

Introduction to applied bioinformatics

PETRA MATOUŠKOVÁ

2024/2025

1/10

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	7	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	12.5.2025 ?		Út 8:00 - 9:30



Information for students

CALENDAR

Pharmaceutical Ball
22/03/2024

The Students Scientific Conference
04/04/2024

The Students Scientific Conference
05/04/2024

BAF (Veletř bioanalýtiky a farmacie)
18/04/2024

Conference Synthesis and Analysis of
Drugs 2024
19/09/2024

Stud
Info
Syst
(SIS)

New

14. Pos
Univers
05/02/20
The Stu

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

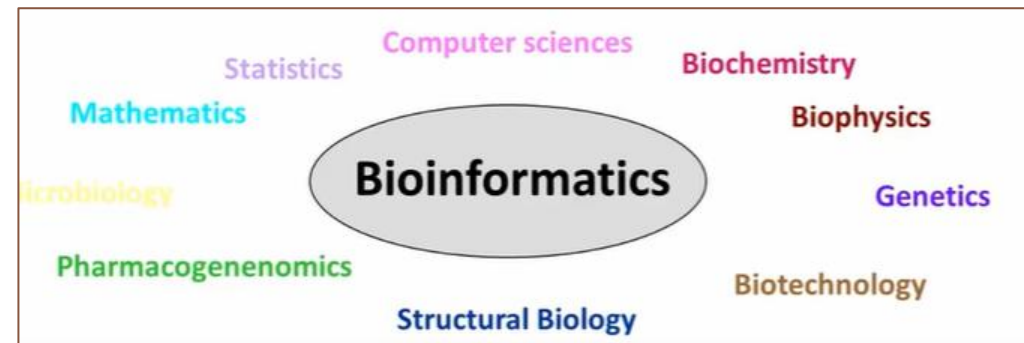
Katedra biologických a lékařských věd

Katedra farmaceutické botaniky

Katedra farmaceutické chemie a farmaceutické analýzy

Bioinformatics is about...

= **computational branch of molecular biology.**

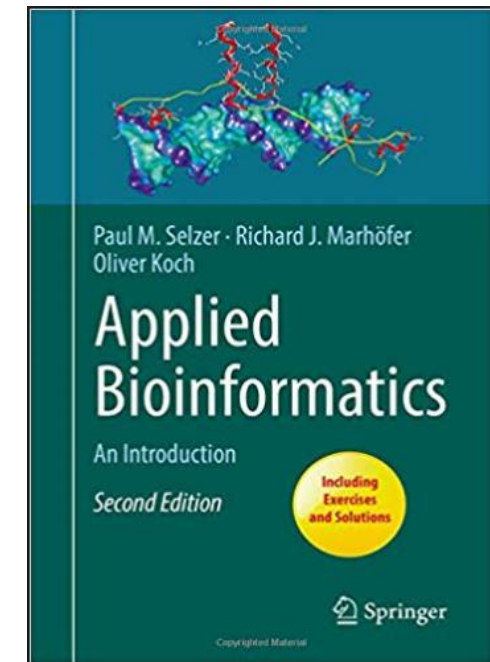


- searching biological databases
- comparing sequences
- looking at protein structures
-asking biological and biomedical questions with a computer.

„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

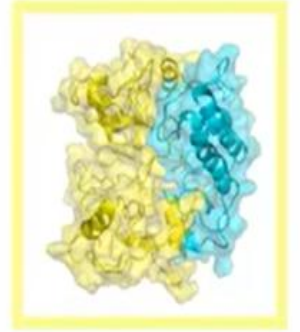
Tissue expression levels

MicoArray

Single gene analysis

Sequence contigs

Protein



Homology modeling

Structure-function prediction

Ligand docking

Protein-protein interactions

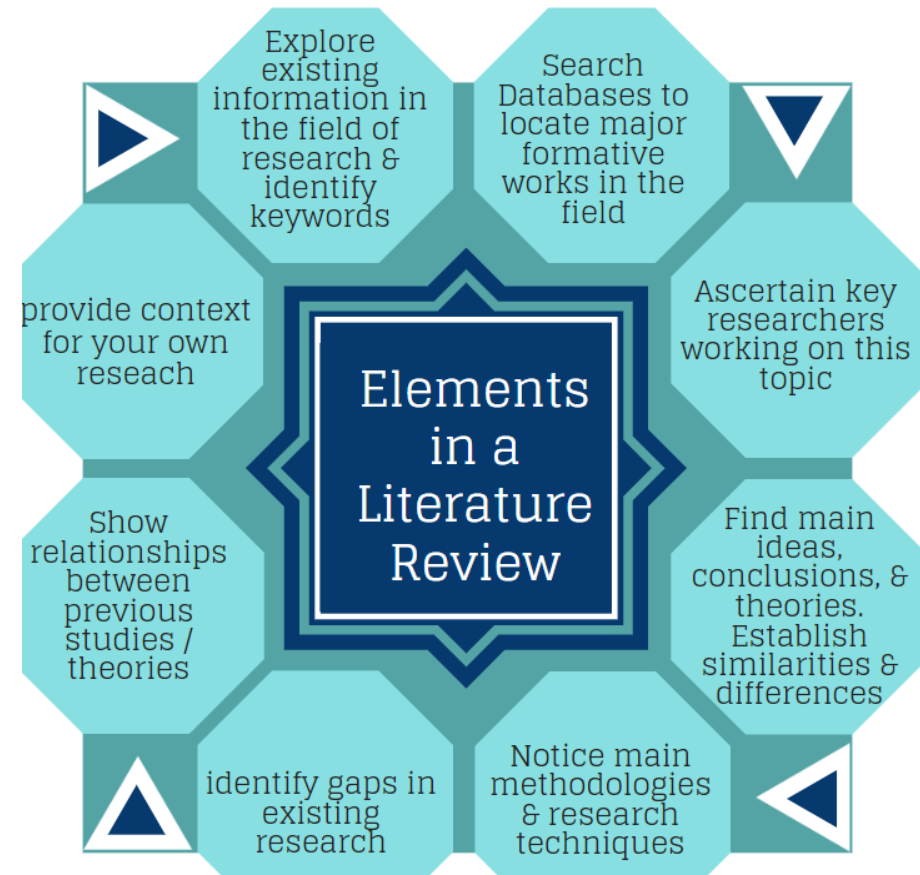
Protein expression

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 inconsistencies: 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



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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]

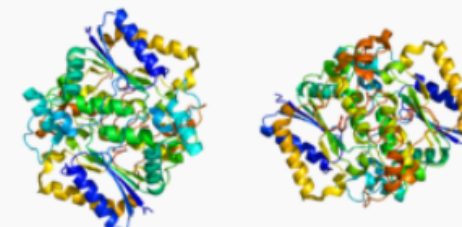
This gene is a member of the NAD(P)H dehydrogenase (quinone) family and encodes a cytoplasmic 2-electron reductase. This FAD-binding protein forms homodimers and reduces [quinones](#) to hydroquinones. This protein's enzymatic activity prevents the one electron reduction of quinones that results in the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

List of PDB id codes [\[show\]](#)

Identifiers

Symbols *NQO1*; DHQU; DIA4; DTD; NMOR1; NMORI; QR1

ChatGPT

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:

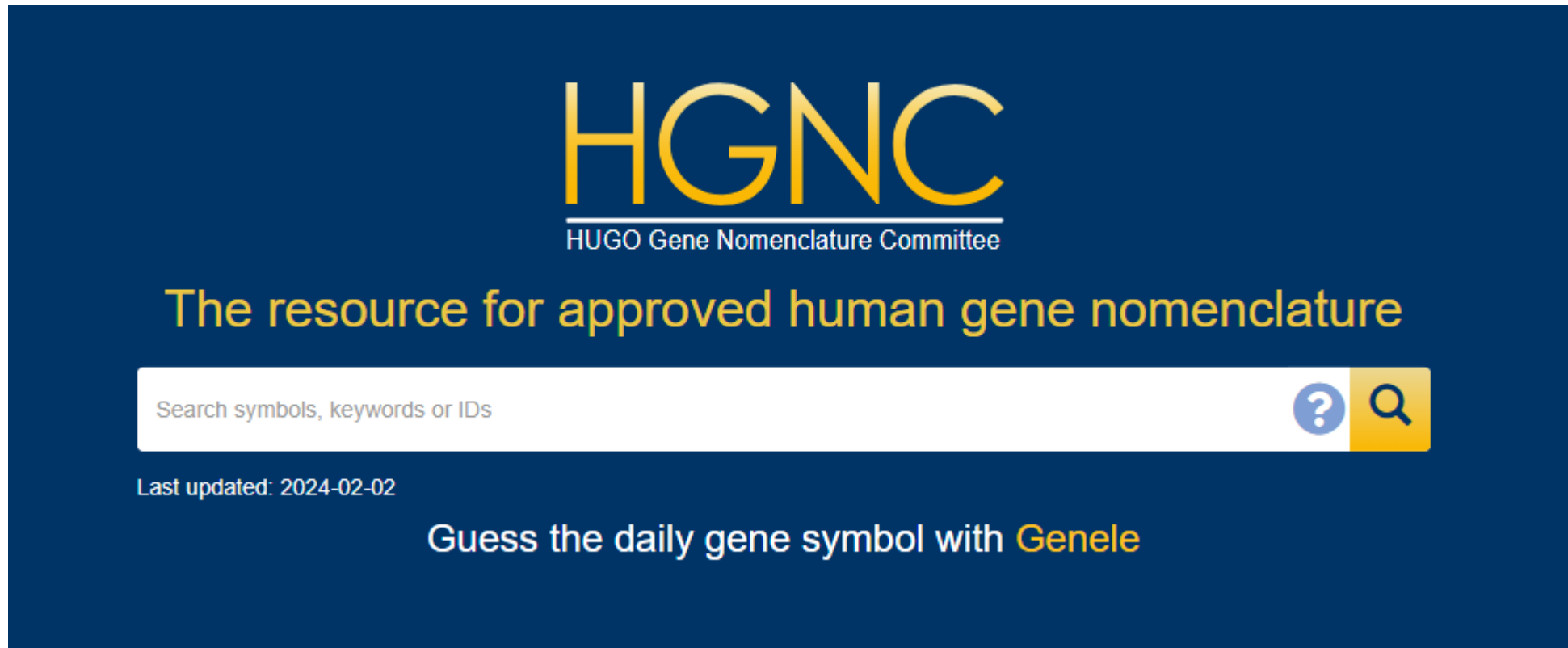
- **Cancer:** NQO1 is overexpressed in many cancers, making it a potential target for cancer therapy. Some anticancer drugs are designed to exploit this overexpression.

Research Project: NQO1

Quinone:NAD(P)H dehydrogenase 1


Identify the gene symbol!

HUGO database



Identify the gene symbol!

HUGO database



Search:

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Search results

Filter by type

● Gene

2

Filter by gene entry status

Approved

2

Filter by gene locus type

Protein-coding gene

1

Non-coding RNA

1

RNA, long non-coding

1

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Items: 1 to 2 of 2

NQO1: NAD(P)H quinone dehydrogenase 1

Gene

HGNC ID

HGNC:2874

Locus type

Gene with protein product

Status

Approved

Matches

Gene symbol:

NQO1

NQO1-DT: NQO1 divergent transcript

Gene

HGNC ID

HGNC:55344

Locus type

RNA, long non-coding

Status

Approved

Matches


Gene name:

NQO1 divergent transcript

Gene symbol:

NQO1-DT


Literature search



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When 1+1 is more than 2 – a hybridization approach yields a new candidate molecule for the treatment of tuberculosis

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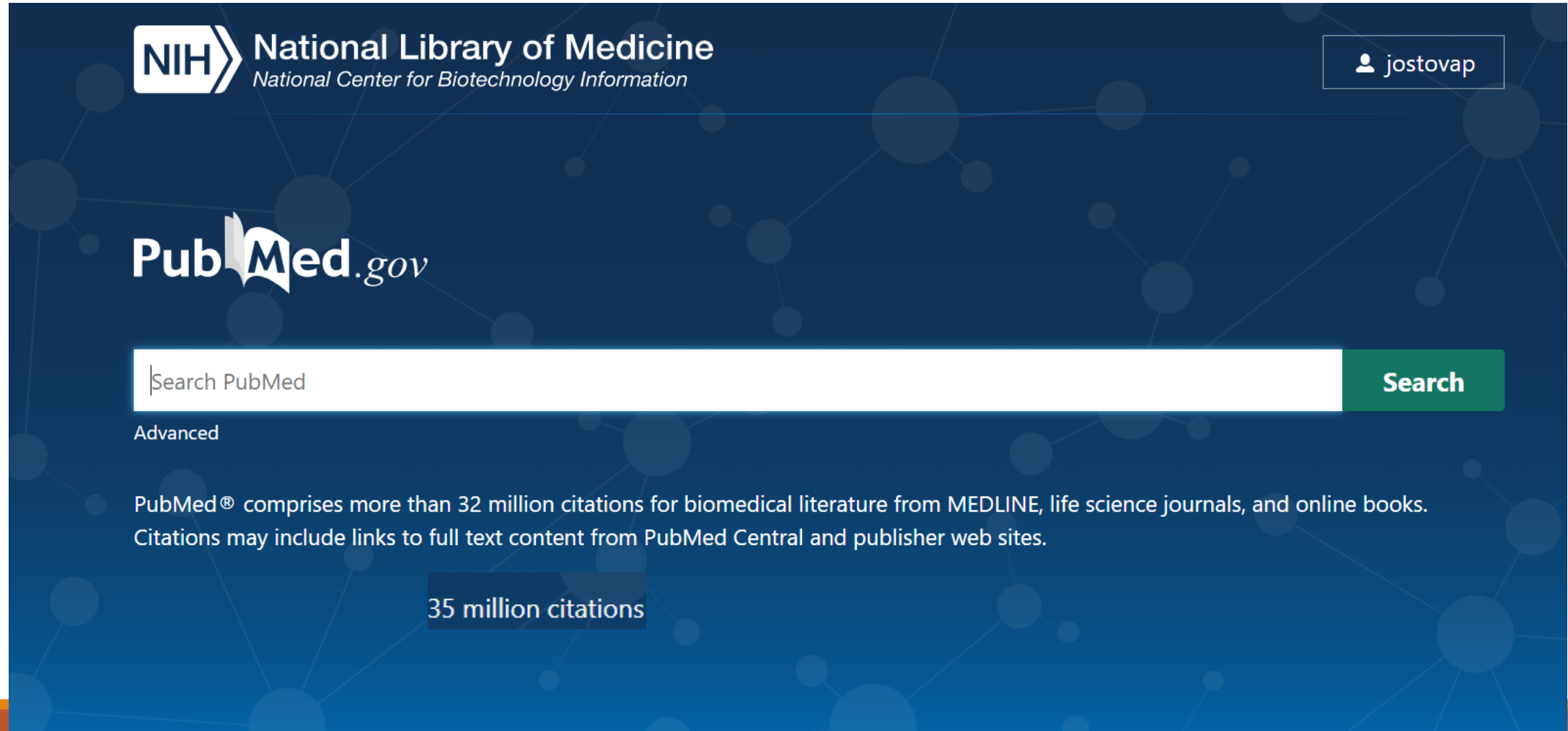
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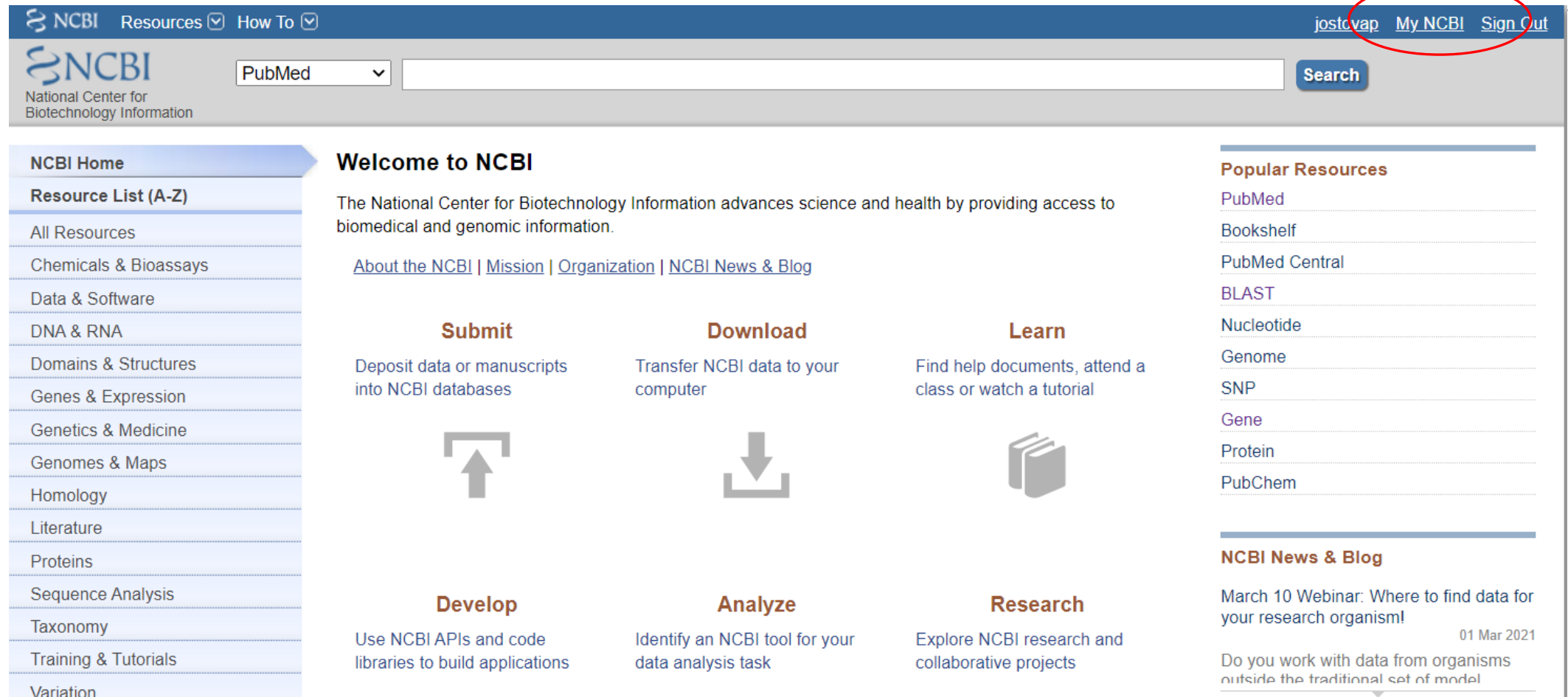
Literature search PubMed

<http://www.ncbi.nlm.nih.gov/pubmed/>

The image is a screenshot of the PubMed.gov homepage. The background is a dark blue gradient with a faint network of white dots and lines. In the top left corner, there is the NIH logo (a white square with 'NIH' in black) followed by the text 'National Library of Medicine' and 'National Center for Biotechnology Information' in a smaller font. In the top right corner, there is a user profile icon and the name 'jostovap'. Below the NIH logo, the 'PubMed.gov' logo is displayed in a large, white, stylized font. In the center, there is a large white search bar with the placeholder text 'Search PubMed'. To the right of the search bar is a green button with the word 'Search' in white. Below the search bar, the word 'Advanced' is written in a small, light blue font. Further down, a paragraph of text states: 'PubMed® comprises more than 32 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full text content from PubMed Central and publisher web sites.' At the bottom center, there is a dark blue rectangular box with the text '35 million citations' in white.

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The screenshot displays the NCBI (National Center for Biotechnology Information) homepage. At the top, there is a navigation bar with links for "Resources" and "How To". On the right side of the top bar, the user's name "jostovap" is displayed, along with links for "My NCBI" and "Sign Out", which are circled in red. Below the top bar, the NCBI logo is on the left, and a search bar is in the center with "PubMed" selected in a dropdown menu. A "Search" button is to the right of the search bar. On the left side, there is a vertical menu titled "NCBI Home" and "Resource List (A-Z)" containing links to various databases and tools. The main content area is titled "Welcome to NCBI" and includes a brief description of the center's mission. Below this, there are six sections: "Submit" (Deposit data or manuscripts into NCBI databases), "Download" (Transfer NCBI data to your computer), "Learn" (Find help documents, attend a class or watch a tutorial), "Develop" (Use NCBI APIs and code libraries to build applications), "Analyze" (Identify an NCBI tool for your data analysis task), and "Research" (Explore NCBI research and collaborative projects). On the right side, there is a "Popular Resources" section with links to PubMed, Bookshelf, PubMed Central, BLAST, Nucleotide, Genome, SNP, Gene, Protein, and PubChem. Below this is an "NCBI News & Blog" section featuring a webinar announcement for March 10, 2021, titled "Where to find data for your research organism!" and a link to a blog post about working with data from organisms outside the traditional set of model organisms.

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NCBI News & Blog


March 10 Webinar: Where to find data for your research organism!

01 Mar 2021

Do you work with data from organisms outside the traditional set of model

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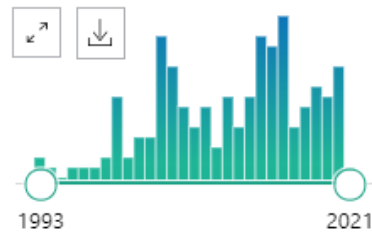
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- ☐ 1
- NAD(P)H:Quinone Oxidoreductase 1 (NQO1) as a Therapeutic and Diagnostic Target in Cancer.**
Cite Zhang K, Chen D, Ma K, Wu X, Hao H, Jiang S.
J Med Chem. 2018 Aug 23;61(16):6983-7003. doi: 10.1021/acs.jmedchem.8b00124. Epub 2018 May 7.
Share PMID: 29712428 Review.
It is abnormally overexpressed in many tumors and intimately linked with multiple carcinogenic processes. **NQO1** is considered to be a cancer-specific target for therapy but currently available **NQO1** inhibitors have not yet led to chemotherapeutic success. ...This arti ...
- ☐ 2
- Alzheimer's Disease and NQO1: Is there a Link?**
Cite Chhetri J, King AE, Gueven N.
Curr Alzheimer Res. 2018;15(1):56-66. doi: 10.2174/1567205014666170203095802.
Share PMID: 28164770 Review.
One of those endogenous defences is NADPH quinone oxidoreductase 1 (**NQO1**). **NQO1** is a cytosolic homodimeric flavoprotein that catalyses the two-electron reduction of quinones and related molecules aimed at increasing their solubility and excretion. In line with its r ...

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Exp Hematol Oncol. 2016 Sep 13;5(1):27. doi: 10.1186/s40164-016-0056-z. eCollection 2015.

Activation of NQO1 in NQO1*2 polymorphic human leukemic HL-60 cells by diet-derived sulforaphane.

Wu JM¹, Oraee A¹, Doonan BB¹, Pinto JT¹, Hsieh TC¹.

Author information

Abstract

BACKGROUND: The

NAD(P)H: quinone oxidoreductase (NQO1) confers protection against semiquinones and also elicits oxidative stress. The C609T polymorphism of the NQO1 gene, designated NQO1*2, significantly reduces its enzymatic activity due to rapid degradation of protein. Since down regulation of NQO1 mRNA expression correlates with increased susceptibility for developing different types of cancers, we investigated the link between leukemia and the NQO1*2 genotype by mining a web-based microarray dataset, ONCOMINE. Phytochemicals prevent DNA damage through activation of phase II detoxification enzymes including NQO1. Whether NQO1 expression/activity in leukemia cells that carry the labile NQO1*2 genotype can be induced by broccoli-derived phytochemical sulforaphane (SFN) is currently unknown.

METHODS AND RESULTS: The ONCOMINE query showed that: (1) acute lymphoblastic leukemia and chronic myelogenous leukemia are associated with reduced NQO1 levels, and (2) under-expressed NQO1 was found in human HL-60 leukemia cell line containing the heterozygous NQO1*2 polymorphism. We examined induction of NQO1 activity/expression by SFN in HL-60 cells. A dose-dependent increase in NQO1 level/activity is accompanied by upregulation of the transcription factor, Nrf2, following 1-10 μ M SFN treatment. Treatment with 25 μ M SFN drastically reduced NQO1 levels, inhibited cell proliferation, caused sub-G1 cell arrest, and induced apoptosis, and a decrease in the levels of the transcription factor, nuclear factor- κ B (NF κ B).

CONCLUSIONS: Up to 10 μ M of SFN increases NQO1 expression and suppresses HL-60 cell proliferation whereas \geq 25 μ M of SFN induces apoptosis in HL-60 cells. Further, SFN treatment restores NQO1 activity/levels in HL-60 cells expressing the NQO1*2 genotype.

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Sub-chronic sulforaphane exposure in CD-1 pregnant mice enhances n [Reprod Toxicol. 2014]

Review Regulation of genes encoding NAD(P) H:quinone oxidoredu [Free Radic Biol Med. 2000]

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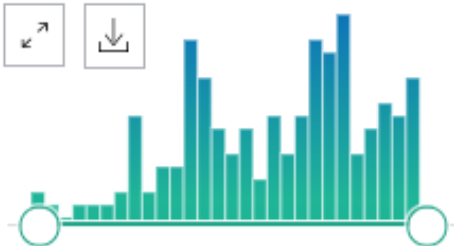
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oxidoreductase 1 (**NQO1**) as a Therapeutic and Diagnostic

X, Hao H, Jiang S.

J Med Chem. 2018 Aug 23;61(16):6983-7003. doi: 10.1021/acs.jmedchem.8b00124. Epub 2018 May 7. PMID: 29712428 Review.

It is abnormally overexpressed in many tumors and intimately linked with multiple carcinogenic processes. **NQO1** is considered to be a cancer-specific target for therapy but currently available **NQO1** inhibitors have not yet led to chemotherapeutic success. ...This arti ...


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1

Rational designed highly sensitive NQO1-activated near-infrared fluorescent probe combir vivo: An innovative strategy for NQO1-overexpressing cancer theranostics

Gong, QJ; Yang, FL; (...); Zhang, XJ

1 | EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY 224

Since NQO1 is overexpressed in many cancer cells, it can be used as a biomarker for cancer diagnosis and targeted t anticancer activity through the redox cycle mediated by NQO1, while the NQO1 probes can monitor NQO1 levels in c needed for diagnostic imaging in clinic. In this study, based on the analysis of NQO1 catalytic pocket, the naphthoqu

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2

LncRNA Nqo1-AS1 Attenuates Cigarette Smoke-Induced Oxidative Stress by Upregulating i

Nqo1

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CHEMOSPHERE

Publisher name: PERGAMON-ELSEVIER SCIENCE LTD

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8.12023

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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](#)
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[Chang, G. J.¹](#)
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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- κ B 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]

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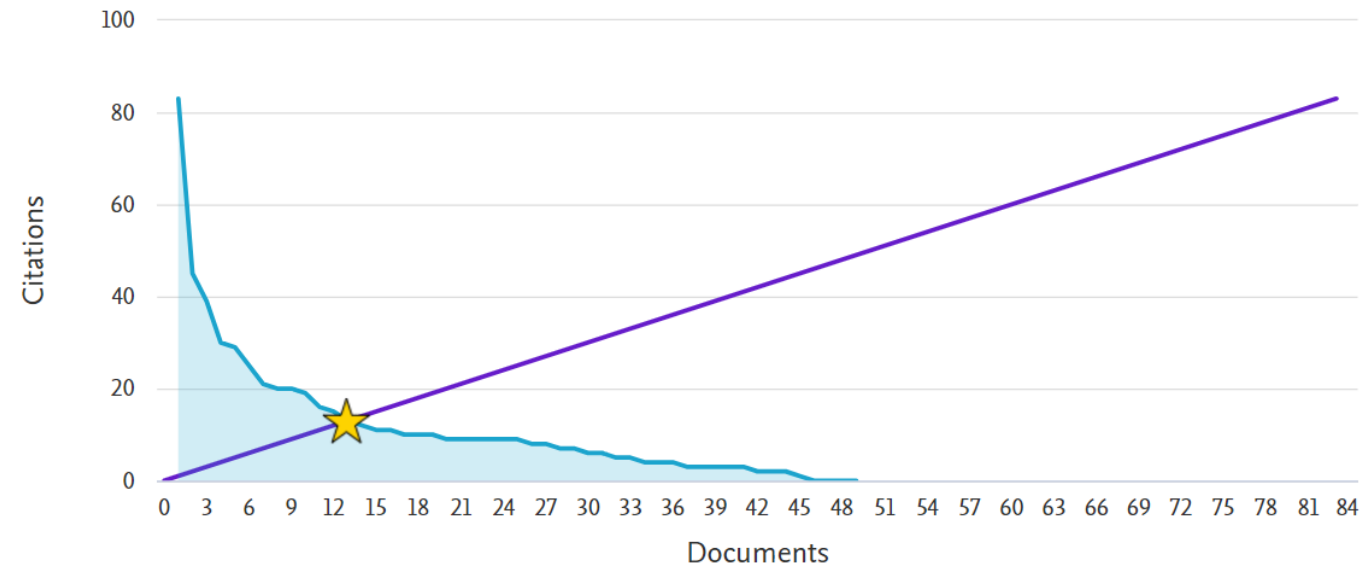
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
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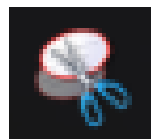
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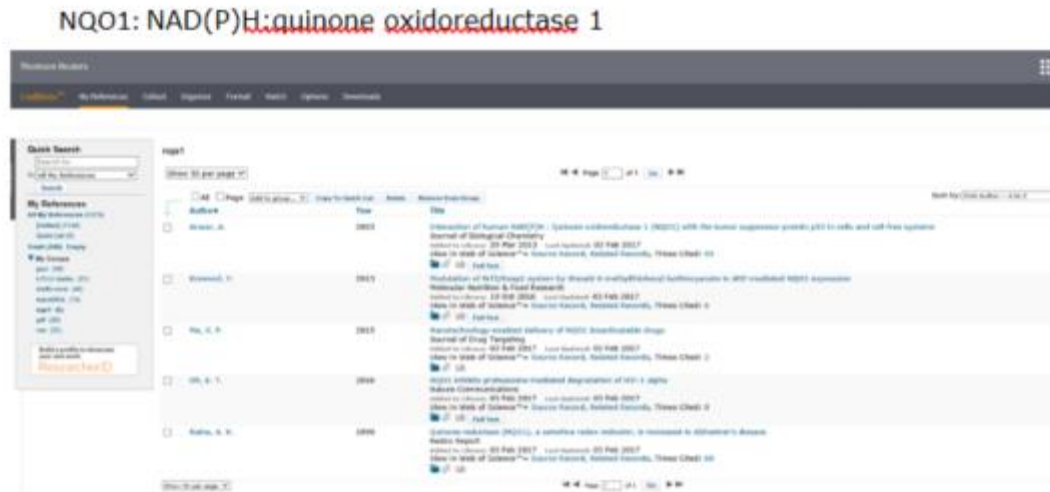
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