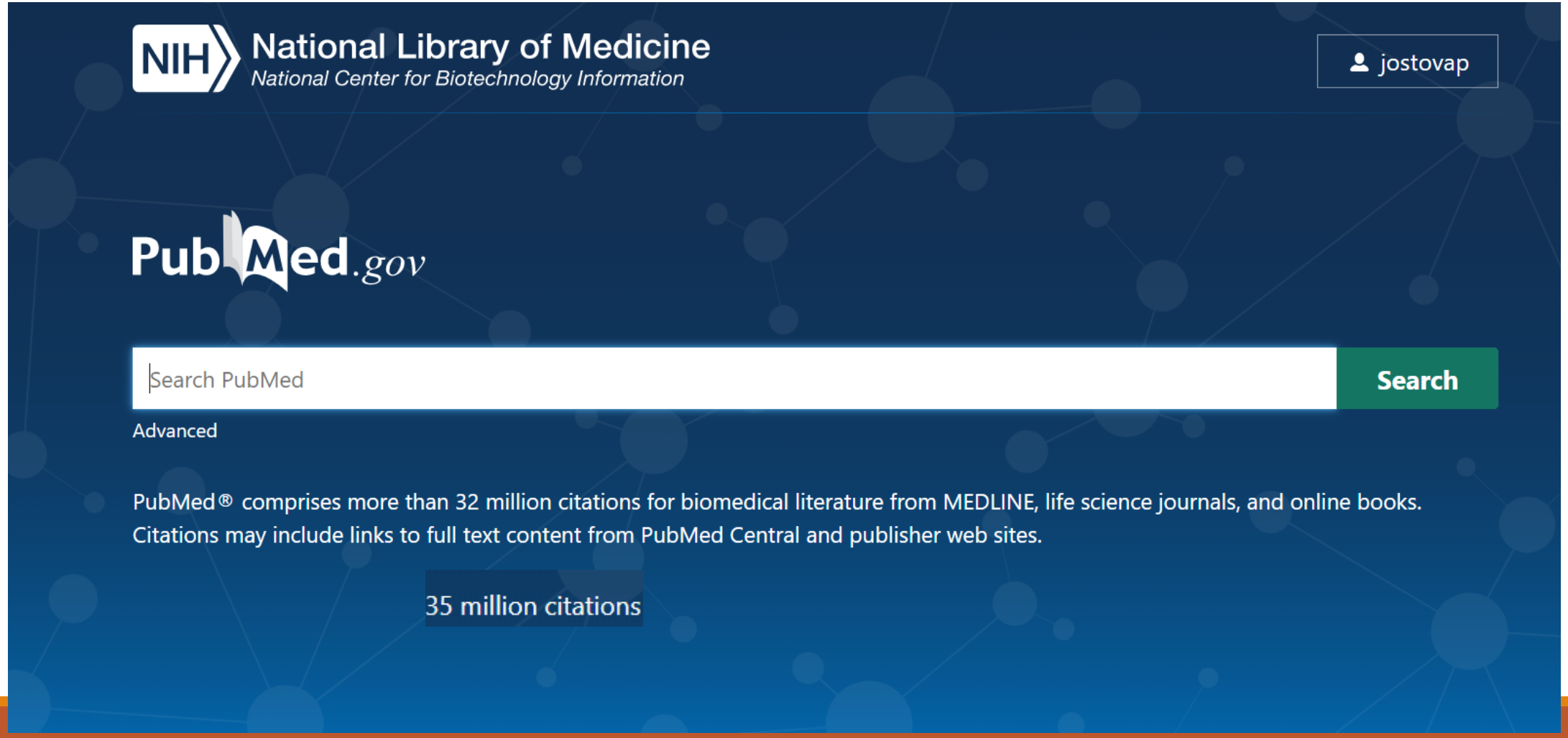
HUGO database



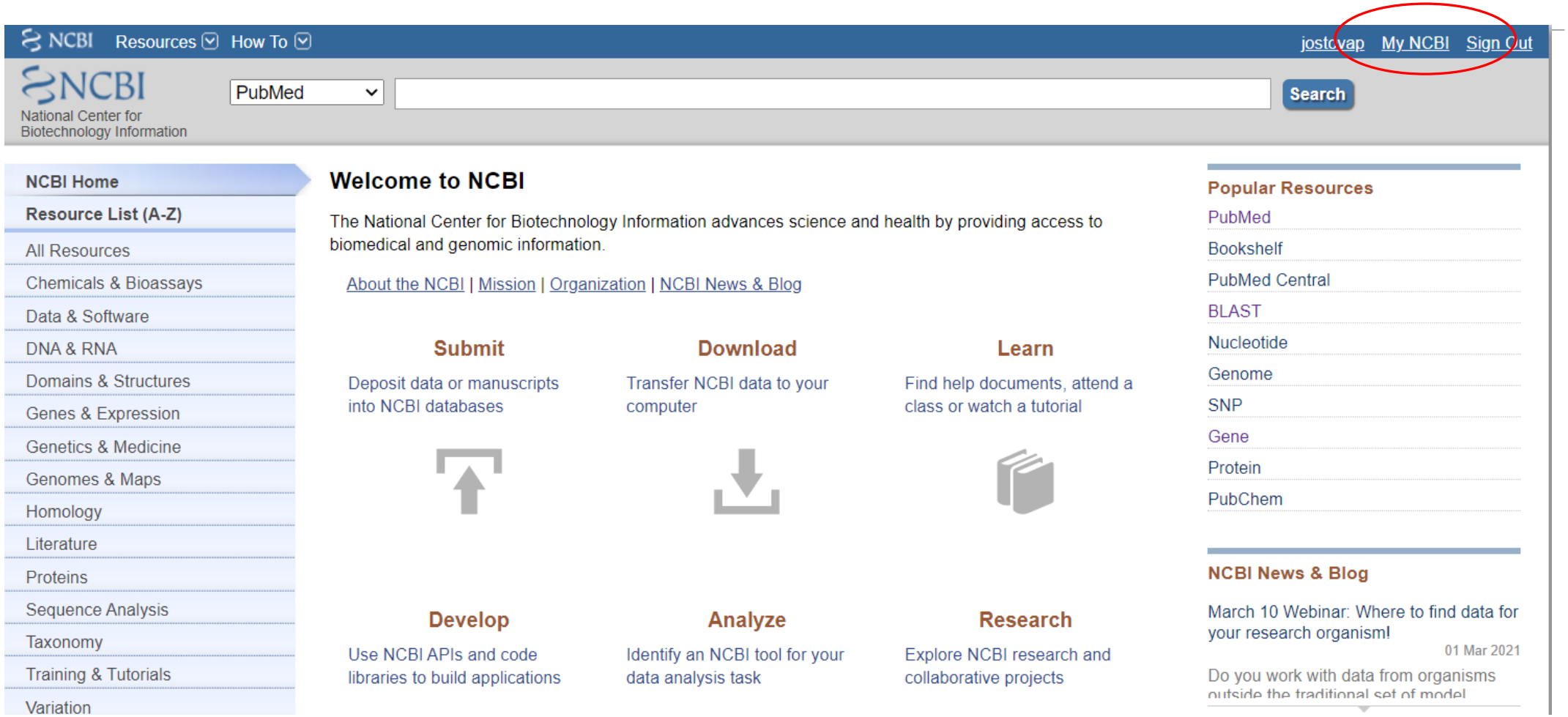
Literature search



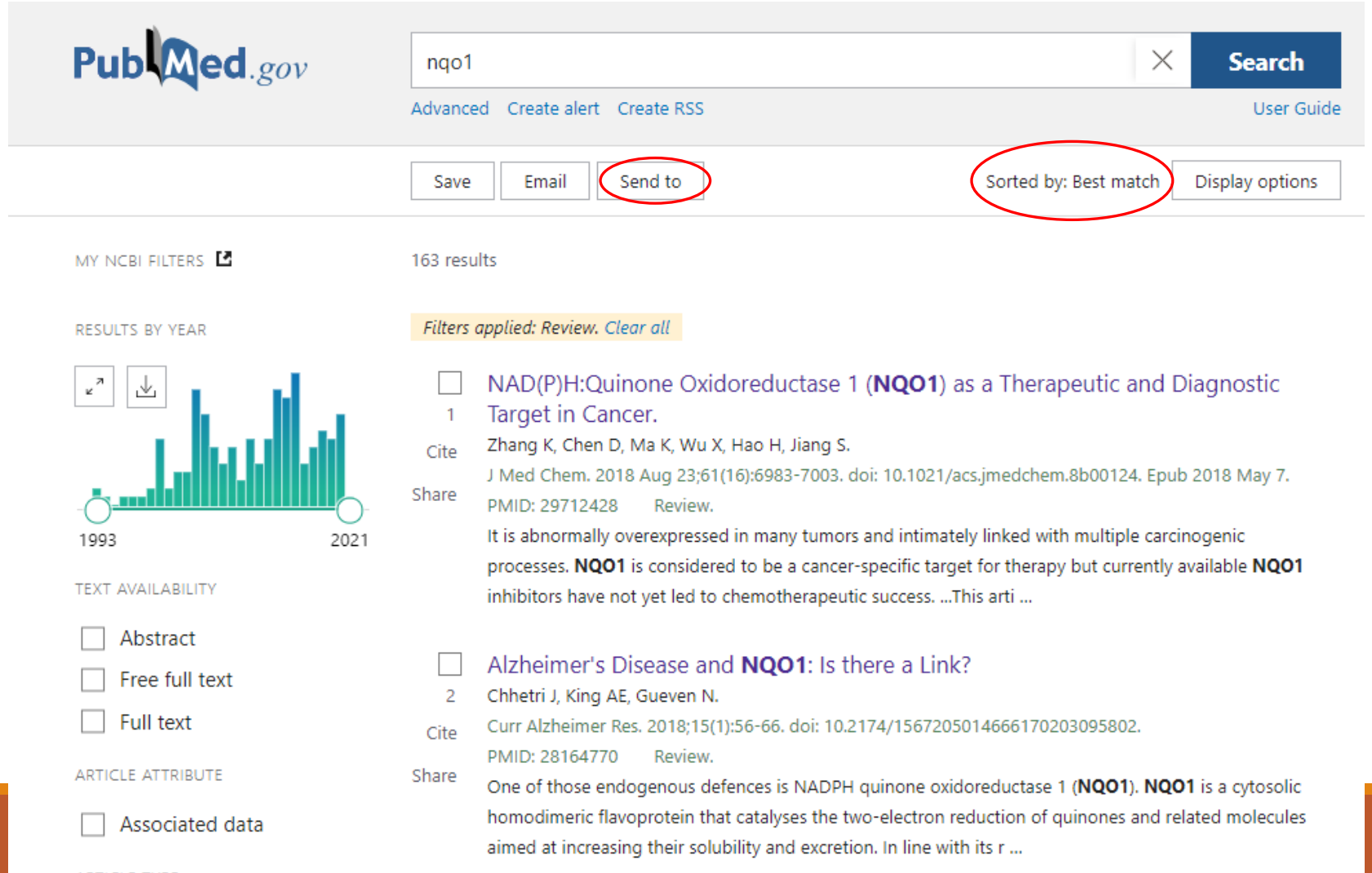
Literature search **PubMed** http://www.ncbi.nlm.nih.gov/pubmed/



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

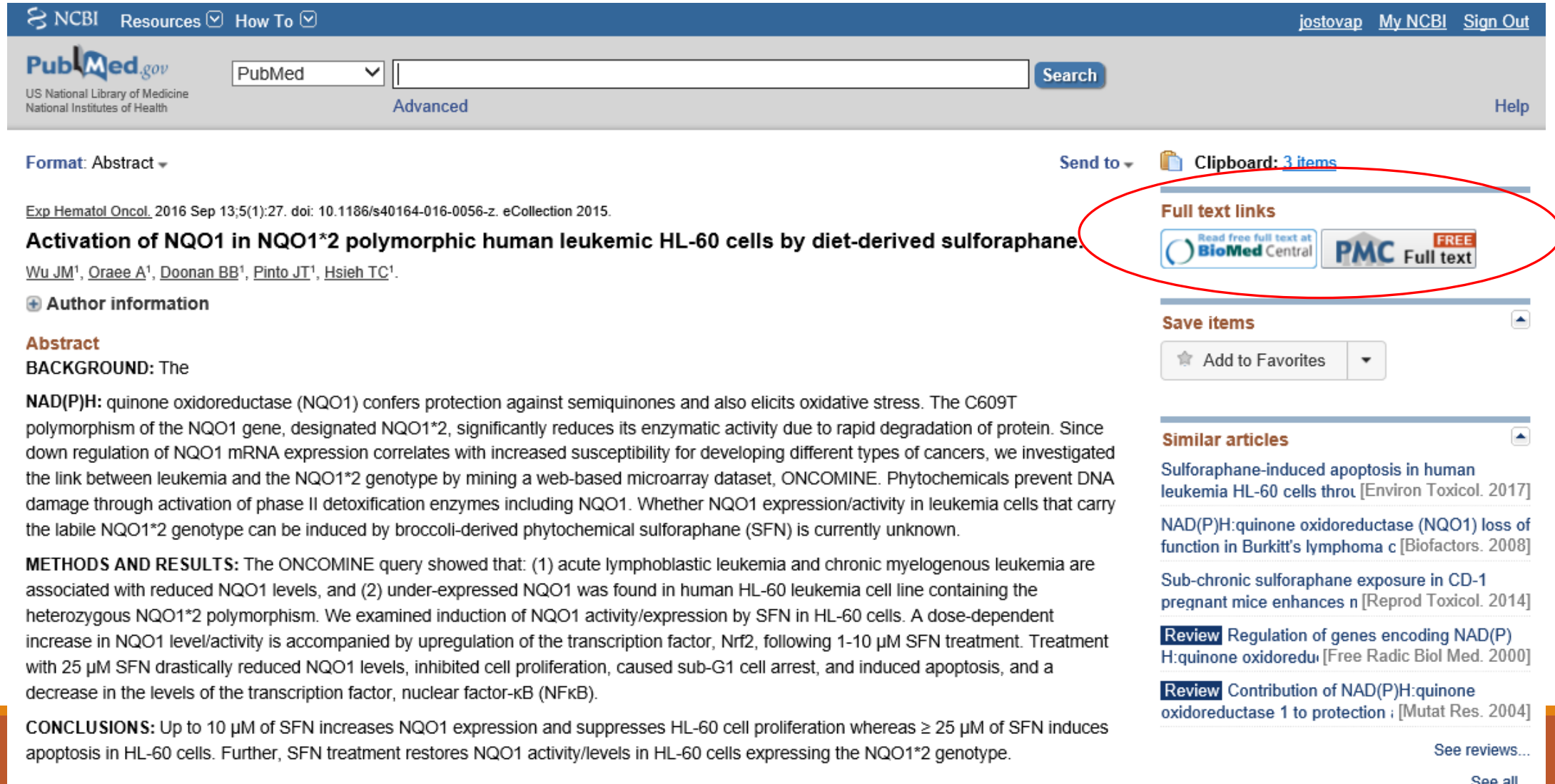


Literature search **PubMed** http://www.ncbi.nlm.nih.gov/pubmed/



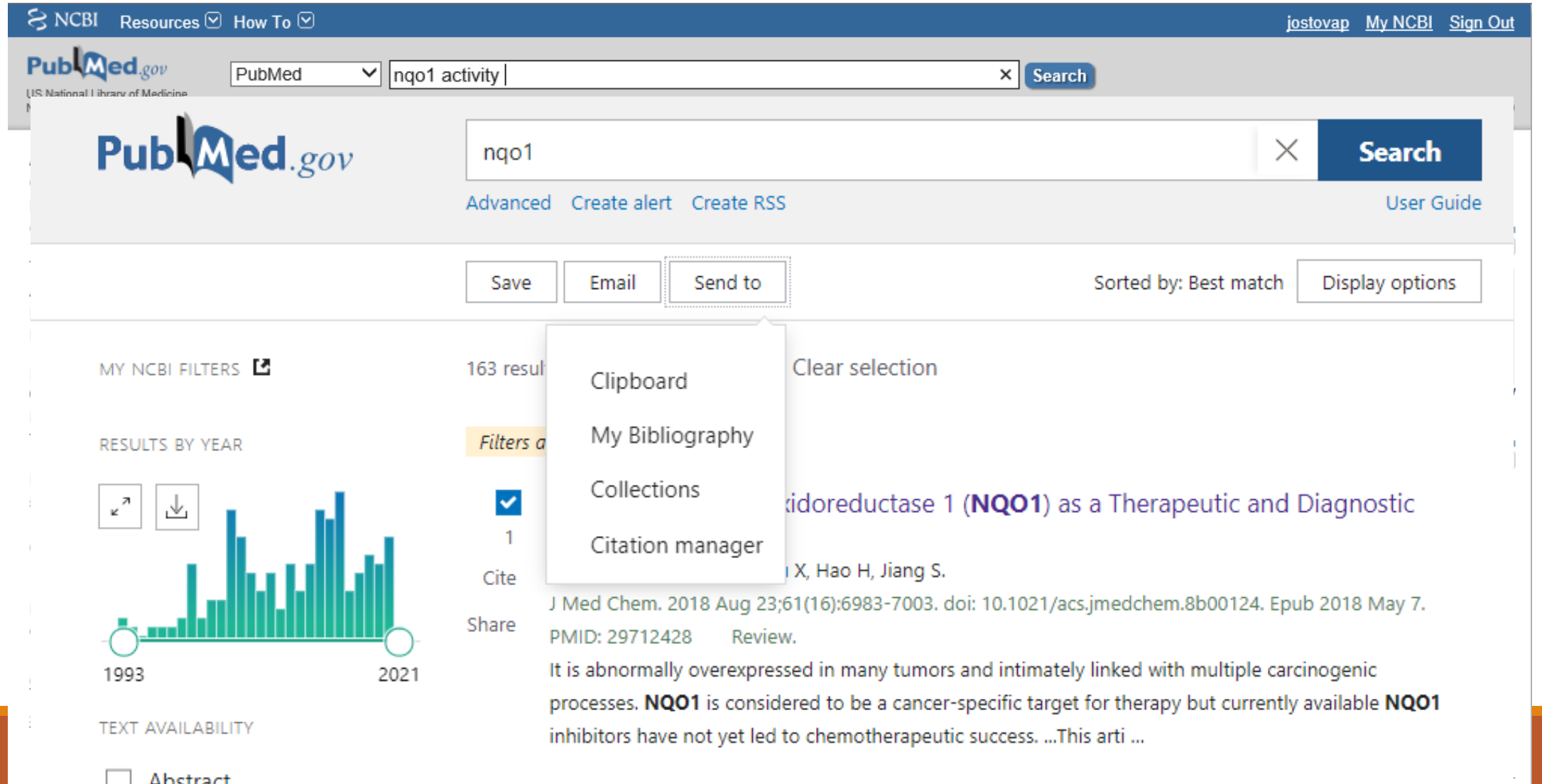
Literature search

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



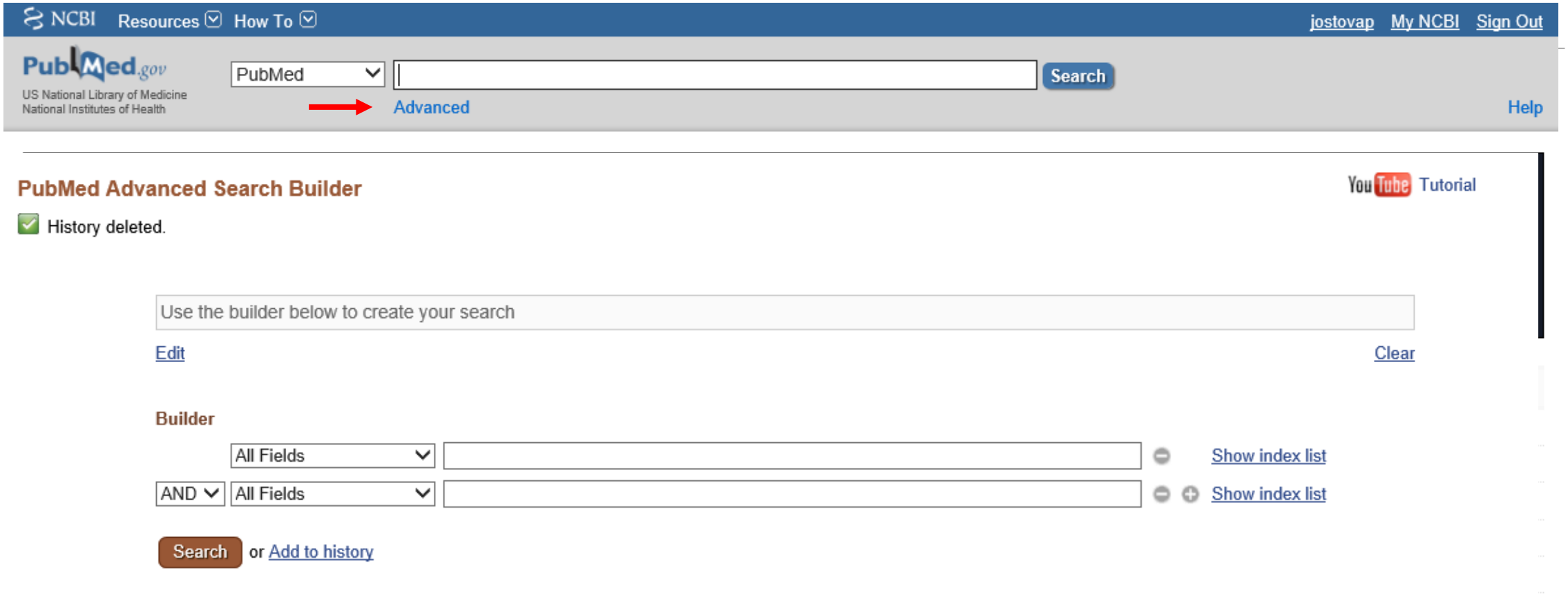
Literature search

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



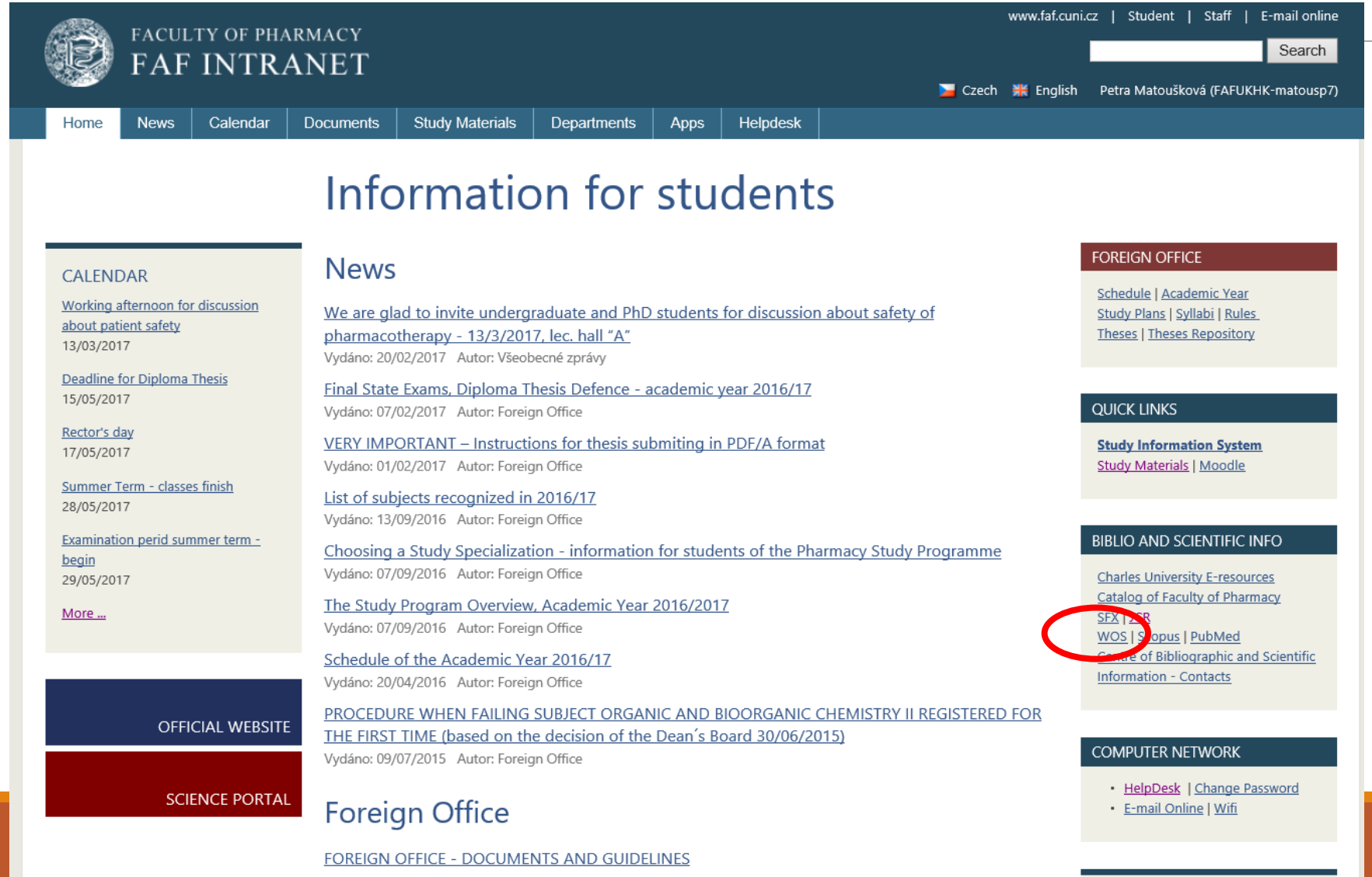
Literature search

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



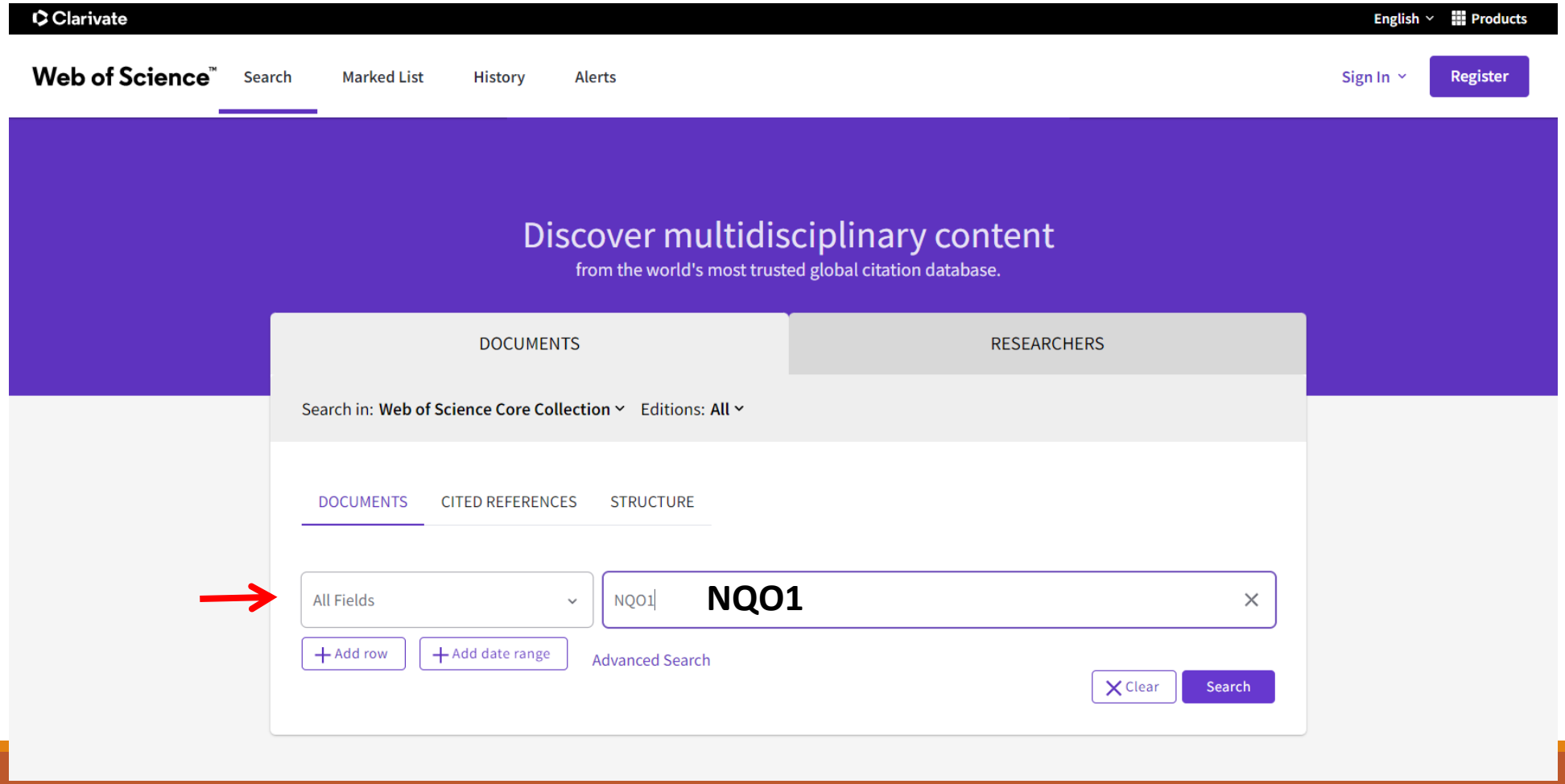
Try PubMed !

Literature search



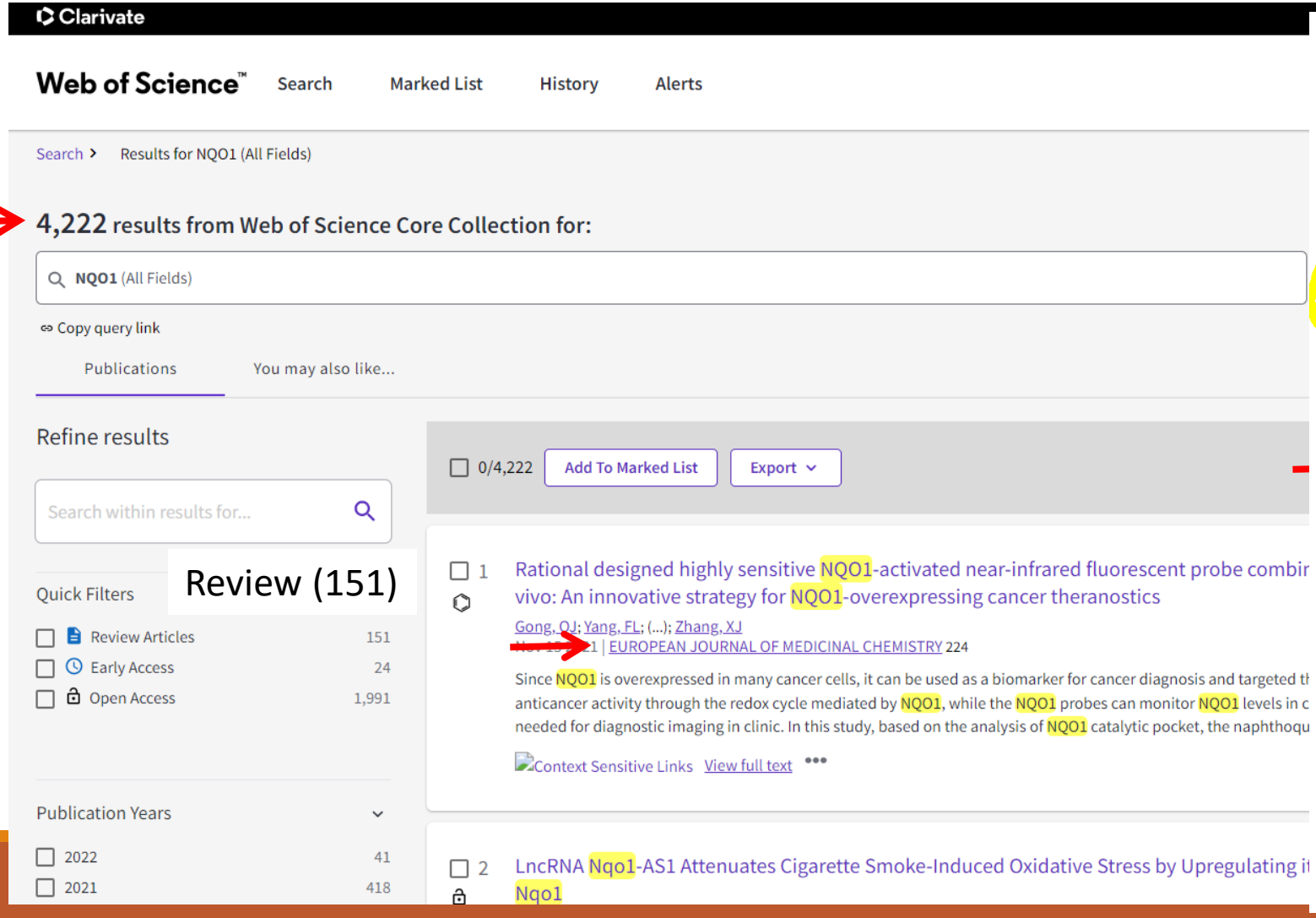
Literature search

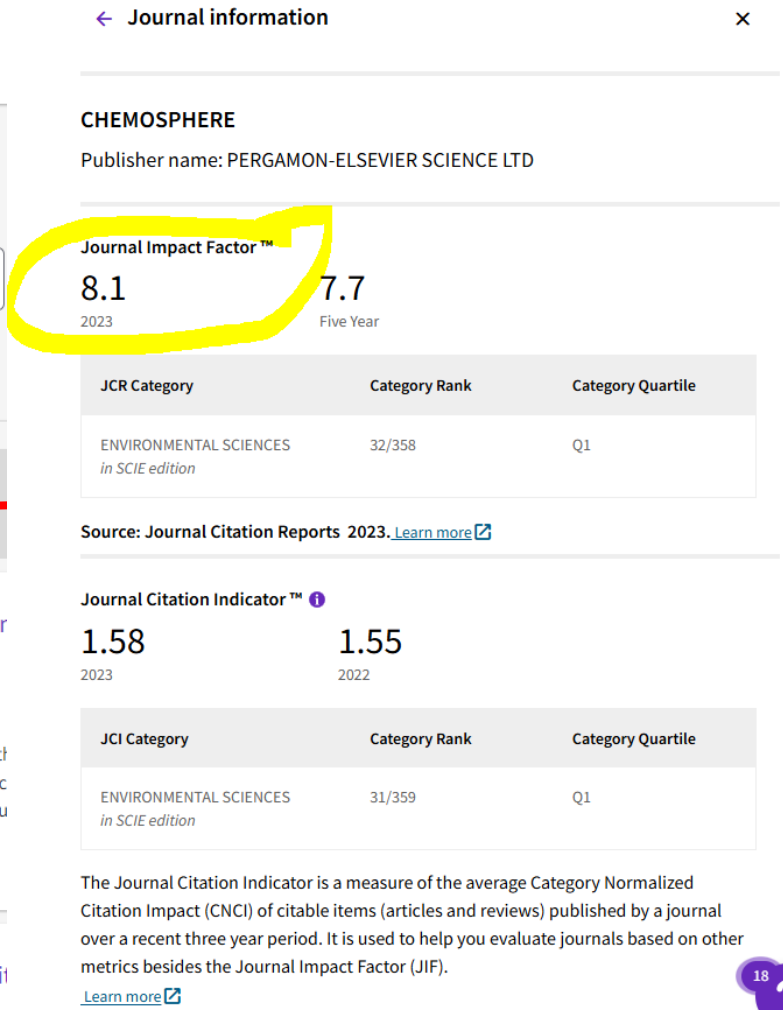
WOS http://apps.webofknowledge.com/



Literature search

Impact factor





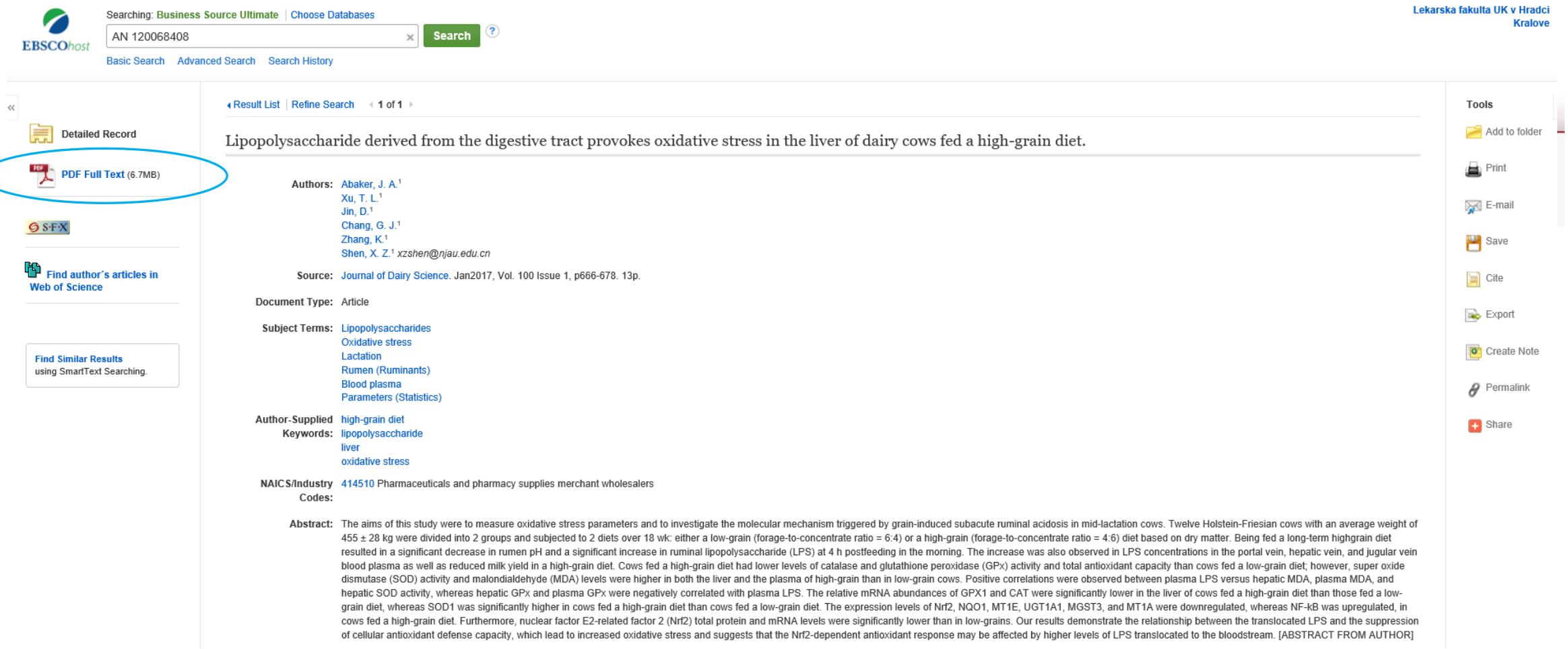
impact factor

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

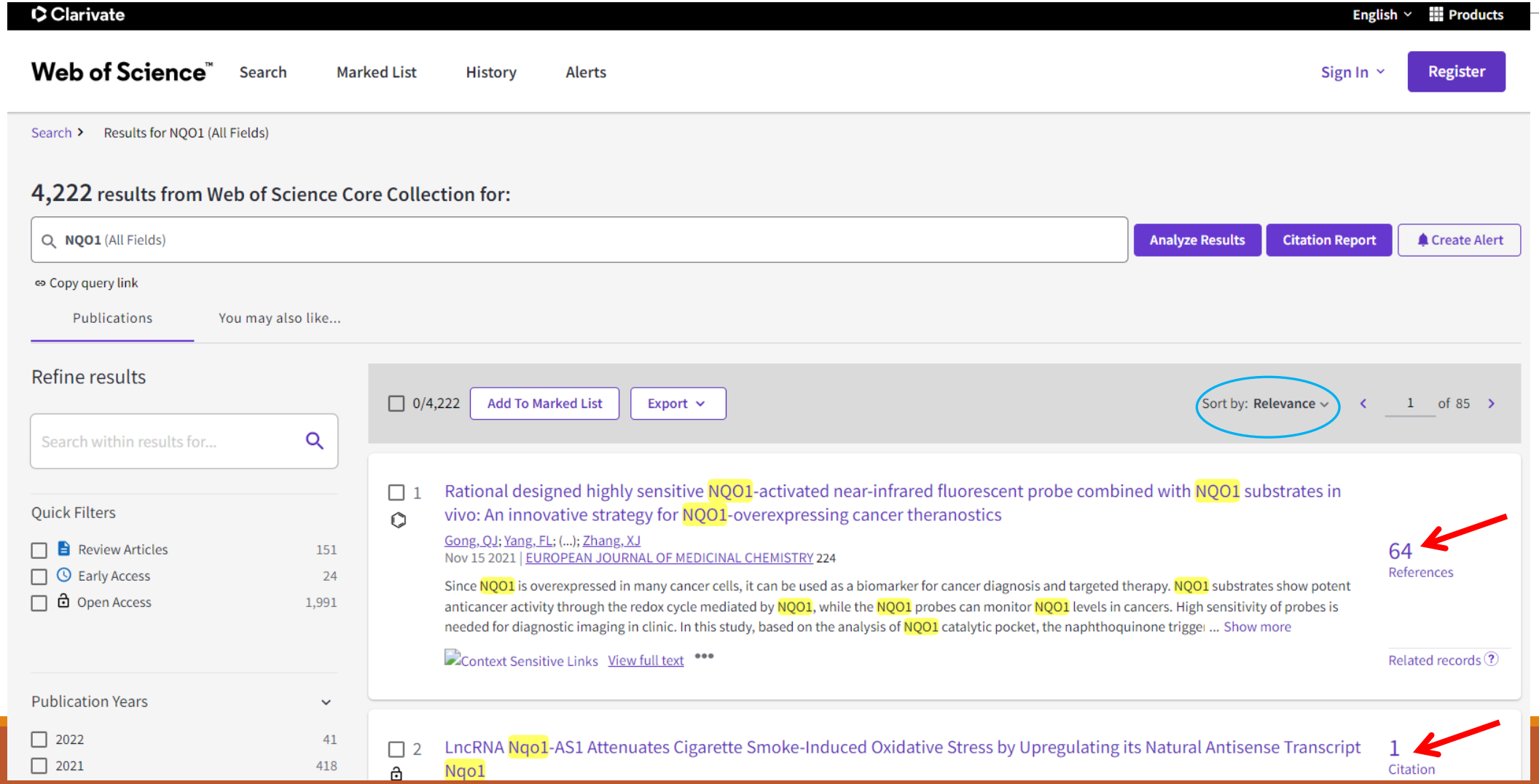
~relative **importance of the journal** within its field

Literature search

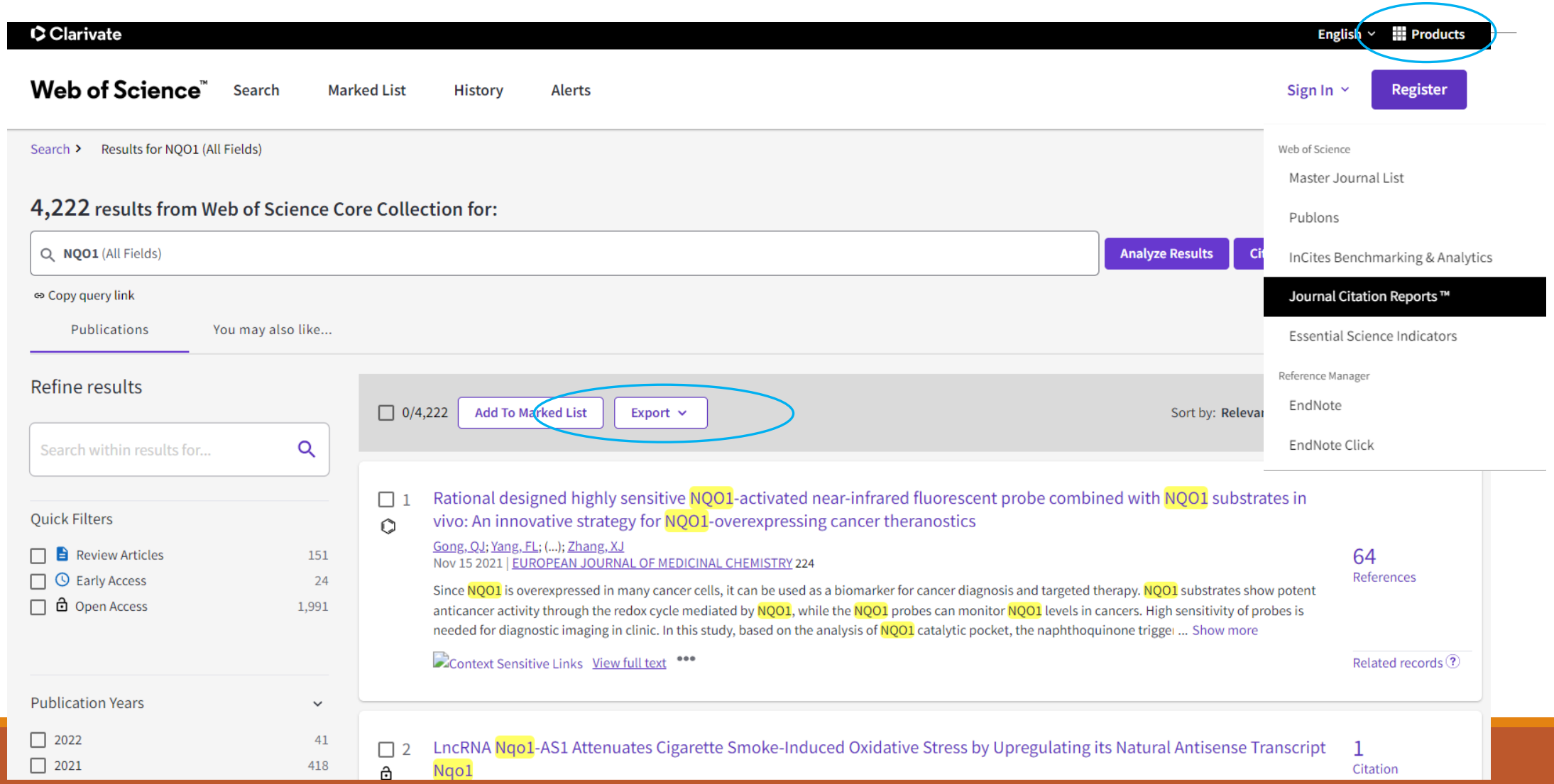
Literature search



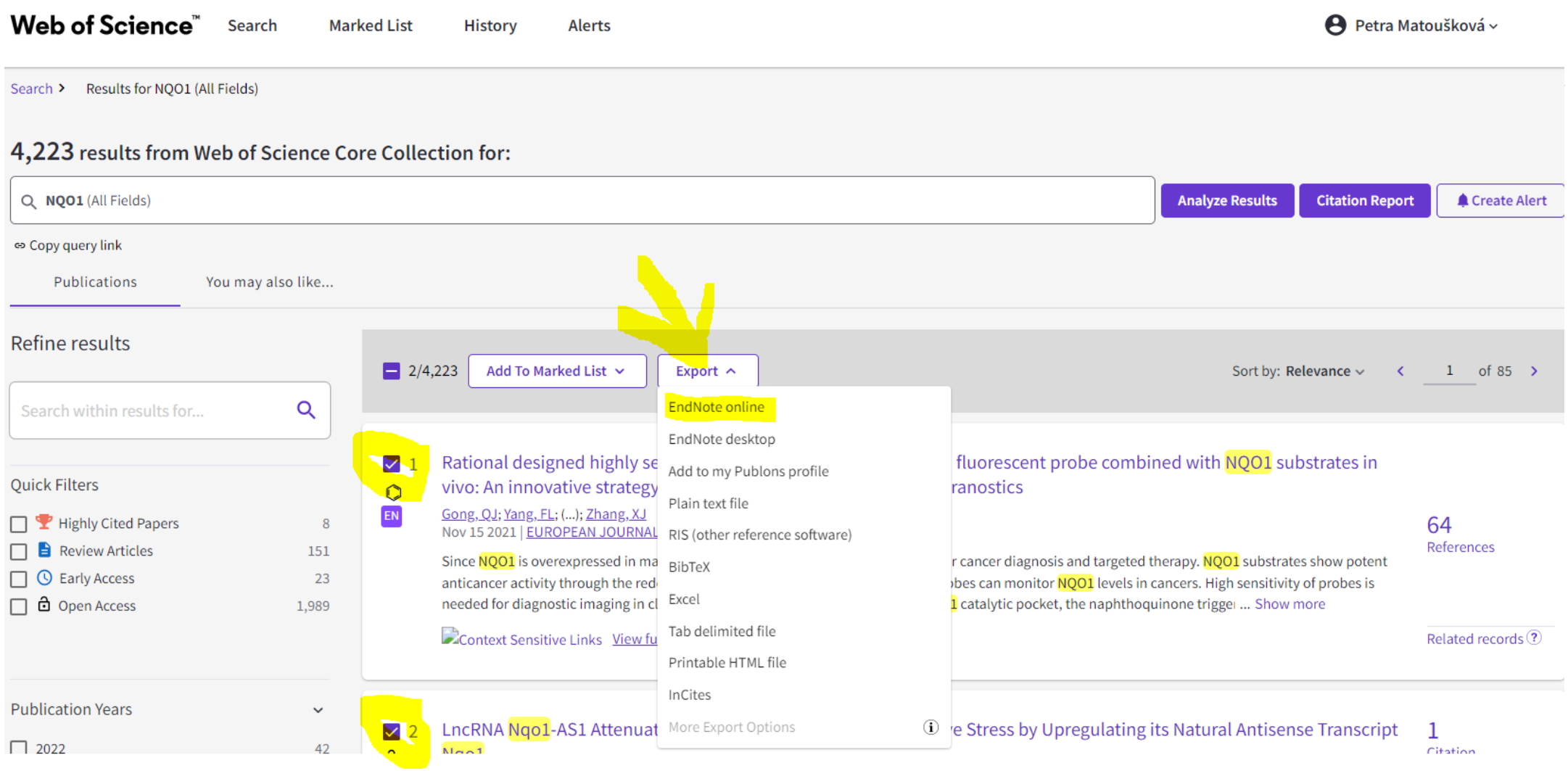
Literature search– citations (EndNote)



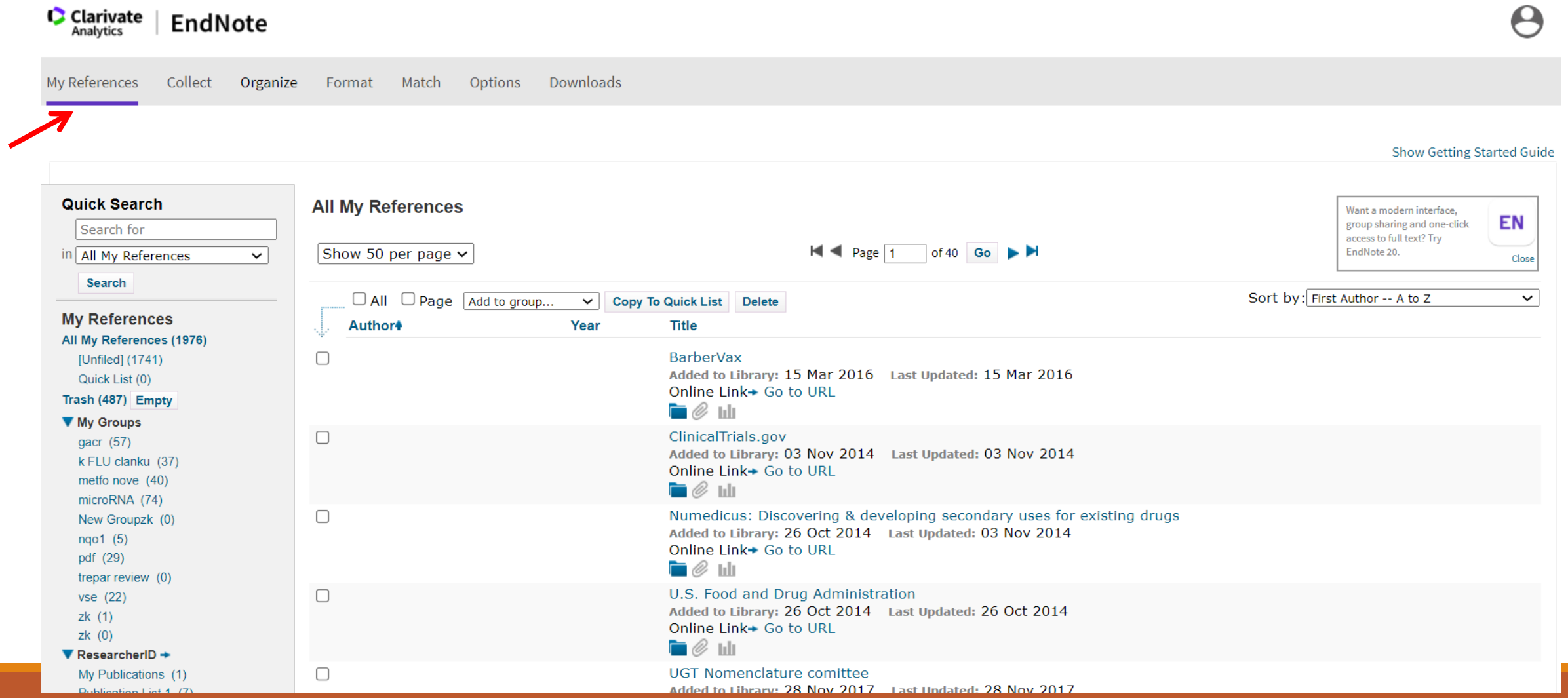
Literature search– citations (EndNote)



Literature search– citations (EndNote)



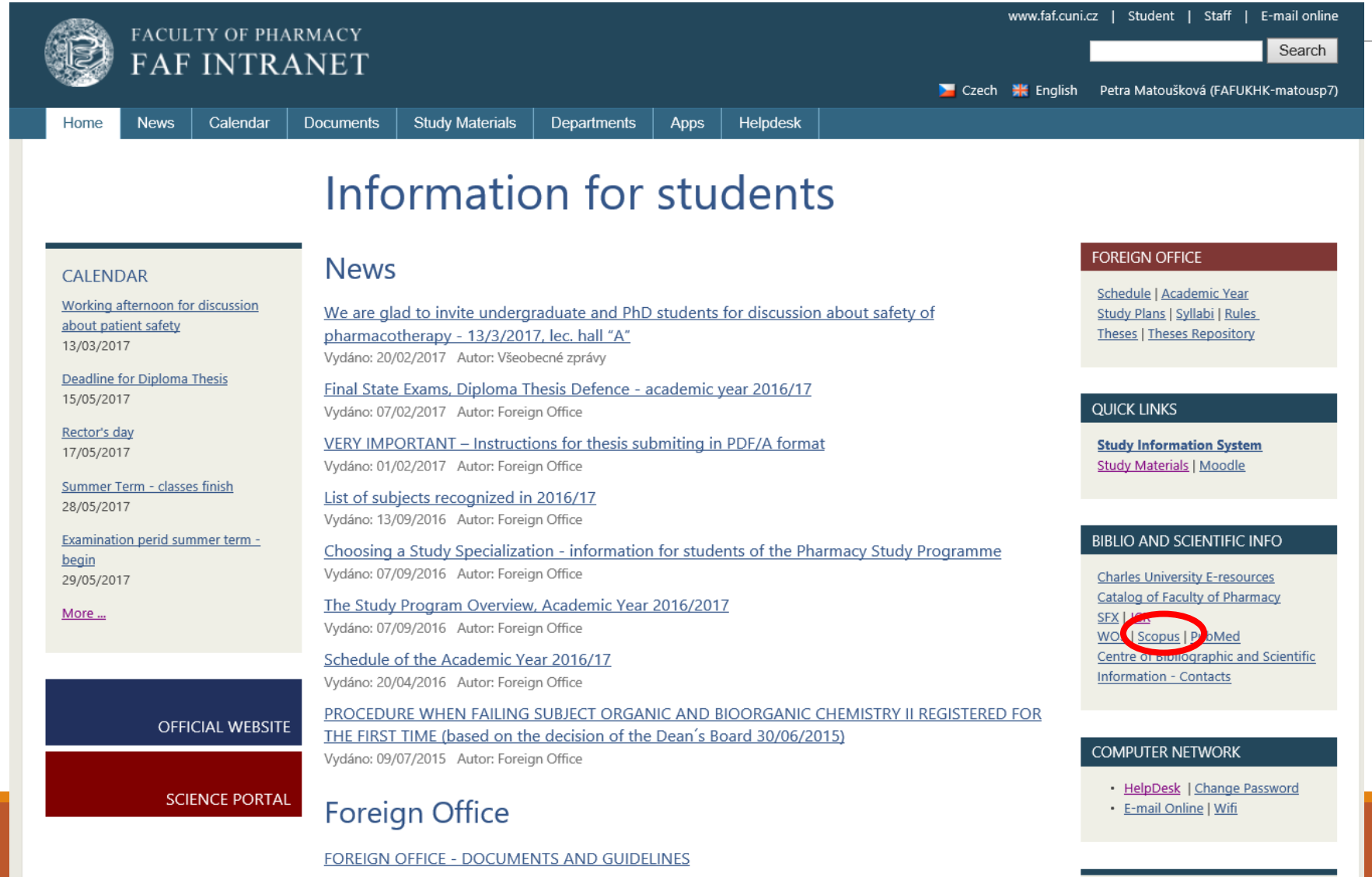
Literature search



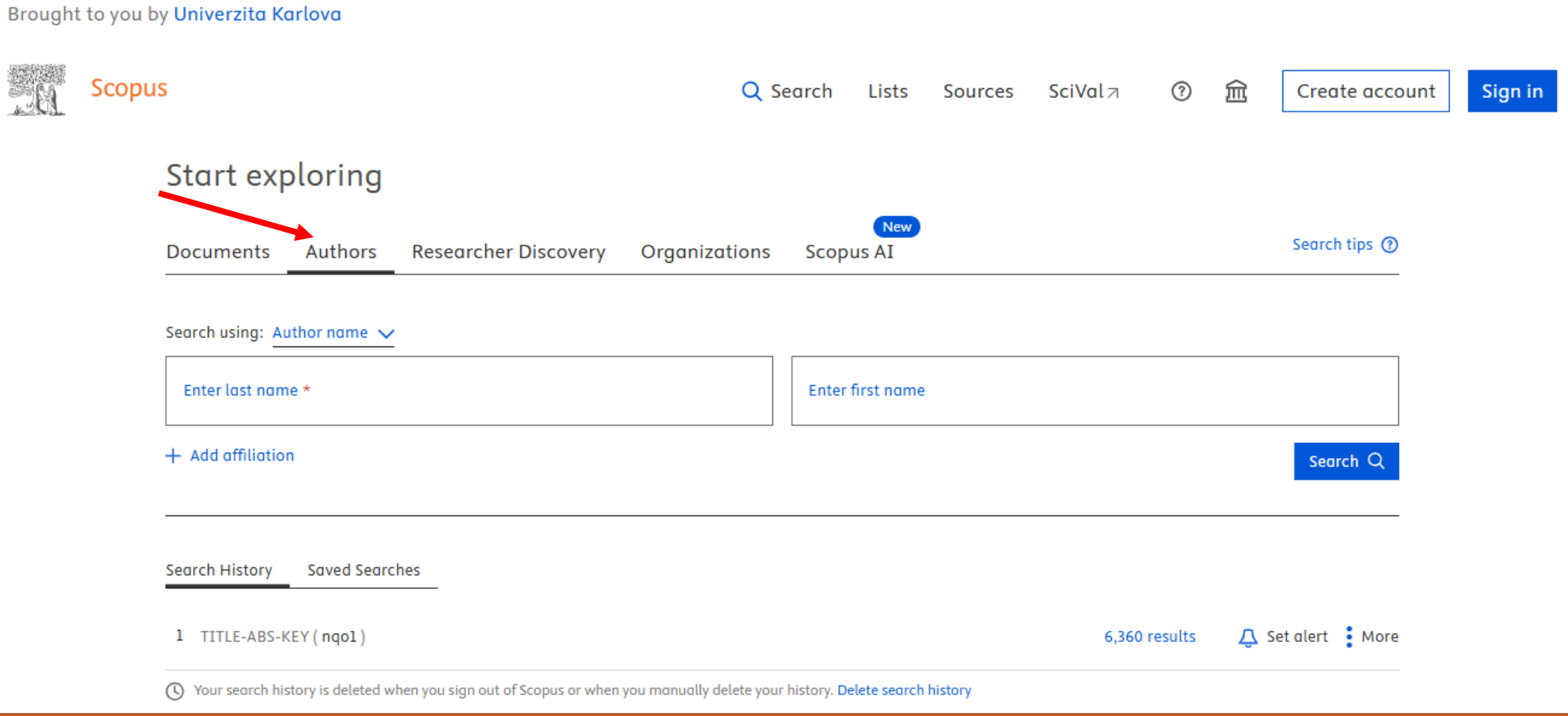
Try WOS !

Register-Login into WebEndnote!

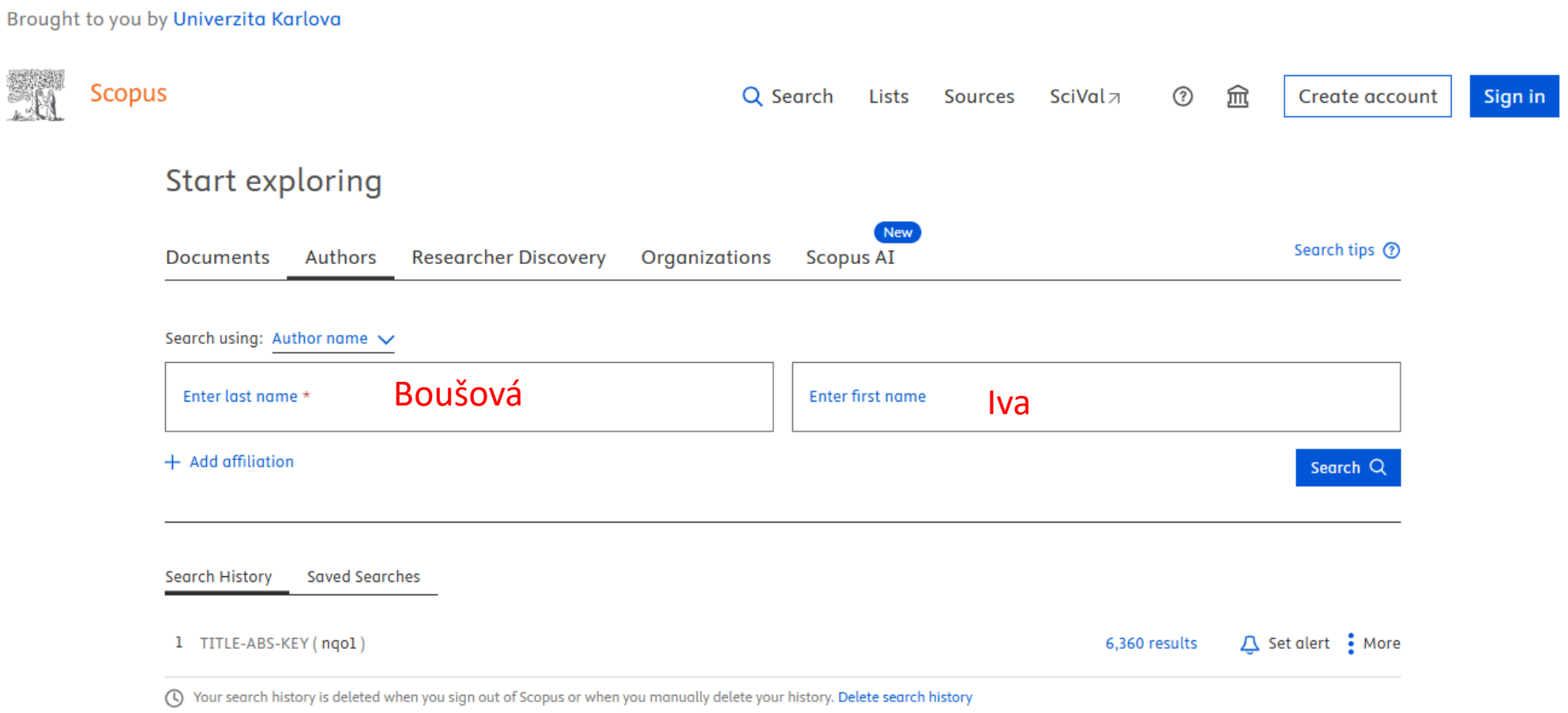
Literature search



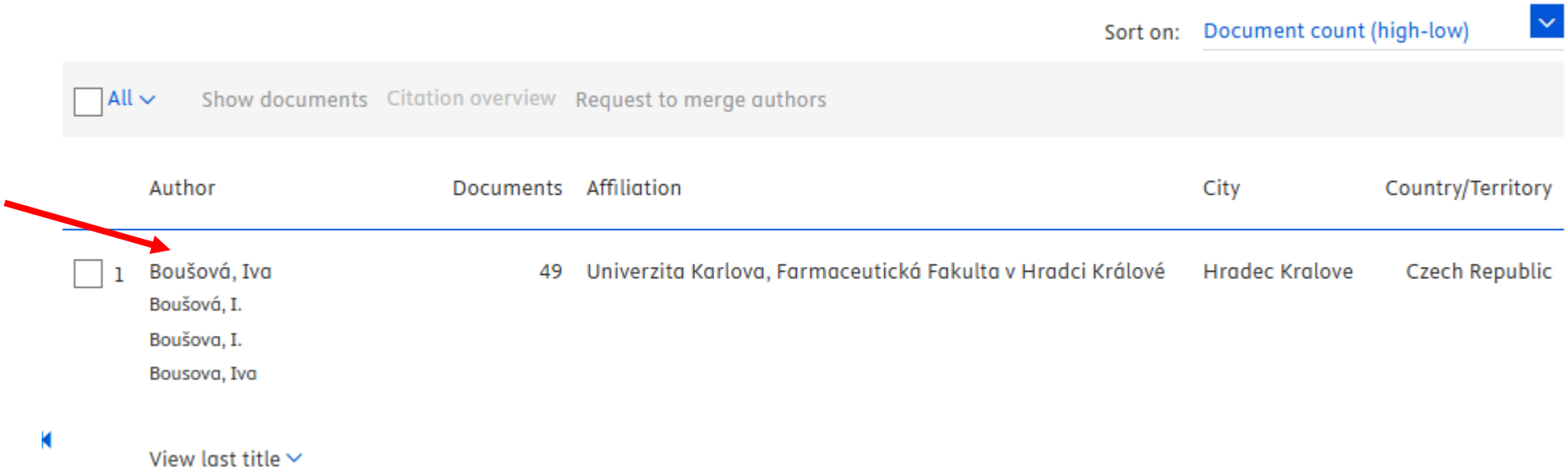
Literature search / H-index



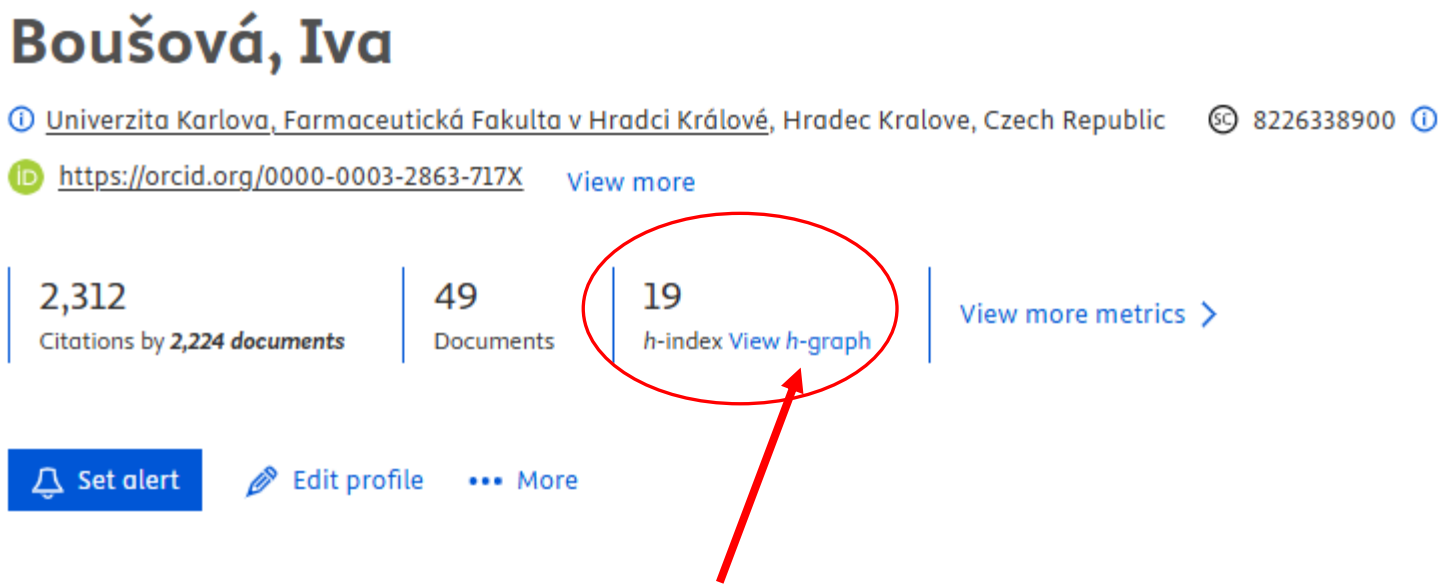
Literature search / H-index



Literature search / H-index

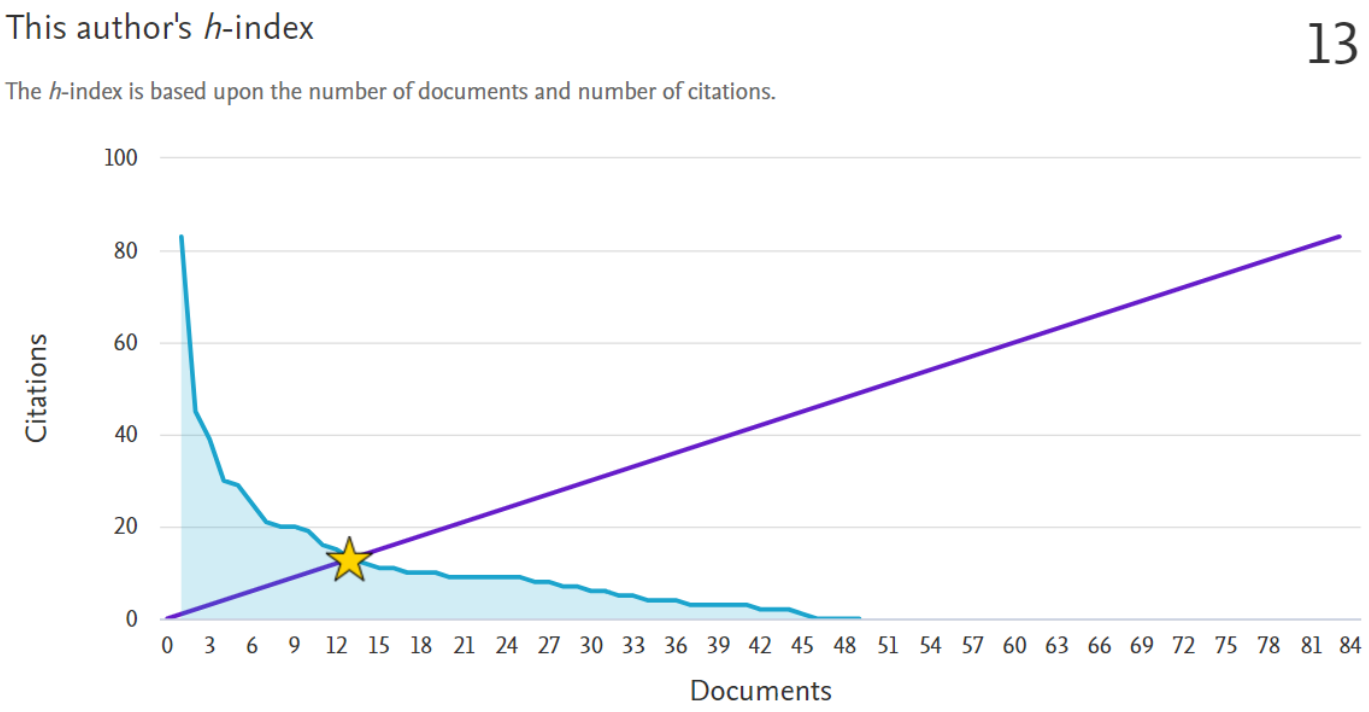


Literature search / H-index

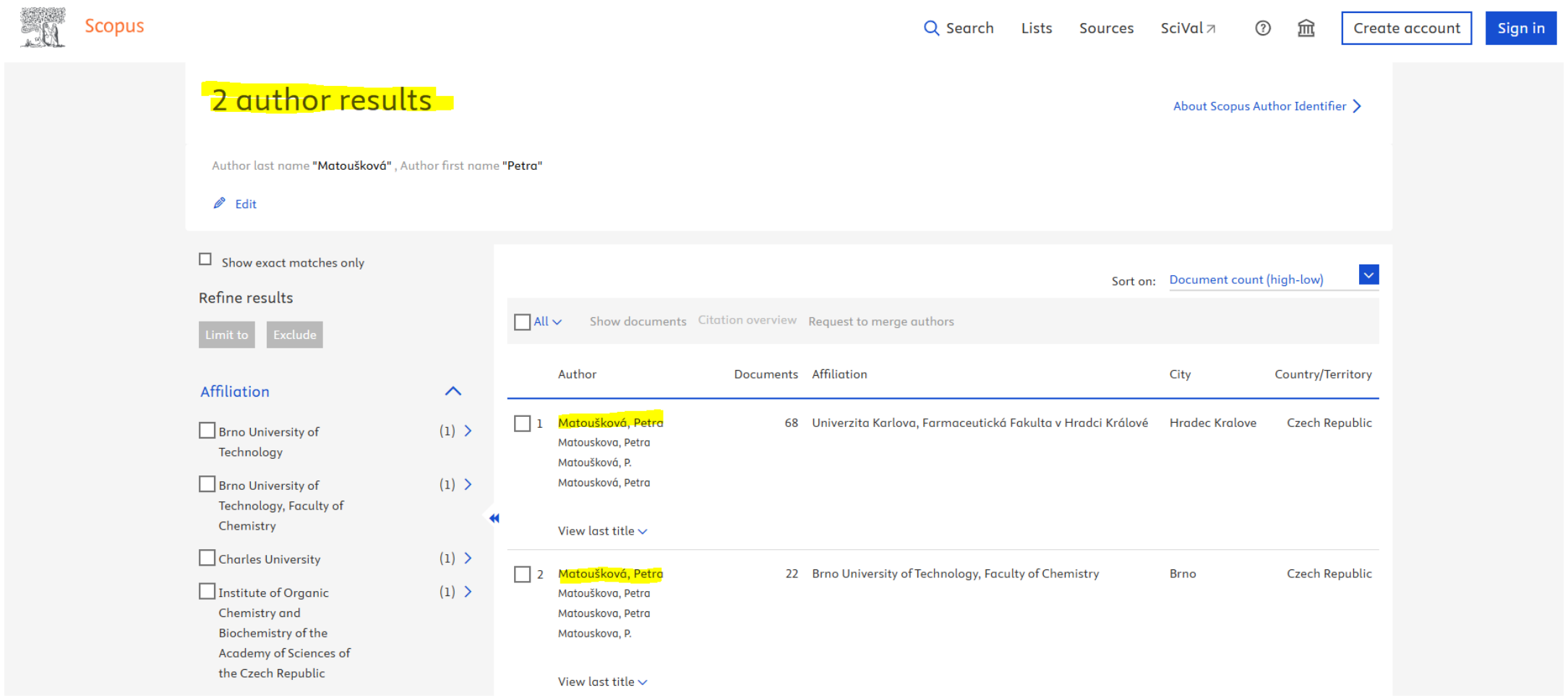


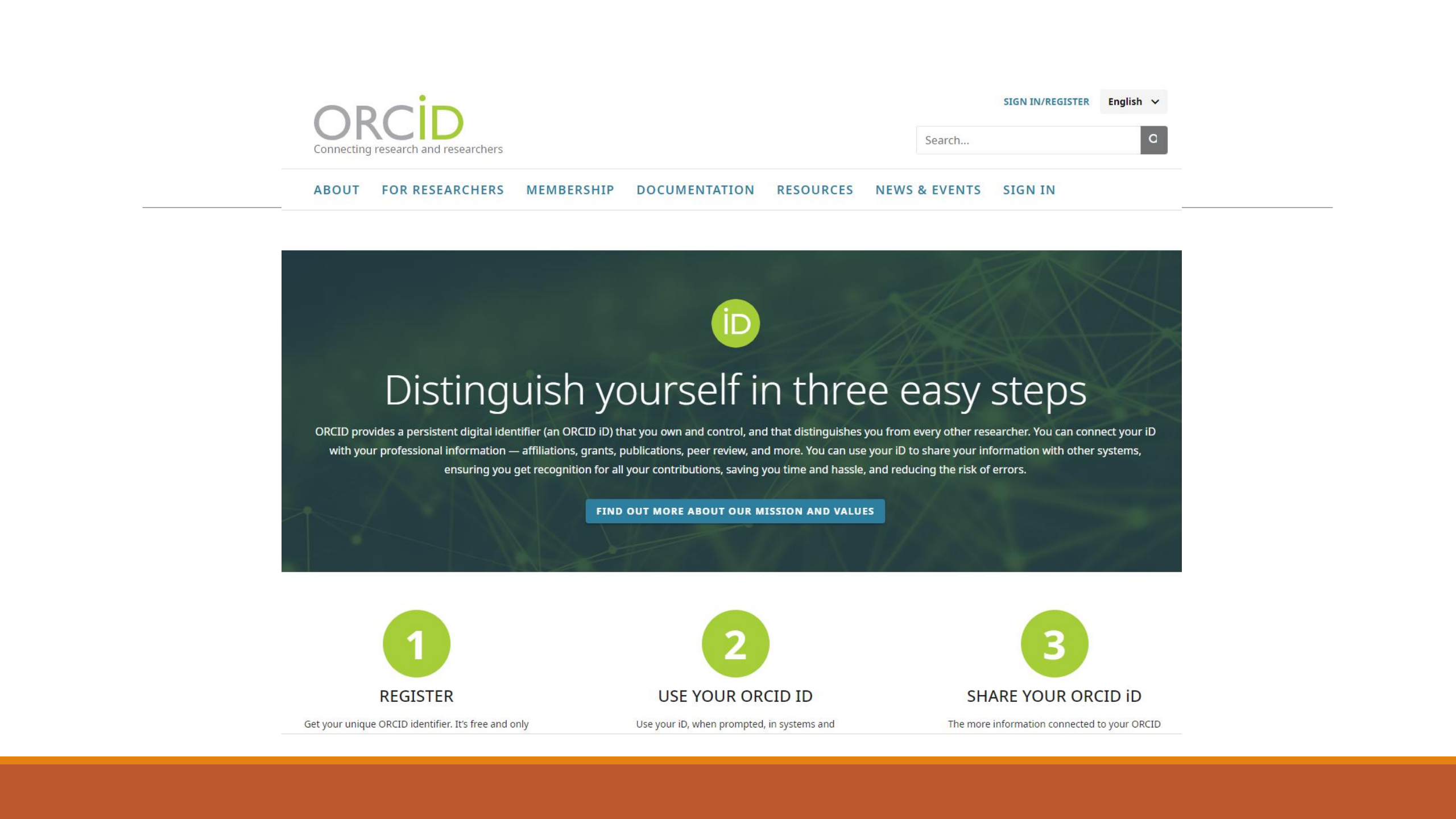
H-index

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

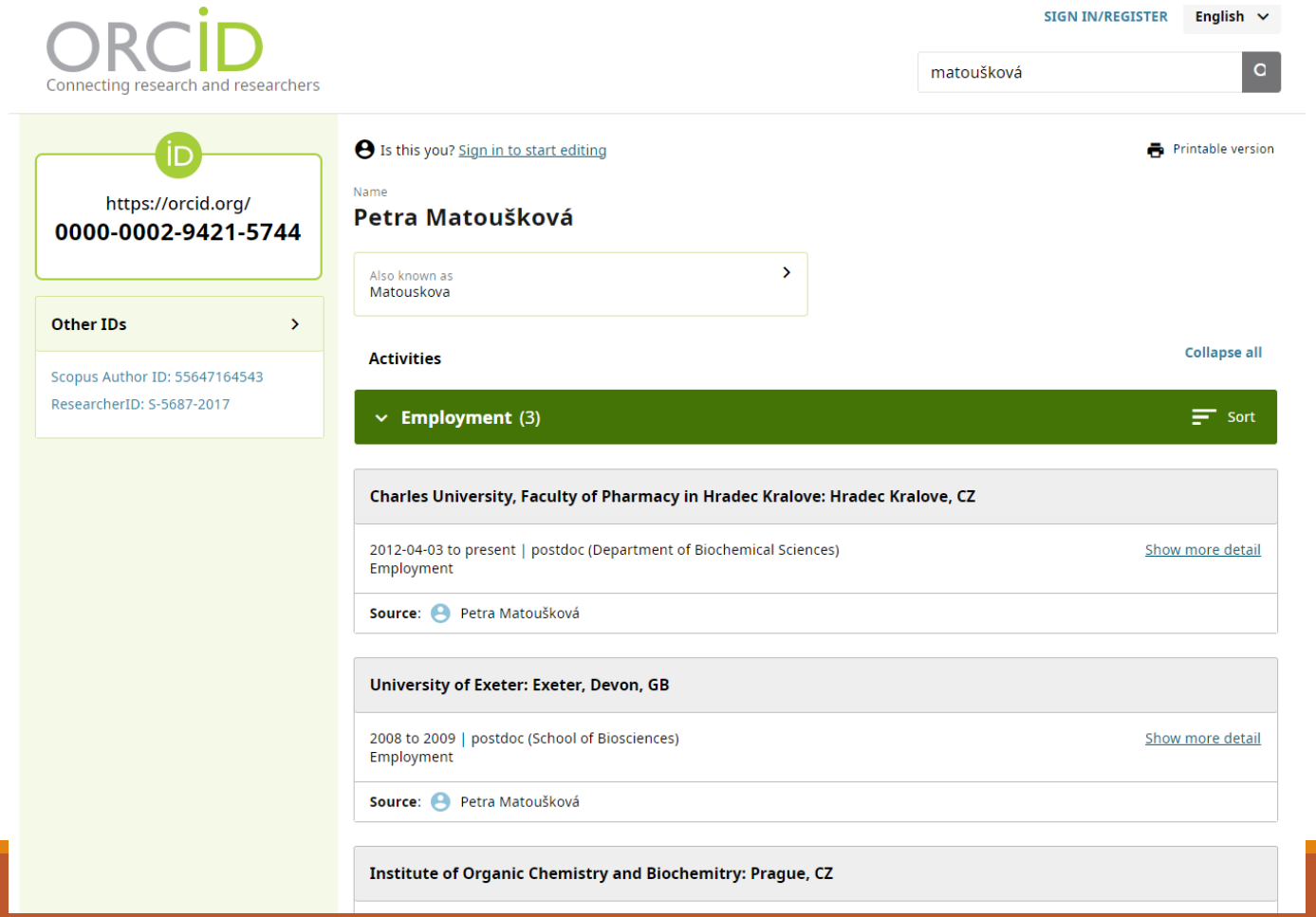


Literature search / H-index




ORCID
Connecting research and researchers
SIGN IN/REGISTER
English
Search...
ABOUT
FOR RESEARCHERS
MEMBERSHIP
DOCUMENTATION
RESOURCES
NEWS & EVENTS
SIGN IN
Distinguish yourself in three easy steps
ORCID provides a persistent digital identifier (an ORCID iD) that you own and control, and that distinguishes you from every other researcher. You can connect your iD with your professional information — affiliations, grants, publications, peer review, and more. You can use your iD to share your information with other systems, ensuring you get recognition for all your contributions, saving you time and hassle, and reducing the risk of errors.
FIND OUT MORE ABOUT OUR MISSION AND VALUES
1
REGISTER
Get your unique ORCID identifier. It's free and only
2
USE YOUR ORCID ID
Use your iD, when prompted, in systems and
3
SHARE YOUR ORCID iD
The more information connected to your ORCID

ORCID ID _ unique identification of scientist



Literature search / Homework 1

1) find full name of your gene

2) find 5 relevant literature

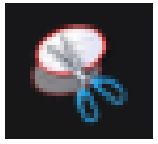
- at least one review
- at least one publication from 2024-25
- 1 older publication than 2005

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

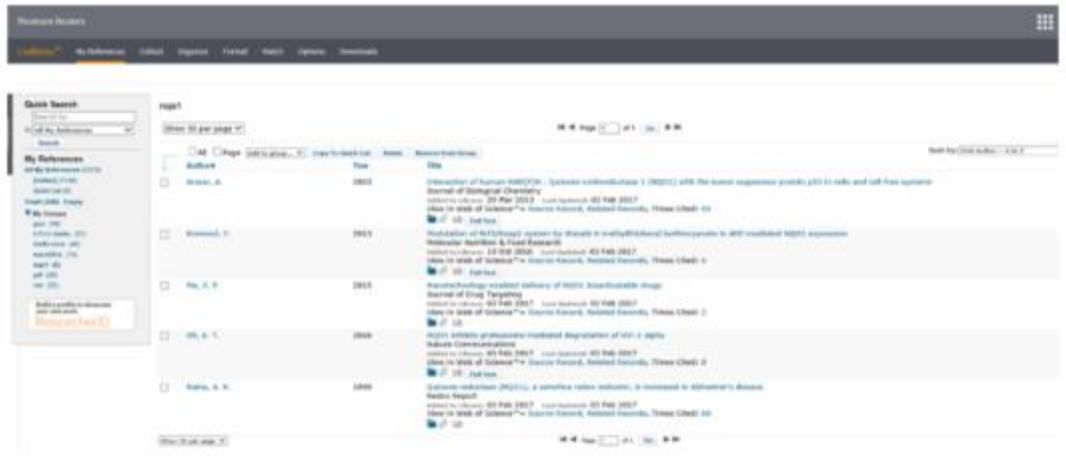
- E.g use „výstřižky“
- Compile in Word, pdf, one note…
- Submit in Moodle



„snipping tool“

Literature search / Homework 1 - example

NQO1: NAD(P)H:quinone oxidoreductase 1



NQO1 is involved in the biotransformation process of many compounds.

Matoušková Petra h-index 20