



DEVELOPMENT OF BIOMEDICAL EDUCATIONAL PROGRAMS

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Development of computer programs for drug discovery needs qualified scientific staff, not only software development and technical support. Growth of biomedical data volume and availability of new experimental technologies give solid background for complex computer modeling limiting rather by human resources than hardware. Bioinformatics education faces new challenges related to changing educational standards, distant education on online meeting formats.



XXVIII Symposium on Bioinformatics
and Computer-Aided Drug Discovery

Moscow (Virtual), 26/05/2022



COVID-19 changed research and development directions in 2020-2021.

We still have consequences (distal conferences and disrupted contacts)

Professor of Sechenov University

Minister of Health of the Russian Federation Mikhail Murashko



Rector Prof., Acad.
P.V.Glybochko

Importance of the digital solutions for medicine was strengthened by COVID-19 and related lockdowns

At the forefront of health care

Monument to the feat of medical workers in the fight against COVID-19

(монумент «Подвигу медицинских работников в борьбе с COVID-19»)

(open 17.09.2021 in campus of Sechenov University in Moscow)



New challenges in digital medicine and education



Scientific challenges in connection with the coronavirus pandemic have raised research and educational problems, changes in the methodology for mastering scientific disciplines.

Medical universities use new E-health technologies, one of the global areas of which is telemedicine. Medical teleconsultations make it possible to increase the availability of medical care for the population of remote areas, elderly and inactive patients, which is especially relevant for monitoring the spread of coronavirus infection.

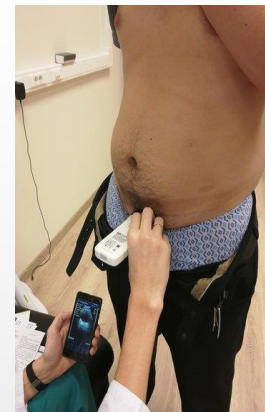
The First Moscow State Medical University of the Ministry of Health of Russia (Sechenov University) and the Institute of Digital Medicine deal with the problems of digitalization of medicine, provide a platform for discussing existing issues in the development of medical technologies, online conferences, and new educational programs.

Publication activity - The Russian Journal of Telemedicine and E-Health continues series of publication on this topic (<https://jtelemed.ru/>). We have arranged series of international journal issues on gene expression regulation as well.

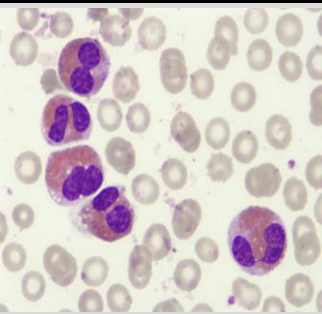
Training a neural network to recognize bladder malady

Dr. I.A.Shaderkin

Laboratory of electronic healthcare,
Sechenov University



3D positioning



Fundus pictures

Peripheral and bone marrow
smear images

Approaches at Sechenov University

- Teaching on informatics, IoT, Machine Learning courses
- Master-classes for students
- Specialized Russian journal on telemedicine (RSCI - ПИНЦ)

Network medicine conception – extension of gene network, drug-disease network, genotype-phenotype network terms

Network medicine: a network-based approach to human disease

Albert-László Barabási , Natali Gulbahce & Joseph Loscalzo

Nature Reviews Genetics 12, 56–68(2011) | [Cite this article](#)

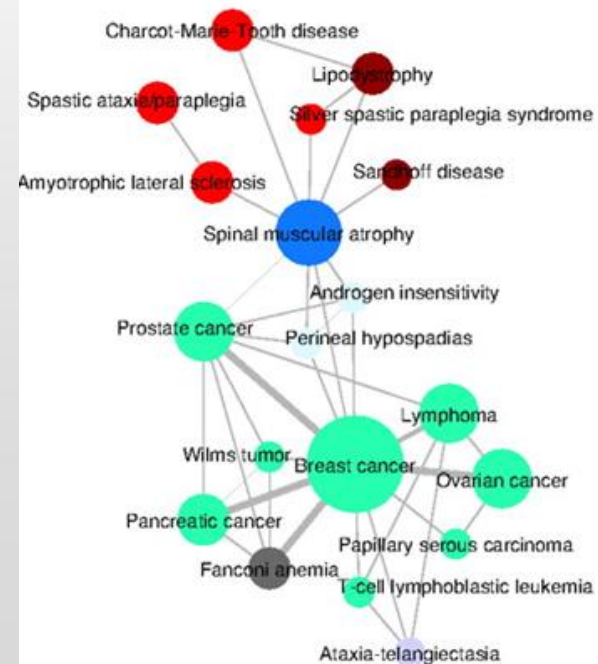
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The idea is to compare diseases by comparing the functions of genes, symptoms, drug compounds - **the network approach**.

Analysis of genes associated with a disease, assessment of their place in the gene network (connectivity) allows us to evaluate them as target genes for drug effects

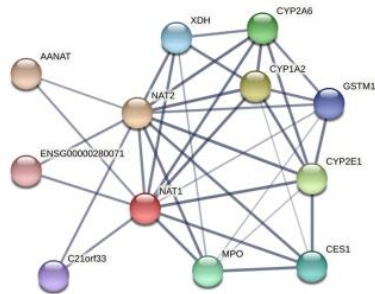
Standard for students' diploma and course works at Sechenov University on gene networks for complex human diseases – cancers, metabolic syndrome, Parkinson's disease

Human Disease Network (HDN)



Work on gene network of
metabolic syndrome with students

R.P. Tiis^{1,2}, L.P. Osipova^{1,2}, E.R. Galieva², D.V. Lichman^{1,2},
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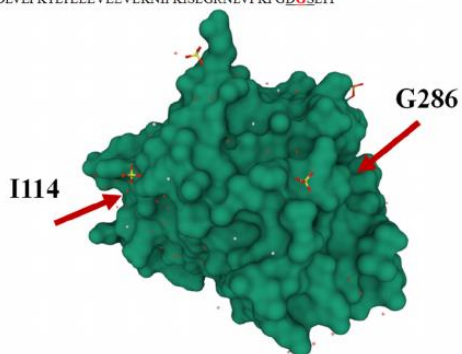
To search for new targets of therapy, it is necessary to reconstruct the gene network of the disease, and identify the interaction of genes, proteins, and drug compounds. Using the online bioinformatics tools we have analyzed the current data set related to the metabolism of xenobiotics, mediated by the N-acetyltransferase 2 (NAT2) gene. The study of allelic polymorphism of the NAT2 gene has a prognostic value, allowing to determine the risk of a number of oncological diseases, the degree of increased risk due to smoking and exposure to chemical carcinogens, including drugs. The aim of this study was to determine the frequencies of two important “slow” variants of the NAT2 gene (NAT2*5, rs1801280 and NAT2*7, rs1799931), which significantly affected the rate of xenobiotic acetylation among the indigenous Nenets population of Northern Siberia. The obtained frequencies of polymorphic variants among the Nenets occupy an intermediate value between those for Europeans and Asians, which might indicate specific features of adaptation. We present a model of the distribution of two polymorphic variants of the NAT2 gene involved in the biotransformation of xenobiotics to study the characteristics of their metabolism in the indigenous inhabitants of Yamal.

Key words: xenobiotics; N-acetyltransferase 2; gene polymorphism; Nenets; bioinformatics; gene networks reconstruction

Funding. The work was supported by the Russian Science Foundation (project no. 19-15-00219).

Received: 23.04.2021, revised: 05.05.2021, accepted: 11.05.2021.

>2PFR_1|Chains A,B|Arylamine N-acetyltransferase 2|Homo sapiens (9606)
GGSGSDIEAYFERIGYKNSRNKLDLETLDILEHQIRAVPFENLNMHCGQAMELGLAIFDHI
VRRNRGGWCLQVNLQYLTWALTTIGFQTTMLGGYFYIPVKNYSTGMVHLLQVITDGRNYI
VDAGSGSSSQMWQPLELISGKDQPOVPCIFCLTEERGIWYLDQIRREQYITNKEFLNSHLLPK
KKHQKIYLFLEPRITIEDFESMNTY/LQTSPTSSFITTSFCSLQTPGEGVYCLVGFILTYRKFNYKD
NTDLVEFKLTLEEEVEVLKNIFKISLGRNLVPKPGDGLTI



Tiis, R. P., Osipova, L. P., Galieva, E. R., Lichman, D. V., Voronina, E. N., Melikhova, A. V., Orlov, Y. L., Filipenko, M. L. (2021). N-acetyltransferase (NAT2) gene polymorphism and gene network analysis. *Biomeditsinskaya khimiya*, 67(3), 213-221.

DOI: 10.18097/PBMC20216703213

Presented at previous “Way2drug” conference in 2021

Due to distant education format in Moscow in 2020-2021 we set priority for online bioinformatics tools

Natalya V. Gubanova, Nina G. Orlova, Arthur I. Dergilev, Nina Y. Oparina and Yuriy L. Orlov*

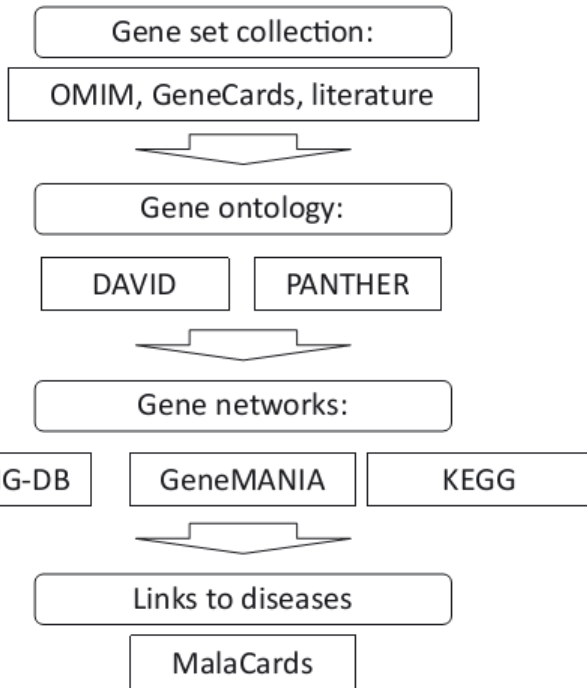
Glioblastoma gene network reconstruction and ontology analysis by online bioinformatics tools

<https://doi.org/10.1515/jib-2021-0031>

Received August 31, 2021; accepted October 18, 2021; published online November 16, 2021

Table 5: Diseases found by prioritization of shared genes to glioblastoma.

No.	Description	Category	Score
1	Glioma	1.882×10^{-25}	9.333×10^{-22}
2	Pilocytic astrocytoma	3.147×10^{-25}	1.561×10^{-21}
3-4	Adult pilocytic astrocytoma/childhood pilocytic astrocytoma	1.829×10^{-22}	9.069×10^{-19}
5	Malignant glioma	3.741×10^{-21}	1.855×10^{-17}
6	Mixed gliomas	3.741×10^{-21}	1.855×10^{-17}
7	Neurofibromatosis 1	6.750×10^{-21}	3.348×10^{-17}
8	Malignant neoplasm of soft tissue	2.560×10^{-20}	1.270×10^{-16}
9	Ganglioglioma	4.231×10^{-20}	2.098×10^{-16}
10-11	Childhood oligodendroglioma/adult oligodendroglioma	4.616×10^{-20}	2.290×10^{-16}
12	Sarcoma	2.272×10^{-19}	1.127×10^{-15}

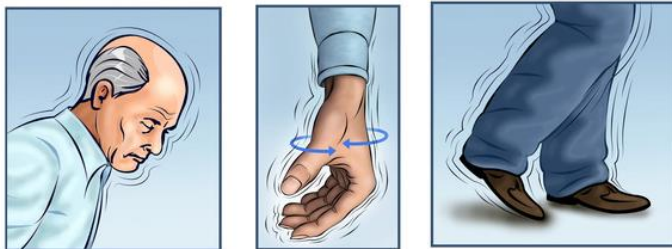
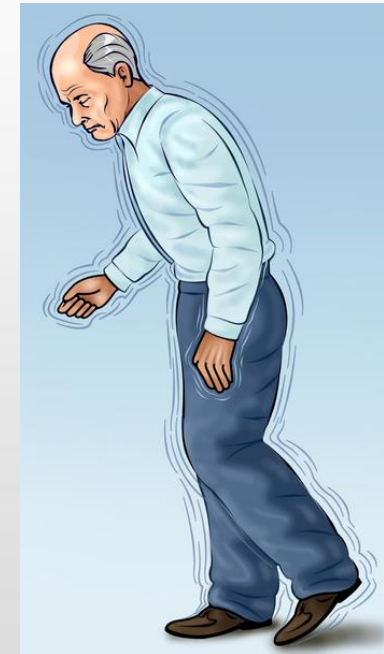


Computer pipeline – using only online tools – appropriate for students and distal education format

The research interest in the study of **Parkinson's disease** is due to the fact that this disease is a medical and economic problem for society and at the moment there are no treatments that can stop or reverse the neurodegenerative process accompanying this disease.



The growth in the volume of genetic data provides a basis for searching for associations with diseases, which is reflected in the replenishment of such databases as **OMIM** (<https://omim.org/>), **GeneCards** (<https://www.genecards.org/>). The development of experimental sequencing technologies leads to an increase in transcriptomic data, which allows the reconstruction of gene networks / signal transduction pathways based on co-expression. Existing online bioinformatics tools allow solving many practical tasks for the reconstruction of gene networks without using additional software (used in the training course for students of the Sechenov University - First Moscow State Medical University of the Ministry of Health of the Russian Federation named after I.M. Sechenov).



Quick links

[Whole genome function views](#)

[Gene expression tools](#)

[cSNP tools](#)

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SEQUENCE SEARCH

Enter a protein sequence: [?](#)

Sequence query limits: Protein - 50kb

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The PANTHER (Protein **AN**alysis **TH**rough Evolutionary Relationships) Classification System is a unique resource that **classifies genes by their functions**, using published scientific experimental evidence and evolutionary relationships to predict function even in the absence of direct experimental evidence. Proteins are **classified by expert biologists** according to:

- [Gene families and subfamilies](#), including annotated phylogenetic trees
- [Gene Ontology classes](#): molecular function, biological process, cellular component
- [PANTHER Protein Classes](#)
- [Pathways, including diagrams](#)

PANTHER is part of the [Gene Ontology Reference Genome Project](#).

PANTHER is supported by a research grant from the National Institute of General Medical Sciences [grant [GM081084](#)] and maintained by the [Thomas lab at the University of Southern California](#).

What can I do on the PANTHER site? [?](#)
Guide to getting started

News

(December 12, 2011)

PANTHER tools are now supporting all 48 organisms.

[Click](#) for additional info.

Publications

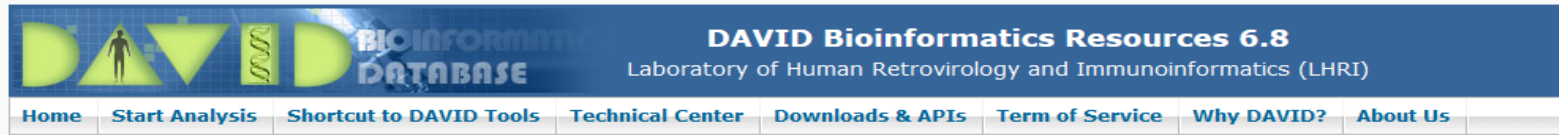
[How to cite PANTHER](#)

"[PANTHER version 7: improved phylogenetic trees, orthologs and collaboration with the Gene Ontology Consortium.](#)" [Mi, et al.](#)

"[Applications for protein sequence-function evolution data: mRNA/protein expression analysis and coding SNP scoring tools.](#)" [Thomas, et al.](#)

"[PANTHER: a library of protein families and subfamilies indexed by function.](#)" [Thomas, et al.](#)

Online tools for gene ontology analysis based on gene list



DAVID Bioinformatics Resources 6.8
Laboratory of Human Retrovirology and Immunoinformatics (LHRI)

Home Start Analysis Shortcut to DAVID Tools Technical Center Downloads & APIs Term of Service Why DAVID? About Us

*** Welcome to DAVID 6.8 ***

*** If you are looking for [DAVID 6.7](#), please visit our [development site](#). ***

Recommending: A [paper](#) published in *Nature Protocols* describes step-by-step procedure to use DAVID!

Welcome to DAVID 6.8

2003 - 2019

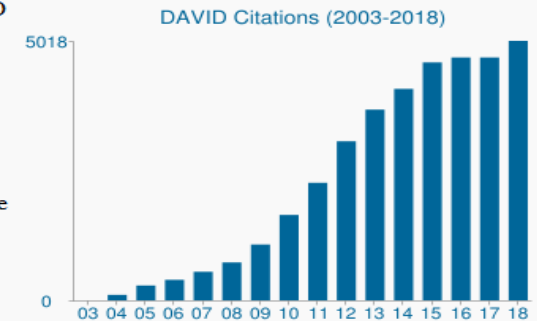
The Database for Annotation, Visualization and Integrated Discovery (DAVID) v6.8 [comprises a full Knowledgebase update to the sixth version](#) of our original web-accessible programs. DAVID now provides a comprehensive set of functional annotation tools for investigators to understand biological meaning behind large list of genes. For any given gene list, DAVID tools are able to:

- Identify enriched biological themes, particularly GO terms
- Discover enriched functional-related gene groups
- Cluster redundant annotation terms
- Visualize genes on BioCarta & KEGG pathway maps
- Display related many-genes-to-many-terms on 2-D view.
- Search for other functionally related genes not in the list
- List interacting proteins
- Explore gene names in batch
- Link gene-disease associations
- Highlight protein functional domains and motifs
- Redirect to related literatures
- Convert gene identifiers from one type to another

What's Important in DAVID?

- [Cite DAVID](#)
- [IDs of Affy Exon and Gene arrays supported](#)
- [Novel Classification Algorithms](#)
- [Pre-built Affymetrix and Illumina backgrounds](#)
- [User's customized gene background](#)
- [Enhanced calculating speed](#)

Statistics of DAVID



• [> 38,000 Citations](#)

Shortcut to DAVID Tools

- Functional Annotation**
Gene-annotation enrichment analysis, functional annotation clustering, BioCarta & KEGG pathway mapping, gene-disease association, homologue match, ID translation, literature match and more
- Gene Functional Classification**
Provide a rapid means to reduce large lists of genes into functionally related groups of genes to help unravel the biological content captured by high throughput technologies. [More](#)
- Gene ID Conversion**
Convert list of gene ID/accessions to others of your choice with the most comprehensive gene ID mapping repository. The ambiguous accessions in the list can also be determined semi-automatically. [More](#)
- Gene Name Batch Viewer**
Display gene names for a given gene list; Search functionally related genes within your list or not in your list; Deep links to enriched detailed information. [More](#)

The tool for gene list manipulations and gene ontology analysis



Preparation of the list of genes associated with the disease

OMIM[®]

Online Mendelian Inheritance in Man[®]

An Online Catalog of Human Genes and Genetic Disorders

The Internet resource OMIM (Online Mendelian Inheritance in Man) (<https://omim.org/>) was used to search for genes of susceptibility to the disease. A list of 229 genes was found, and the categories and analysis of gene ontologies were calculated using the PANTHER resource (Protein ANalysis THrough Evolutionary Relationships) (<http://pantherdb.org/>) (Mi et al., 2013).

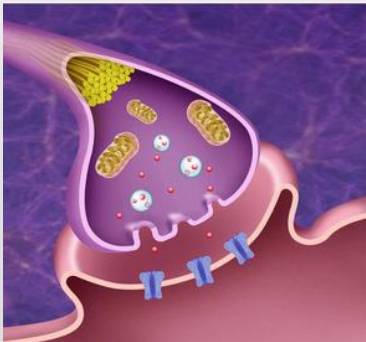
Of the 229 original genes, 170 identifiers were recognized, 59 identifiers were not recognized or could not be unambiguously mapped. In total, 20851 genes were used in the PANTHER reference genome. With the help of PANTHER, we built a table of ontologies for categories of biological processes, in order to obtain the most informative results, the p-values were limited to E-20.

The most significant categories for the genes of Parkinson's disease are general regulation of cell death, regulation of cell death of neurons, regulation of apoptosis and programmed cell death, negative regulation of cell death, which confirms the etiology of the disease - death of substantia nigra neurons.

These data confirm the key etiological features of the disease, among which the central aspect of the pathophysiology of Parkinson's disease is the progressive death of dopamine neurons in the midbrain and their axonal projections.

(Published recently at "Biomedical chemistry" (2021))

Some findings on gene ontologies for Parkinson's disease using these tools

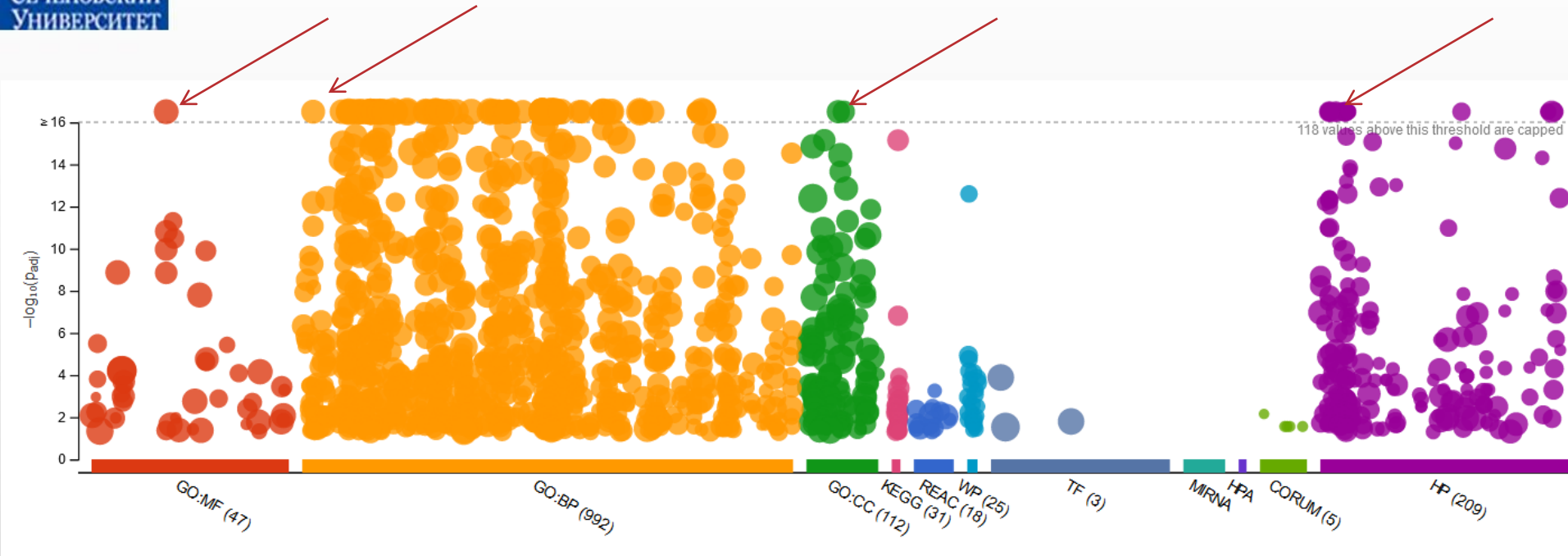


GO molecular functions	Number of genes	P-value (corrected)
enzyme binding	59	2,48E-12
protein binding	150	2,22E-11
ubiquitin protein ligase binding	22	7,08E-11
ubiquitin-like protein ligase binding	22	1,94E-10
signaling receptor binding	46	2,15E-09
heatshock protein binding	15	2,41E-09
binding	164	2,80E-08
identical protein binding	46	9,35E-08
tau protein binding	9	1,69E-06
kinase binding	26	4,88E-06
protein domain specific binding	25	6,55E-06
catalytic activity	86	1,38E-05
protein kinase binding	22	1,99E-04

The most significant are the categories of enzyme binding, protein binding, binding of ubiquitin ligase and ubiquitin-like proteins, and binding of signaling proteins and heat shock proteins.

Autophagy is one of the main pathways for intracellular degradation of α -synuclein, and current research shows that dysfunctional autophagy in Parkinson's disease is one of the main risk factors for the development of the disease (Hale et al. 2016).

Plot of pointwise values of the categories of gene ontologies of Parkinson's disease genes, calculated using the GOST program for a list of 293 genes.

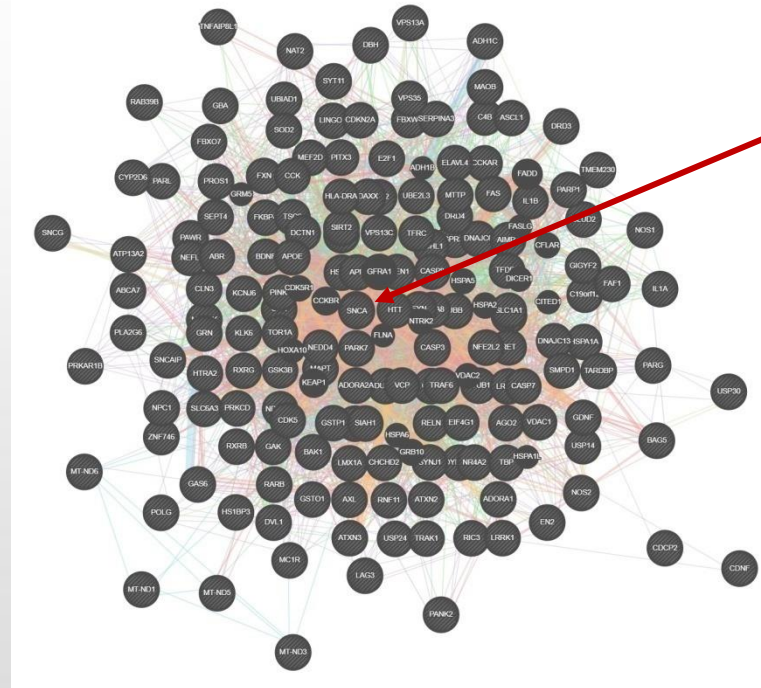


Findings on gene ontologies
for Parkinson's disease
using these tools

The most significant categories of this list of genes include the death of neurons, Lewy bodies, regulation of cell death, and the somatodendritic compartment.

GeneMANIA and STRING-DB resources were used to reconstruct the gene network of interactions between Parkinson's disease genes. The figure shows a gene network of 187 genes for Parkinson's disease, reconstructed using GeneMANIA.

Gene network reconstruction
for Parkinson's disease
using same gene list



To date, it is known that the SNCA gene encoding α -synuclein is pleiomorphic, and any, both rare mutations and common, variations in this locus change the risk of developing the disease.

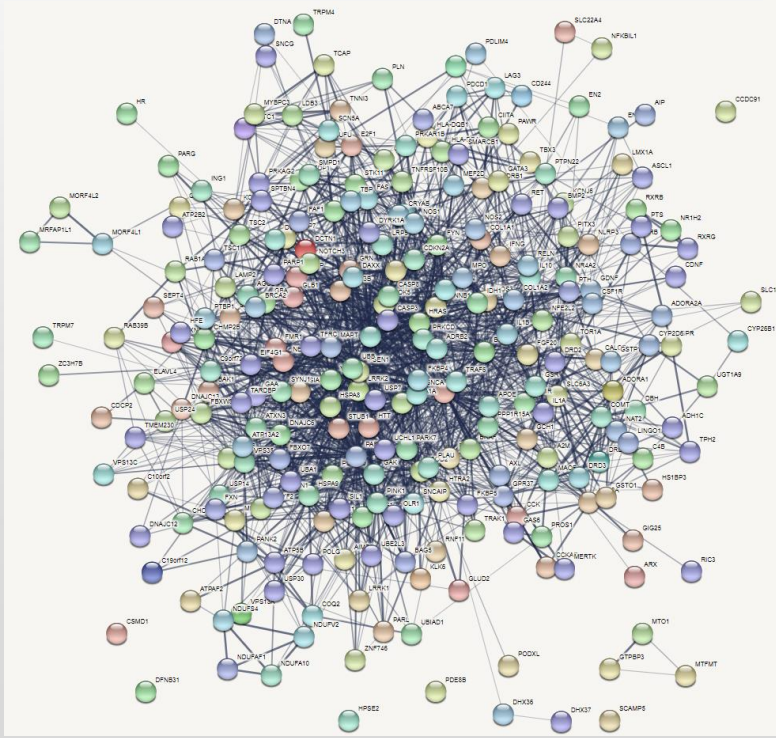
In the center of the constructed network are genes (proteins) that have a large number of connections with other elements - **SNCA, CASP3, GFRA1, HTT, PARK7.**

This trend is supported by current studies of candidate gene associations (Billingsley *et al.* 2018), in which the most statistically significant signals associated with Parkinson's disease are common variants located close to SNCA, LRRK2 and MAPT, as well as low-frequency coding variants in GBA.



<https://string-db.org/>

Gene network for the same disease reconstructed using STRING-DB



Version: 11.0

STRING

[Search](#) [Download](#)

Protein by name >

Protein by sequence >

[Multiple proteins](#) >

Multiple sequences >

Proteins with Values/Ranks **New** >

Organisms >

Protein families ("COGs") >

Examples >

Random entry >

SEARCH

Multiple Proteins by Names / Identifiers

List Of Names: (one per line, examples: #1 #2 #3)

A2M
ABCA7
ACTC1
AD17
AD7CNTP
ADH1C

... or, upload a file:

[Browse ...](#)

Organism:

auto-detect

[Advanced Settings](#)

SEARCH

number of nodes: 268
number of edges: 2079
average node degree: 15.5
avg. local clustering coefficient: 0.428
expected number of edges: 942
PPI enrichment p-value: < 1.0e-16



Integrative database tool – GeneCards.org



According to the GeneCards resource, the following 10 genes are the most significant for Parkinson's disease

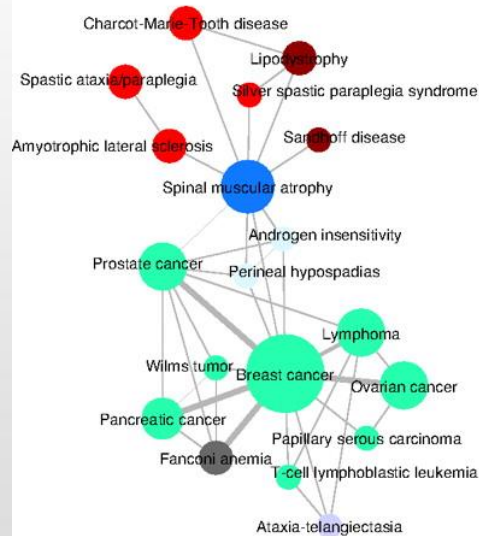
	Gene	Full name	Score
1	SNCA	Synuclein Alpha	157.73
2	LRRK2	Leucine Rich Repeat Kinase 2	151.68
3	PRKN	Parkin RBR E3 Ubiquitin Protein Ligase	142.61
4	PARK7	Parkinsonism Associated Deglycase	119.70
5	PINK1	PTEN Induced Kinase 1	114.13
6	MAPT	Microtubule Associated Protein Tau	106.49
7	ATP13A2	ATPase Cation Transporting 13A2	104.18
8	GBA	Glucosylceramidase Beta	103.77
9	APOE	Apolipoprotein E	94.18
10	APP	Amyloid Beta Precursor Protein	85.19

The first place in this hierarchical list is occupied by the *SNCA* gene encoding the alpha-synuclein protein, mutations in this gene lead to the development of autosomal dominant forms of the disease, the severity of the disease correlates with the number of copies of the *SNCA* gene. Mutations in the *LRRK2* gene have been identified as the causes of the autosomal dominant nature of Parkinson's disease as the most common monogenic form of the disease identified to date (Paisán-Ruíz *et al.*, 2004; Zimprich *et al.*, 2004). Genetic variants in *LRRK2* are associated with most of all known inherited manifestations of Parkinson's disease.

DISEASOME

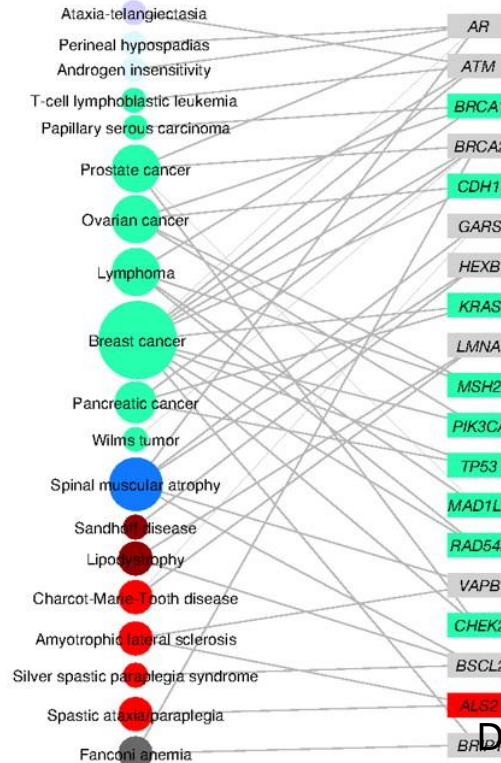
Kwang-II Goh et al. PNAS 2007;104:21:8685-8690

Human Disease Network (HDN)

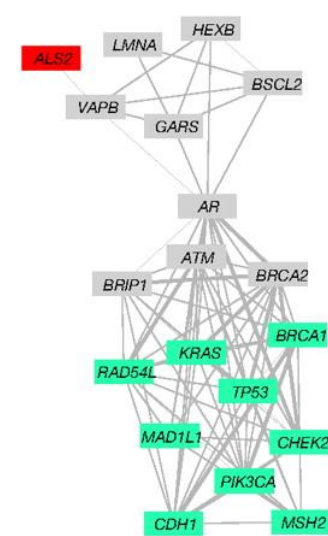


disease phenome

disease genome



Disease Gene Network (DGN)



Disease Network (left panel)
Gene network (right)
And the link between diseases through genes (center).

Generating human disease-drug networks

Online tools (some not free)
GeneGO
(www.genego.com),
Ingenuity
(www.ingenuity.com)
and Biocarta
(www.biocarta.com).

The human disease network
Kwang-II Goh, M.E. Cusick, D.Valle, B.Children, M.Vidal, A.-L. Barabási
PNAS, 2007 104 (21) 8685-8690;
<https://doi.org/10.1073/pnas.0701361104>



Reconstruction of gene networks associated with Parkinson's disease leads to the identification of network structures. Such a discovery of functional connections opens the way to the creation of new drugs. The same network modeling approach is applied to series on complex diseases.



Acknowledgements

Sechenov University, Novosibirsk State University

Students:

A.G.Galieva

Y.A.Mozyleva

E.N.Ivanova

R.R.Shakirova

N.A.Makarov

A.V.Korobeinikova

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The development of education programs using online bioinformatics tools was supported in 2022 by Potanin Foundation (grant **ГК22-000797**) :

Natalya V. Gubanova, Nina G. Orlova, Arthur I. Dergilev, Nina Y. Oparina, Yuriy L. Orlov. Glioblastoma gene network reconstruction and ontology analysis by online bioinformatics tools. *Journal of Integrative Bioinformatics*.2021.Vol. 18, pp. 20210031.

Орлов Ю.Л., Галиева А.Г., Орлова Н.Г., Иванова Е.Н., Мозылева Ю.А., Анашкина А.А. (2021) Реконструкция генной сети болезни Паркинсона для поиска генов-мишеней. *Биомедицинская химия*, 2021, том 67, выпуск 3, с. 222-230 doi: 10.18097/PBMC20216703222

Тийс Р.П., Осипова Л.П., Галиева Э.Р., Личман Д.В., Воронина Е.Н., Мелихова А.В., Орлов Ю.Л., Филипенко М.Л. Полиморфизм вариантов гена N-ацетилтрансферазы 2 (*NAT2*) и анализ генной сети. *Биомедицинская химия*, 2021, 67(3): 213-221 doi:10.18097/PBMC20216703213

Yuriy L. Orlov, Ayya G. Galieva, Anton N. Luzin, Anastasia A. Anashkina (2021). Reconstruction of Gene Networks Associated with Complex Disorders on Example of Parkinson Disease //In: *Biologia Serbica* Vol. 43 - No. 1 Special Edition. Book of Abstracts Belgrade Bioinformatics Conference 2021, 21-25 June 2021, Vinča, Serbia, P.62.

Orlova N.G., Orlov Y.L. (2022) Problems of developing online training courses for students in digital disciplines using bioinformatics as an example // In: *Proceedings of the International Conference "Scientific research of the SCO countries: synergy and integration"*. Part 3 - Reports in English. March 31, 2022. Beijing, PRC). Scientific publishing house Infinity P. 58-65



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Molecular Sciences

Special Issue "Medical Genetics, Genomics and Bioinformatics—2022"

Special Issue Editors

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Guest Editor

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Interests: medical genomics; e-Health; bioinformatics; systems biology

Special Issues, Collections and Topics in MDPI journals



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Interests: diabetes; obesity; chronic kidney disease; metabolism; biomedicine; e-health

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Institute of Personalized Oncology, I.M. Sechenov First Moscow State Medical University of the Ministry of Health of the Russian Federation (Sechenov University), Moscow, Russia

Interests: oncology; medicine; medical genetics; genomics



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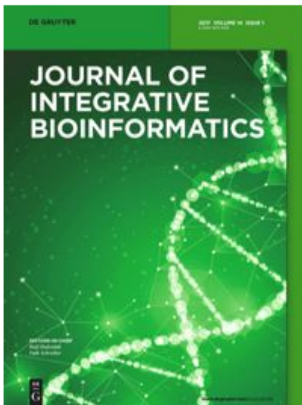
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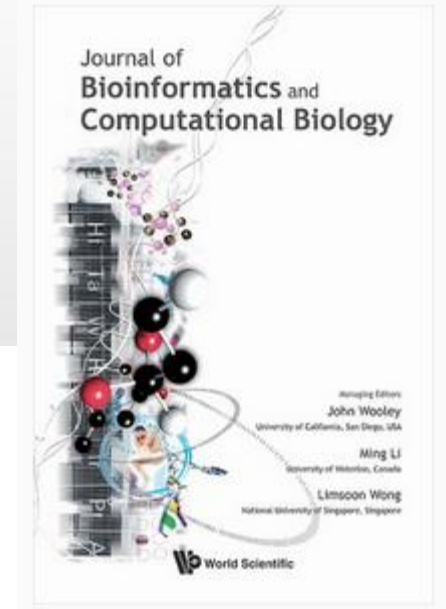
First published: January 1, 2017

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ISSN print 2712-9217 ISSN online 2712-9225 DOI: 10.29188/2712-9217

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Сетевое издание Основано в 2015 году

Письма

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