

Introduction to applied bioinformatics

PETRA MATOUŠKOVÁ

2023/2024

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
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)

www.faf.cuni.cz | Student | Staff | E-mail online

FACULTY OF PHARMACY
IN HRADEC KRÁLOVÉ
Charles University

Petra Matoušková (FAFUKHK-matousp7)

Home News Calendar Documents DL 1 Titulní stránka Nástěnka Moje kurzy Podpora uživatelů

Katedra biochemických věd

Nástěnka / M Kategorie Další

Farmac

Farmaceutická fakulta / Katedra biochemických věd

Kategorie Vyhledat kurzy

Rozbalit vše

- ▶ Klinická biochemie a patobiochemie
- Farmaceutická fakulta ▶
Ambasador na FAF →
Teacher: Petra Matoušková
- ▶ Praktická cvičení z molekulární biologie →
Teacher: Petra Matoušková
- Vyhledat kurzy
Introduction to applied bioinformatics 🔒 →
Teacher: Petra Matoušková

Kurzy

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- ▶ Filozofická fakulta
- ▶ Lékařské fakulty
- ▶ Matematicko-fyzikální fakulta

- ▶ 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

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

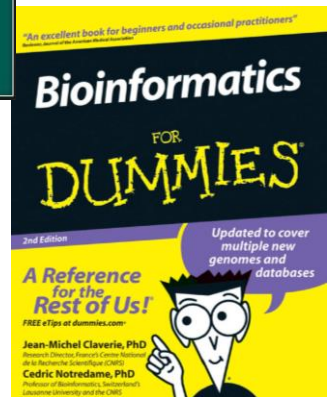
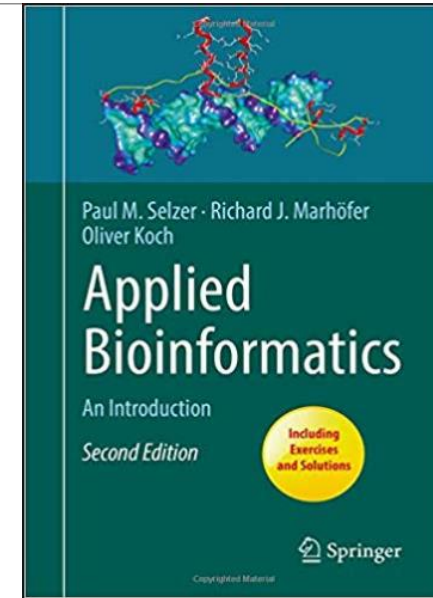
Bioinformatics is about...

= **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

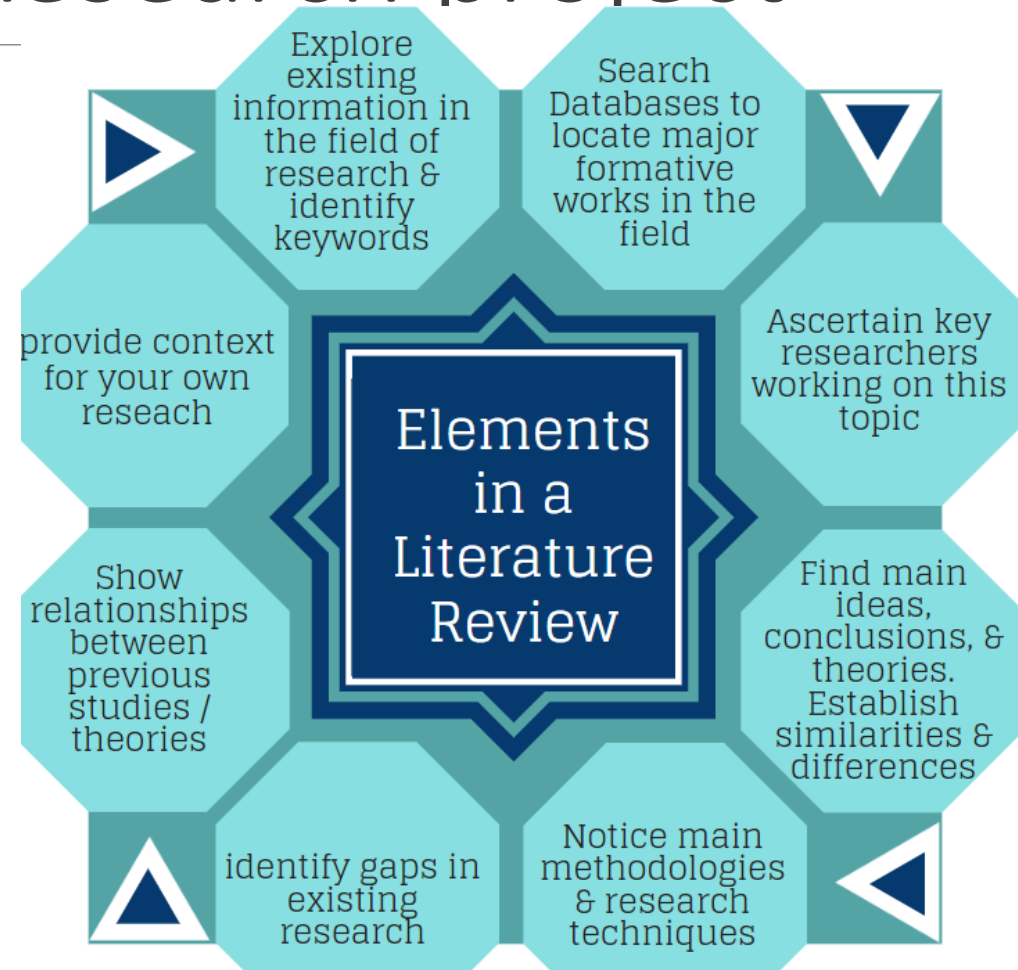
Finding polymorphic sites in genes (single nucleotide polymorphisms, SNPs)

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 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 *v*, SDHA *v*...)



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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]

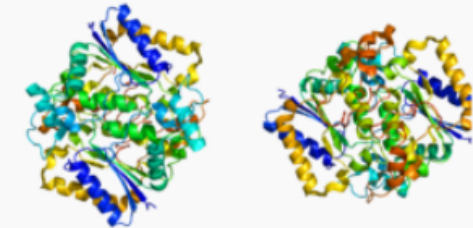
This gene is a member of the NAD(P)H dehydrogenase (quinone) family and encodes a cytoplasmic 2-electron reductase. This FAD-binding protein forms homodimers and reduces [quinones](#) to hydroquinones. This protein's enzymatic activity prevents the one electron reduction of quinones that results in the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

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

Identifiers

Symbols [NQO1](#); [DHQU](#); [DIA4](#); [DTD](#); [NMOR1](#); [NMORI](#); [QR1](#)

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Články Přibližný počet výsledků: 27 600 (0,06 s) [Můj profil](#) [Moje knihovna](#)

Kdykoli
Od 2018
Od 2017
Od 2014
Vlastní období...

Seřadit podle relevance
Seřadit podle data

zahrnout patenty
 zahrnout citace

Vytvořit upozornění

[\[HTML\]](#) NAD (P) H: quinone oxidoreductase 1 (**NQO1**): chemoprotection, bioactivation, gene regulation and genetic polymorphisms
D Ross, JK Kupa, SL Winski, HD Beall, A Anwar... - *Chemico-biological ...*, 2000 - Elsevier
Abstract NAD (P) H: quinone oxidoreductase 1 (**NQO1**) is an obligate two-electron reductase that is involved in chemoprotection and can also bioactivate certain antitumor quinones. This review focuses on detoxification reactions catalyzed by **NQO1** and its role in antioxidant
☆ [Počet citací tohoto článku: 577](#) [Související články](#) [Všechny verze \(počet: 8\)](#) [Web of Science: 398](#) [\[HTML\] sciencedirect.com](#)
[Full-text @ SFX UK](#)

[\[HTML\]](#) NAD (P) H: quinone acceptor oxidoreductase 1 (**NQO1**), a multifunctional antioxidant enzyme and exceptionally versatile cytoprotector
[AT Dinkova-Kostova](#), P Talalay - *Archives of biochemistry and biophysics*, 2010 - Elsevier
Abstract NAD (P) H: quinone acceptor oxidoreductase 1 (**NQO1**) is a widely-distributed FAD-dependent flavoprotein that promotes obligatory 2-electron reductions of quinones, quinoneimines, nitroaromatics, and azo dyes, at rates that are comparable with NADH or
☆ [Počet citací tohoto článku: 372](#) [Související články](#) [Všechny verze \(počet: 8\)](#) [Web of Science: 252](#) [\[HTML\] sciencedirect.com](#)
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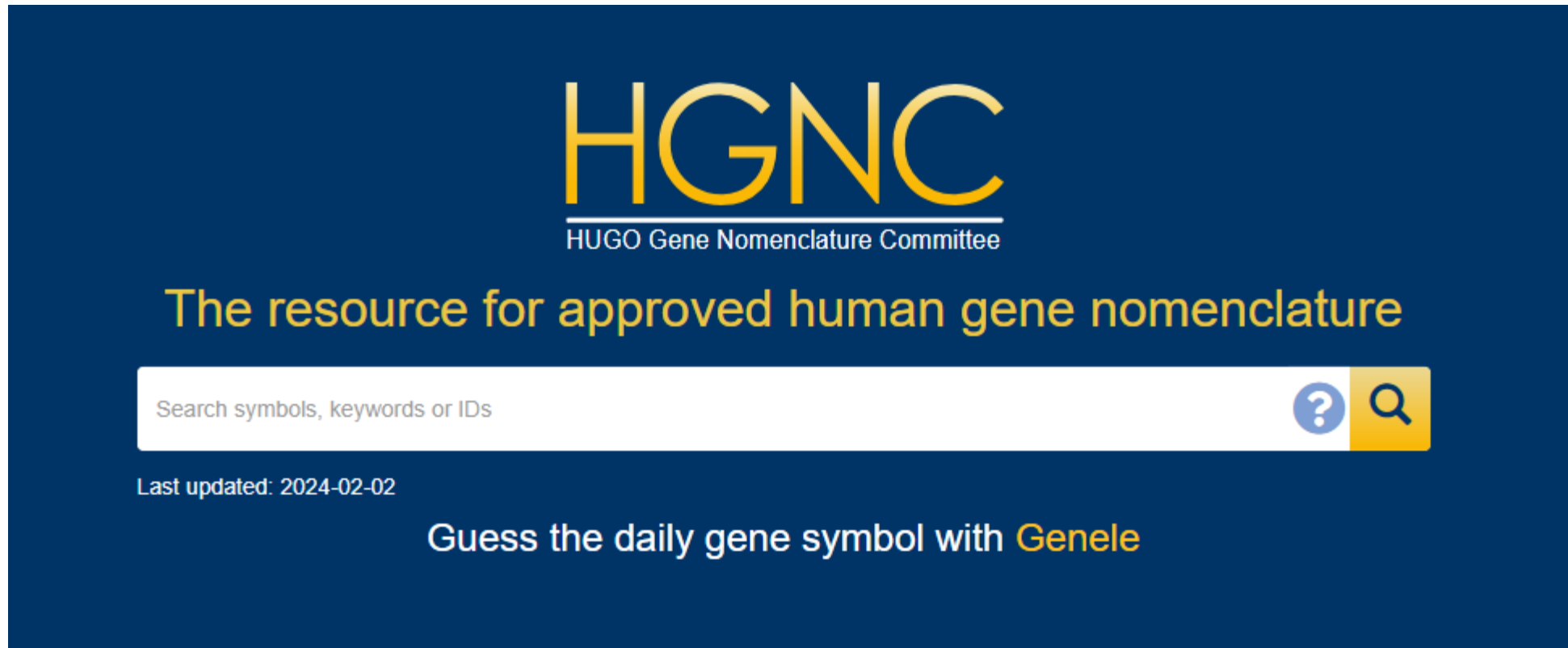
Benzene poisoning, a risk factor for hematological malignancy, is associated with the **NQO1** 609C→ T mutation and rapid fractional excretion of chlorzoxazone
N Rothman, [MT Smith](#), RB Hayes, RD Traver, B Hoener... - *Cancer Research*, 1997 - AACR
Abstract Benzene is a ubiquitous occupational hematotoxin and leukemogen, but people vary in their response to this toxic agent. To evaluate the impact of interindividual variation in enzymes that activate (ie, CYP2E1) and detoxify (ie, **NQO1**) benzene and its metabolites, we
☆ [Počet citací tohoto článku: 333](#) [Související články](#) [Všechny verze \(počet: 8\)](#) [Web of Science: 221](#) [\[PDF\] aacrjournals.org](#)
[Full-text @ SFX UK](#)

Research Project: NQO1

Quinone:NAD(P)H dehydrogenase 1

Identify the gene symbol!

HUGO database



The image shows the homepage of the HUGO Gene Nomenclature Committee (HGNC). The background is a dark blue color. At the top center, the HGNC logo is displayed in large, bold, yellow letters. Below the logo, the text "HUGO Gene Nomenclature Committee" is written in a smaller, white font. Underneath that, the tagline "The resource for approved human gene nomenclature" is written in yellow. A white search bar is positioned below the tagline, containing the placeholder text "Search symbols, keywords or IDs". To the right of the search bar, there are two icons: a blue circle with a white question mark and a yellow square with a white magnifying glass. Below the search bar, the text "Last updated: 2024-02-02" is written in white. At the bottom of the page, the text "Guess the daily gene symbol with Genele" is written in white, with "Genele" in yellow.

HGNC
HUGO Gene Nomenclature Committee

The resource for approved human gene nomenclature

Search symbols, keywords or IDs

Last updated: 2024-02-02

Guess the daily gene symbol with **Genele**

Identify the gene symbol!

HUGO database

HGNC ? 🔍

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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

Download all results



20 items per page

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**


Items: 1 to 2 of 2

Literature search

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Search

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Information for students

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Sample preparation of biological material, microbiological analysis of clinical isolates and advanced methods of drug design
23/02/2023

Dr. Russell Kitson: From chemical biology to chemical education and back again
24/02/2023

51st Pharmaceutical Ball
17/03/2023

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- CU Point Newsletter – February 2023
10/02/2023 | Student Services
- Dean's Directive No. 2/2023: Rules that students are obliged to adhere to during the examination
07/02/2023 | Student Services
- 13. Postgraduate and Postdoctoral Scientific Conference of the Faculty of Pharmacy of Charles University
07/02/2023 | Student Services
- Summer School: Automation and miniaturization in sample preparation, 19 – 22 September 2023, Hradec Králové
07/02/2023 | Student Services
- Dean's Bulletin – January 2023
31/01/2023 | Student Services
- When 1+1 is more than 2 – a hybridization approach yields a new candidate molecule for the treatment of tuberculosis

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Literature search PubMed

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

The image shows a screenshot of the PubMed.gov website. At the top left is the NIH logo with the text "National Library of Medicine" and "National Center for Biotechnology Information". At the top right is a user profile icon labeled "jostovap". The main heading "PubMed.gov" is prominently displayed. Below it is a search bar with the placeholder text "Search PubMed" and a green "Search" button. Under the search bar, the word "Advanced" is visible. A paragraph of text describes the database: "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, a dark box contains the text "35 million citations". The background features a network diagram of nodes and lines.

NIH National Library of Medicine
National Center for Biotechnology Information

jostovap

PubMed.gov

Search PubMed Search

Advanced

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.

35 million citations

Literature search PubMed

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- SNP
- Gene
- Protein
- PubChem

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

Literature search PubMed

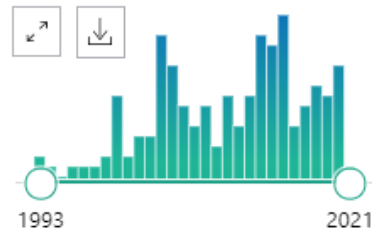
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PubMed.gov

MY NCBI FILTERS

163 results

RESULTS BY YEAR



Filters applied: Review. [Clear all](#)

TEXT AVAILABILITY

- Abstract
- Free full text
- Full text

ARTICLE ATTRIBUTE

- Associated data

- NAD(P)H:Quinone Oxidoreductase 1 (NQO1) as a Therapeutic and Diagnostic Target in Cancer.**
1
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 ...
- Alzheimer's Disease and NQO1: Is there a Link?**
2
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 ...

Literature search

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US National Library of Medicine
National Institutes of Health

Advanced

Format: Abstract ▾

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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.

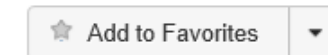
METHODS AND RESULTS: The ONCOMINE query showed that: (1) acute lymphoblastic leukemia and chronic myelogenous leukemia are associated with reduced NQO1 levels, and (2) under-expressed NQO1 was found in human HL-60 leukemia cell line containing the heterozygous NQO1*2 polymorphism. We examined induction 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 μM SFN treatment. Treatment with 25 μM 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-κB (NFκB).

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

Full text links



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Similar articles

Sulforaphane-induced apoptosis in human leukemia HL-60 cells thro [Environ Toxicol. 2017]

NAD(P)H:quinone oxidoreductase (NQO1) loss of function in Burkitt's lymphoma c [Biofactors. 2008]

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]

Review Contribution of NAD(P)H:quinone oxidoreductase 1 to protection ; [Mutat Res. 2004]

See reviews...

See all

Literature search

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

The screenshot shows the PubMed website interface. At the top, there is a navigation bar with 'NCBI Resources' and 'How To' menus, and a user profile for 'jostovap'. The main search area contains the text 'nqo1 activity' in the search box and a 'Search' button. Below this, a larger search box contains 'nqo1' and another 'Search' button. A dropdown menu is open over the 'Send to' button, listing options: 'Clipboard', 'My Bibliography', 'Collections', and 'Citation manager'. The search results show 163 results, with the first result highlighted: 'NAD(P)H dehydrogenase 1 (NQO1) as a Therapeutic and Diagnostic Target'. The abstract text for this result is visible, starting with '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 ...'. On the left side, there is a 'RESULTS BY YEAR' bar chart showing the number of publications from 1993 to 2021. The chart shows a steady increase in publications over time, with a notable peak around 2018-2021. Below the chart, there is a 'TEXT AVAILABILITY' section with a checkbox for 'Abstract'.

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Builder


<input type="text" value="All Fields"/>	<input type="text"/>	-	Show index list
AND <input type="text" value="All Fields"/>	<input type="text"/>	- +	Show index list

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Literature search



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Literature search

WOS

<http://apps.webofknowledge.com/>

The screenshot displays the Web of Science search interface. At the top, the Clarivate logo is on the left, and 'English' and 'Products' are on the right. Below this, the 'Web of Science' logo is followed by navigation links: 'Search', 'Marked List', 'History', and 'Alerts'. On the far right of this navigation bar are 'Sign In' and a 'Register' button. The main header area has a purple background with the text 'Discover multidisciplinary content from the world's most trusted global citation database.' Below this, there are two tabs: 'DOCUMENTS' (selected) and 'RESEARCHERS'. The search area shows 'Search in: Web of Science Core Collection' and 'Editions: All'. Underneath, there are three sub-tabs: 'DOCUMENTS', 'CITED REFERENCES', and 'STRUCTURE'. A search input field contains 'NQO1' with a dropdown menu set to 'All Fields'. Below the input field are buttons for '+ Add row' and '+ Add date range', followed by the text 'Advanced Search'. At the bottom right of the search area are 'Clear' and 'Search' buttons. A red arrow points to the 'All Fields' dropdown menu.

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Search > Results for NQO1 (All Fields)

→ 4,222 results from Web of Science Core Collection for:

Q NQO1 (All Fields) Analyze Results Citation Report Create Alert

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1 Rational designed highly sensitive probes for **NQO1** substrates in vivo: An innovative strategy for early diagnosis of cancer. **EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY** Gong, QJ; Yang, FL; (...); Zhang, XJ; ... | EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY

Since **NQO1** is overexpressed in many types of cancer, it is considered a potential anticancer activity through the redox cycle. The development of highly sensitive probes is needed for diagnostic imaging in clinic.

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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](#)
[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 high-grain 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, superoxide 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-κB 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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Gong, QJ; Yang, FL; (...); Zhang, XJ
Nov 15 2021 | 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 therapy. NQO1 substrates show potent anticancer activity through the redox cycle mediated by NQO1, while the NQO1 probes can monitor NQO1 levels in cancers. High sensitivity of probes is needed for diagnostic imaging in clinic. In this study, based on the analysis of NQO1 catalytic pocket, the naphthoquinone trigger ... Show more
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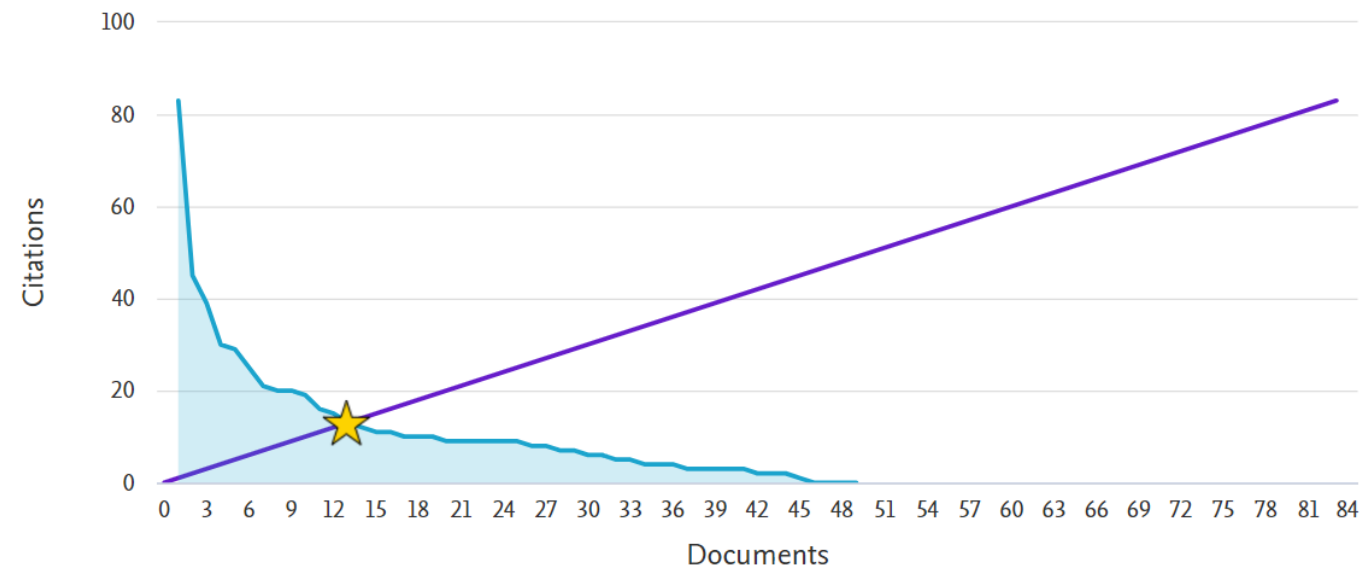
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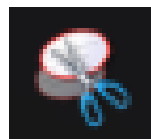
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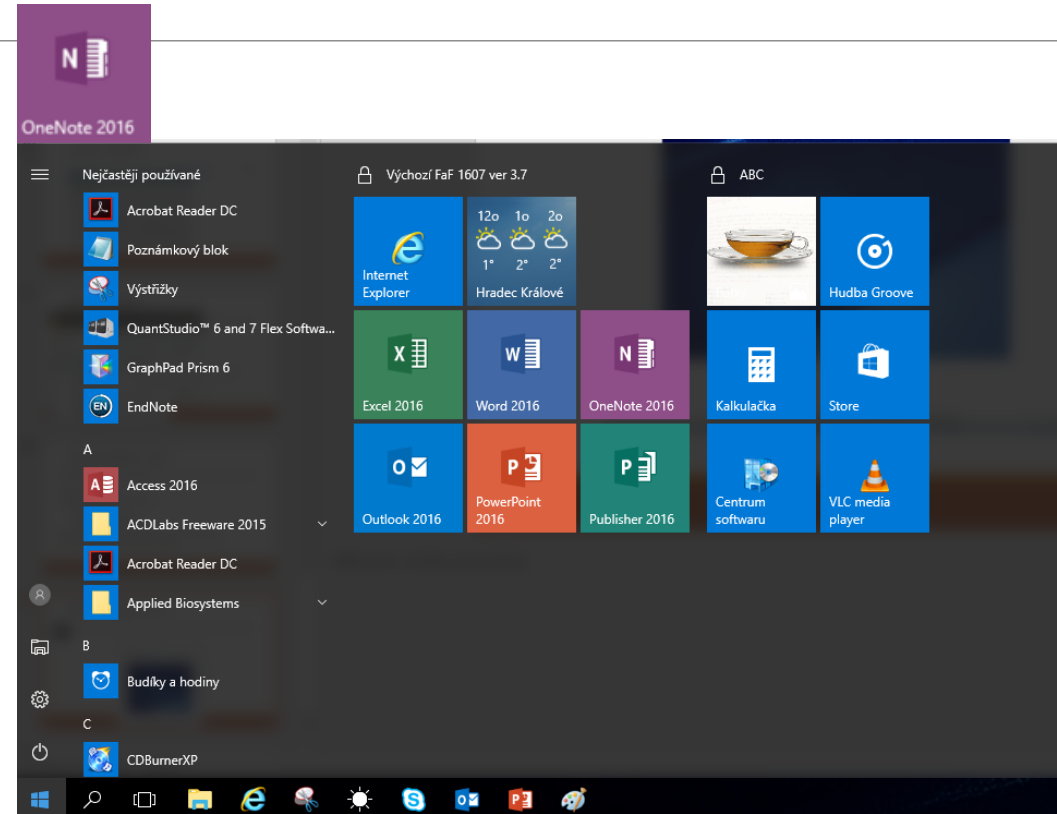
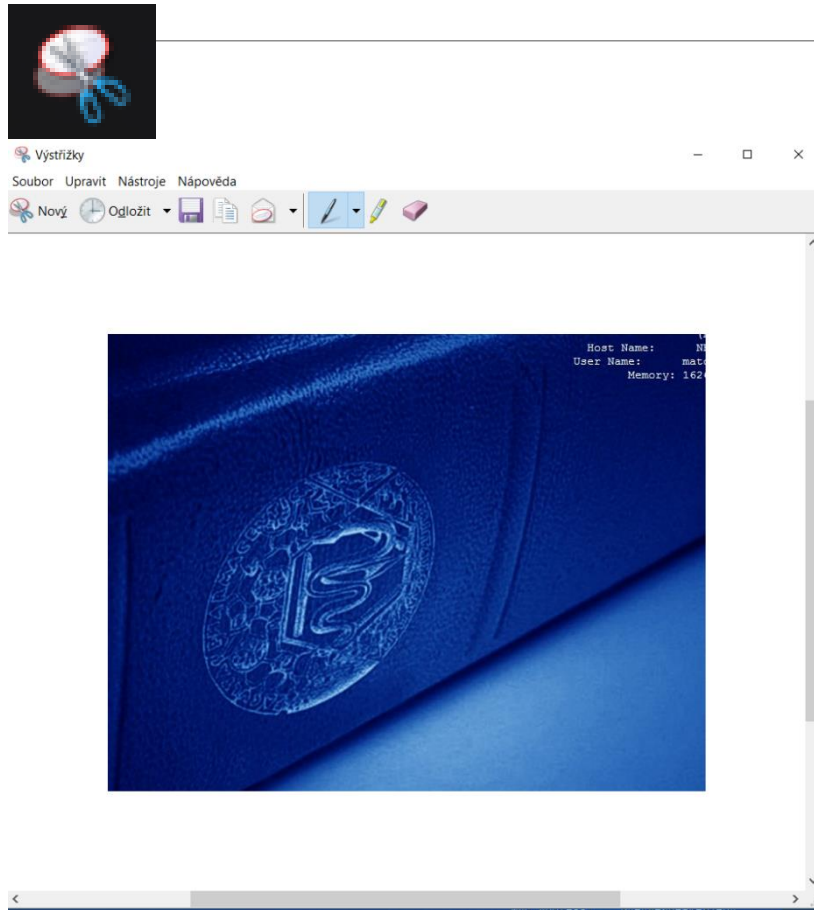
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NQO1: NAD(P)H:quinone oxidoreductase 1

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Kawanishi, Y.	2003	Reduction of 6-(7-hydroxyl) guanine by NAD(P)H:quinone oxidoreductase 1 (NQO1) in the presence of hydrogen peroxide
Fu, X. P.	2005	Nanotechnology-mediated delivery of NQO1: bioavailable drugs
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Kishi, A. S.	2009	Quinone reductase (NQO1), a sensitive redox indicator, is increased in Alzheimer's disease