



Recent Advances in Graph Analytics and Its Applications in Healthcare

KDD 2020 Tutorial

August 23, morning

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http://www.calvinzang.com/kdd2020 tutorial medical graph analytics.html

Outline

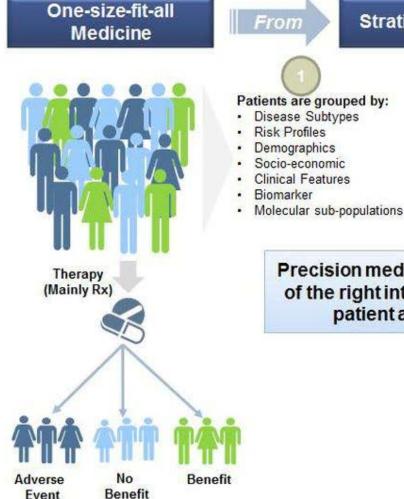
- Introduction
- Network Embedding & GNNs
- Knowledge Graph Mining
- Graph Generative Models & Drug Discovery
- Discussions

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New Paradigm Shift in Treatment

Transitioning From the 'one-size-fits-all' to 'precision medicine' model with multi-level patient stratification.



From

Stratified Medicine



Individual patient level:

- Genomics and Omics
- Lifestyle
- Preferences
- Health History
- Medical Records
- Compliance
- Exogenous Factors



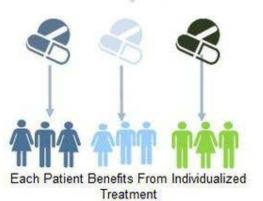
Precision Medicine



Biomarker Therapy

(Rx + Dx = CDx)

Precision medicine ensures delivery of the right intervention to the right patient at the right time.



https://www.forbes.com/sites/reenitadas/2017/03/08/drug-development-industry-bets-big-on-precision-medicine-5-top-trends-shapingfuture-care-delivery/#30fbc5835d3a



The NEW ENGLAND JOURNAL of MEDICINE

Perspective

A New Initiative on Precision Medicine

Francis S. Collins, M.D., Ph.D., and Harold Varmus, M.D. N Engl J Med 2015; 372:793-795 | February 26, 2015 | DOI: 10.1056/NEJMp1500523

Comments open through March 4, 2015

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Article

References

Citing Articles (784)

Comments (7)

Metrics

"Tonight, I'm launching a new Precision Medicine Initiative to bring us closer to curing diseases like cancer and diabetes - and to give all of us access to the personalized information we need to keep ourselves and our families healthier."

President Barack Obama, State of the Union Address, January 20, 2015

President Obama has long expressed a strong conviction that science offers great potential for improving health. Now, the President has announced a research initiative that aims to accelerate progress toward a new era of precision medicine (www.whitehouse.gov/precisionmedicine). We believe that the time is right for this visionary initiative, and the National Institutes of Health (NIH) and other partners will work to achieve this vision.

AUDIO INTERVIEW



Interview with Dr. Francis Collins on what to expect from the recently announced Precision Medicine Initiative. (10:07)

√li>≥ Listen

"The initiative will encourage and support the next generation of scientists to develop creative new approaches for detecting, measuring, and analyzing a wide range of biomedical information - including molecular, genomic, cellular, clinical, behavioral, physiological, and environmental parameters"

Science Translational Medicine MAAAS

PERSPECTIVE HUMAN HEALTH

Precision medicine: Beyond the inflection point

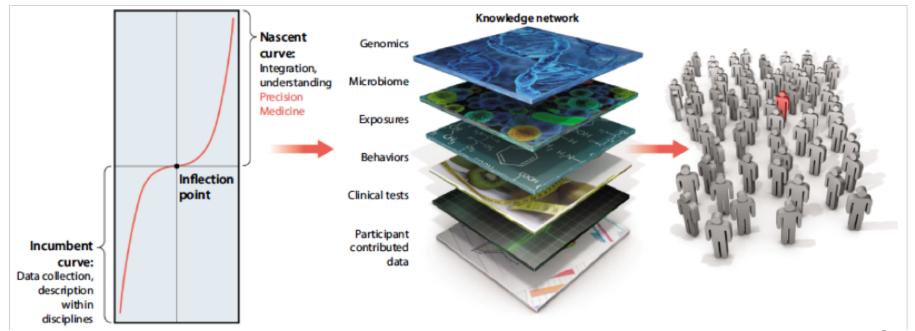
Sam Hawgood¹, India G. Hook-Barnard¹, Theresa C. O'Brien¹ and Keith R. Yamamoto^{1,2,*}

+ See all authors and affiliations

Science Translational Medicine 12 Aug 2015:

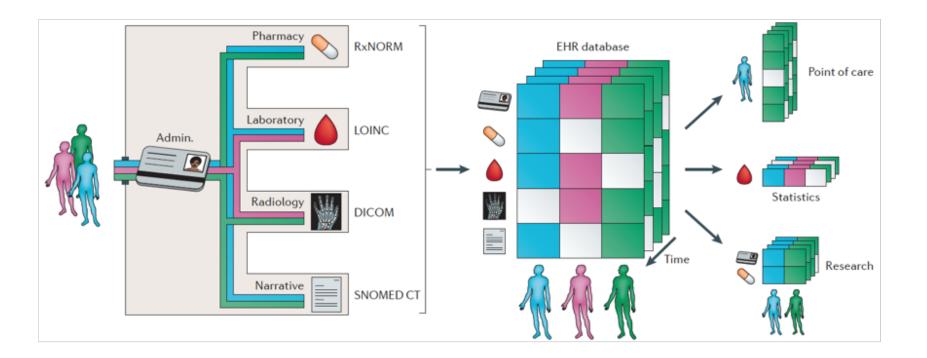
Vol. 7, Issue 300, pp. 300ps17

DOI: 10.1126/scitransImed.aaa9970



Electronic Health Records (EHR)

Electronic Health Record (EHR) is an evolving concept defined as a systematic collection of electronic health information about individual patients or populations



Medical Imaging





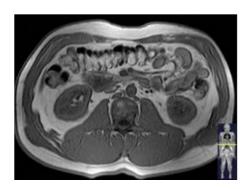
X-ray Computed Tomography (CT)





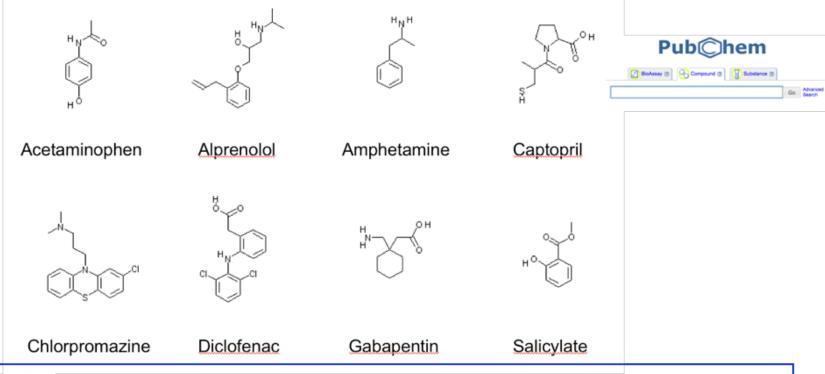
Positron Emission Tomography (PET)





Magnetic Resonance Imaging (MRI)

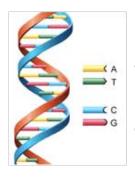
Drug





A chemical compound is a pure chemical substance consisting of two or more different chemical elements that can be separated into simpler substances by chemical reactions

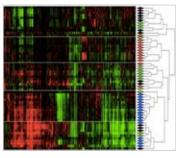
Gene



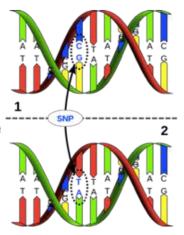
DNA: A long molecule that looks like a twisted ladder. It is made of four types of simple units and the sequence of these units carries information, just as the sequence of letters carries information on a page.



Gene: A segment of DNA. Genes are like sentences made of the "letters" of the nucleotide alphabet, between them genes direct the physical development and behavior of an organism. Genes are like a recipe or instruction book, providing information that an organism needs so it can build or do something like making an eye or a leg, or repairing a wound.



Gene expression: The process in which the information encoded in a gene is converted into a form useful for the cell. The first step is transcription, which produces a messenger RNA molecule complementary to the DNA molecule on which a gene is encoded. For protein-coding genes, the second step is translation, in which the messenger RNA is read by the ribosome to produce a protein.



A Single Nucleotide Polymorphism (SNP,

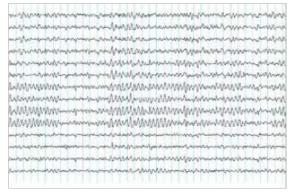
pronounced snip; plural snips) is a DNA sequence variation occurring commonly within a population (e.g. 1%) in which a single nucleotide — A, T, C or G — in the genome (or other shared sequence) differs between members of a biological species or paired chromosomes.

Physiology

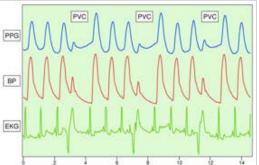


Physiology is the scientific study of function in living systems. A sub-discipline of biology, its focus is in how organisms, organ systems, organs, cells, and bio-molecules carry out the chemical or physical functions that exist in a living system









Patient Survey

	Church Hea		
73.	SURVEY QUEST an separate response from, SA – Strongly Agree, A – Agree, U – Und Our worship services are prayerful experiences.		
74. 75.	Our church does a very good job at discipling members. I pray for my pastor / minister / clergy, their family(ies), and the staff of our church regularly.	100.	I believe you have to be called to be a lifetime missionary to do international missions.
6.	I regularly attempt to establish relationships with people who do not have a church home.	101.	I am excited to be a part of this church. Our church is strong in benevolence ministry.
7.	I believe my voice is heard in this church.	103.	I have been to other churches, and I think our worship services are among the best.
78.	Most of the ministry in our church is done by a small number of people.	104.	The lifestyles of the members at our church are
79.	We have good participation in singing in our worship services.	105.	significantly different than the world's lifestyle. I believe the Bible teaches that prayer should be a daily
80.	We have many people involved in one-on-one discipling	106	part of every Christian's life. I believe that one of the surposes of Sunday school

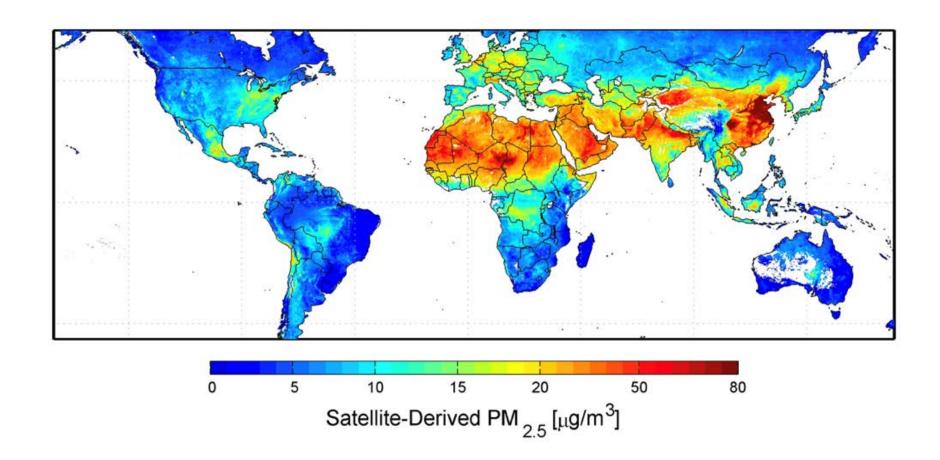
Patient Name:	Date Completed: Date Received:					
Mond and Beltoviors Over the Part 2 Weeks		Barok	Sentimes	Month	Abrays	Comments
I feel sad, unhappy or depressed	1	2	3.	4	5	
2 I feel lethangic, apathetic, or as though I have no energy	- 1	2	3.	4	-5	
3 I feel hopeless about the fature	1	2	3.	4	.5	
4 I feel lonely, isolated or alene	1	2	3.	- 6	.5	
5 Univerticable deeping	1	2	3.	4	.5	
6 E sleep too much	1	2	3.	4	- 5	
7 Ehave no appetite	- 1	2	3.	4	5	
f Covered	1	2	3.	4	5	
9 If feel amproductive or get distracted easily at work	1	1.2	3-	4	.5	
 I have trouble fiscusing on projects, work or activities 	1	2.	3.	4	.5	
Activities and work to longer interest me	1	2	3.	4	5	
2. I have trouble getting along with family/friends/coworkers	1	2	3.	4	5	
3 Effect tense or nervous	1	2.	3.	- 4	5	
4 I feel agitated, angry or irritable	1	2.	3.	4	5	
5 Ethink about hurting myself	1	2	3.	4	5	
16 Lonnider suicide	1	2	3.	4	5	
T. I. drink or de-drugs to escape or dull the pain	1	2	3.	- 4	.5	
8 Ebinge drink (more than 5 drinks in one hour)	1	- 2	3.	4	- 5	
9 People express concern about my drinking or drug use	1	2	3	4	5	
20 I have had trouble at work or school due to alcohol/drags	- 1	2	3.	4	5	

Please answer questions 6 to 19 as follows; 0 = never, 1 = hardly ever, 2 = occasionally, 3 = fairly often, 4 = very often
IN THE PAST 12 MONTHS HAVE YOU Question 4. Had trouble pronouncing any words because of problems with your teeth mouth or dentures?
Question 5. Felt that your sense of taste has worsened because of problems with your teeth mouth or dentures? Question 6. Had any painful aching in your mouth?
Question 7. Found it uncomfortable to eat any foods because of problems with your teeth mouth or dentures?
Question 8. Been self conscious because of problems with your teeth mouth or dentures?
Question 9. Felt tense because of problems with your teeth mouth or dentures?
Question 10. Has your diet been unsatisfactory because of problems with your teeth, mouth or dentures? (Question relates to function - not about quality of food in prisons)
Question 11. Had to interrupt meals because of problems with your teeth mouth or dentures?
Question 12. Found it difficult to relax because of problems with your teeth mouth or dentures?
Question 13. Been a bit embarrassed because of problems with your teeth mouth or dentures?
Question 14. Been a bit irritable with other people because of problems with your teeth mouth or dentures?
Question 15. Had difficulty doing your usual activity because of problems with your teeth mouth or dentures?
Question 16. Falt that life in general is less satisfying because of problems with your teeth mouth or dentures?
Question 17. Been totally unable to function because of problems with your teeth mouth or dentures?
If you have lost some, or all your natural teeth, we would like you to answer the following question.
Question 18. Have you ever had any kind of denture? (False teeth which you can take out) (Please tick one box) YES 1 NO 2
IF YES , PLEASE ANSWER THE FOLLOWING, IF NO, PLEASE GO TO QUESTION 22.
Question 19. What type of denture do you have? (Please tick all relevant boxes)
YES NO YES NO SOMETIMES Full TOP denture. Do you wear
Full BOTTOM denture. Do you wear
TOP part denture. Do you wear
to part deriture.

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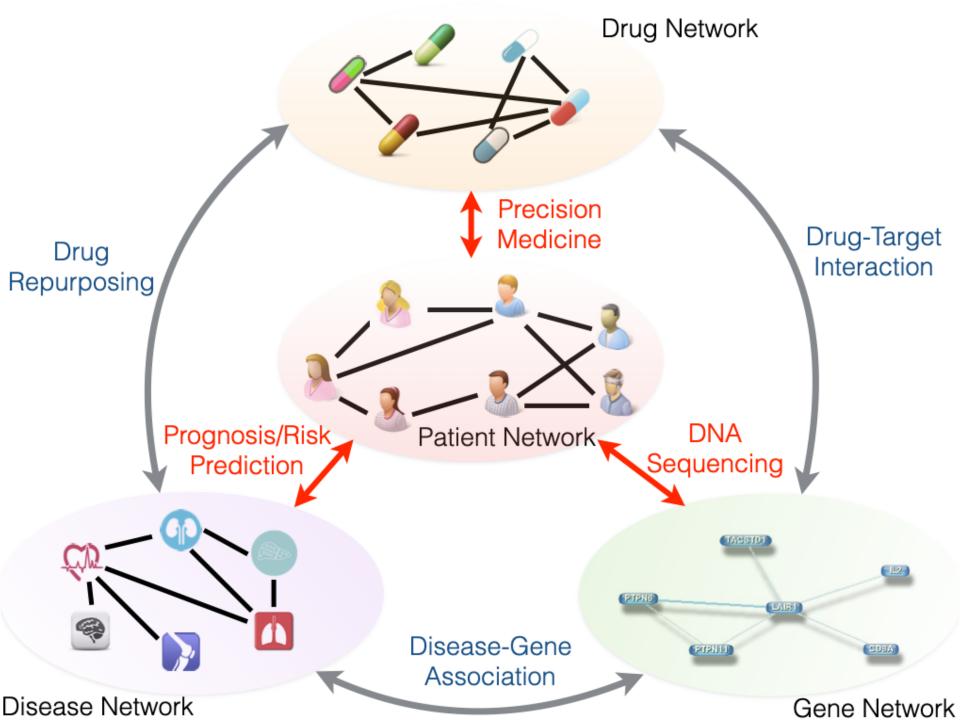
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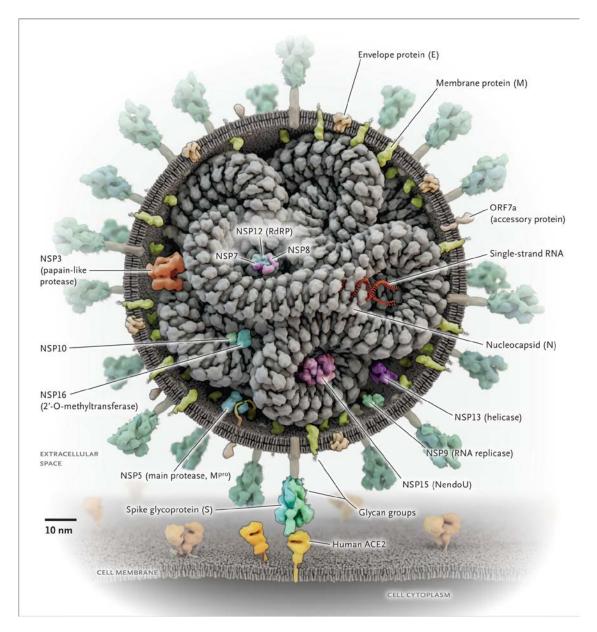
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Explore

MeSH Database Journals Legacy PubMed (available until at least 10/31/2020)





Parks, Jerry M., and Jeremy C. Smith. "How to discover antiviral drugs quickly." *New England Journal of Medicine* (2020).



19 687 156

Confirmed cases

Last update: 9 August 2020, 20:00 GMT-4

727 435

Confirmed deaths

Last update: 9 August 2020, 20:00 GMT-4

215

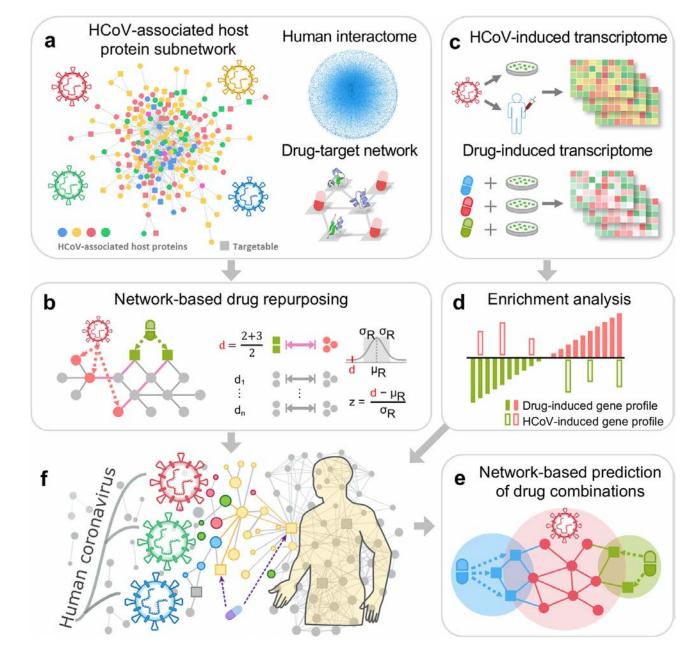
Countries, areas or territories with cases

Last update: 9 August 2020, 20:00 GMT-4

https://www.who.int/emergencies/diseases/novel-coronavirus-2019

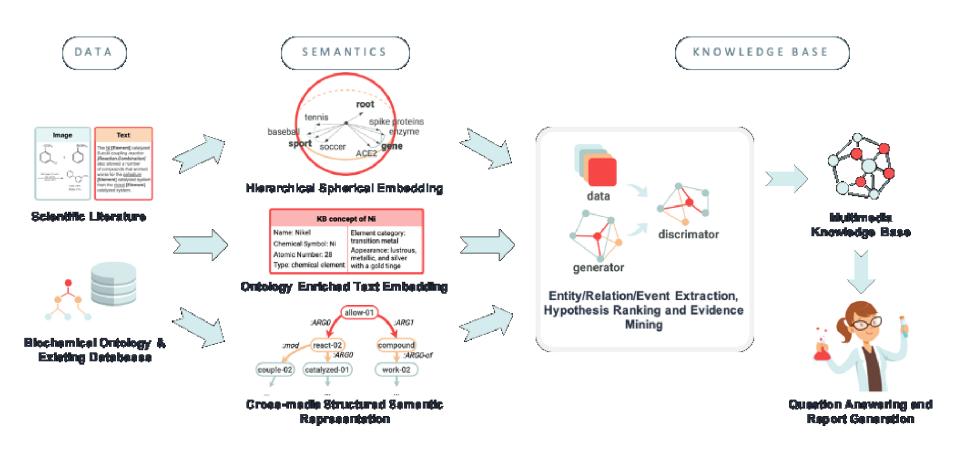
Application:

Drug Repurposing



Zhou, Yadi, Yuan Hou, Jiayu Shen, Yin Huang, William Martin, and Feixiong Cheng. "Network-based drug repurposing for novel coronavirus 2019-nCoV/SARS-CoV-2." *Cell discovery* 6, no. 1 (2020): 1-18.

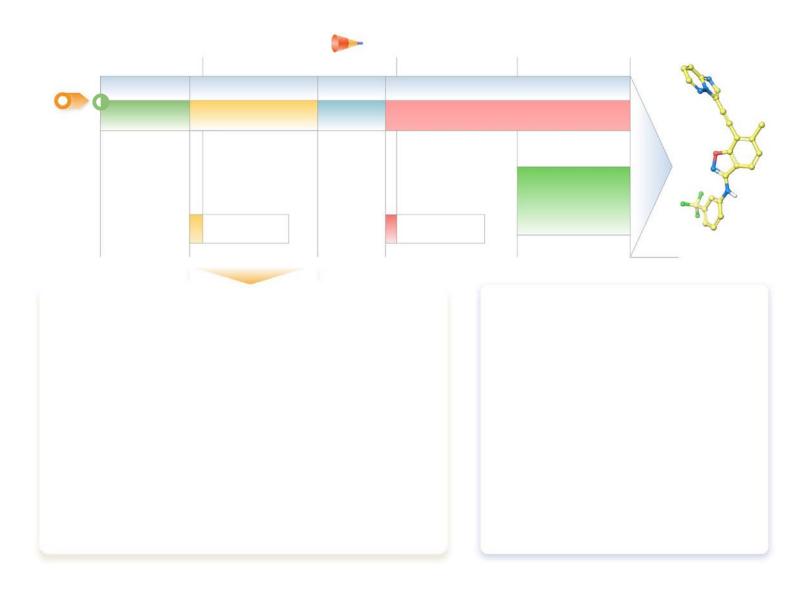
Application: Question Answering and Decision Support with Knowledge Graph Mining



Wang, Qingyun, Manling Li, Xuan Wang, Nikolaus Parulian, Guangxing Han, Jiawei Ma, Jingxuan Tu et al. "COVID-19 Literature Knowledge Graph Construction and Drug Repurposing Report Generation." arXiv preprint arXiv:2007.00576 (2020).

Application:

In-silico Drug Molecule Design



Zhavoronkov, Alex, Yan A. Ivanenkov, Alex Aliper, Mark S. Veselov, Vladimir A. Aladinskiy, Anastasiya V. Aladinskaya, Victor A. Terentiev et al. "Deep learning enables rapid identification of potent DDR1 kinase inhibitors." *Nature biotechnology* 37, no. 9 (2019): 1038-1040.

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