Atviro mokslo gairių projektas

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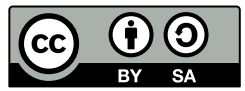


Mokslo rezultatai yra bendras turtas

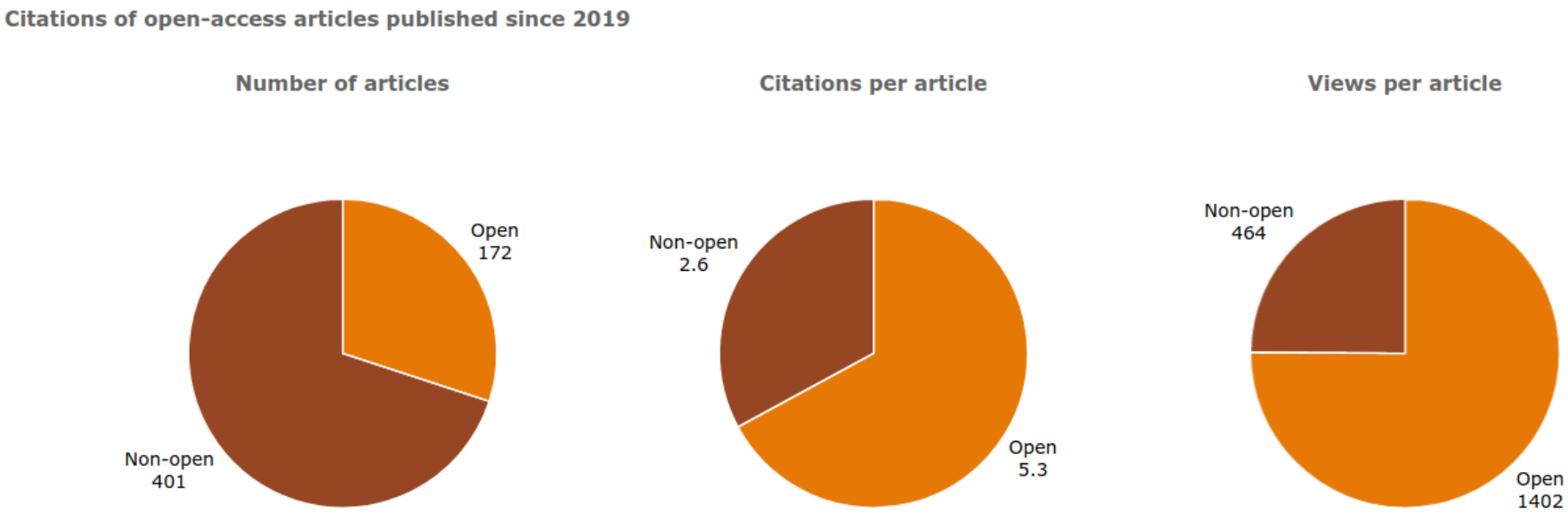
- Prieiga prie mokslo žinių yra *universali žmogaus teisė*[1]
- Visuomenė *turi teisę* pamatyti mokslinių tyrimų, padarytų už mokesčių mokėtojų pinigus, rezultatus;
- Mokslas yra bendra vertybė (“public good”) [Boulton(2021)];

$\Rightarrow$ Mokslo rezultatai turėtų būti publikuojami atvirai.

[1] https://en.unesco.org/udhr, žiūrėta 2022-01-13

Atviro mokslo cituojamumas

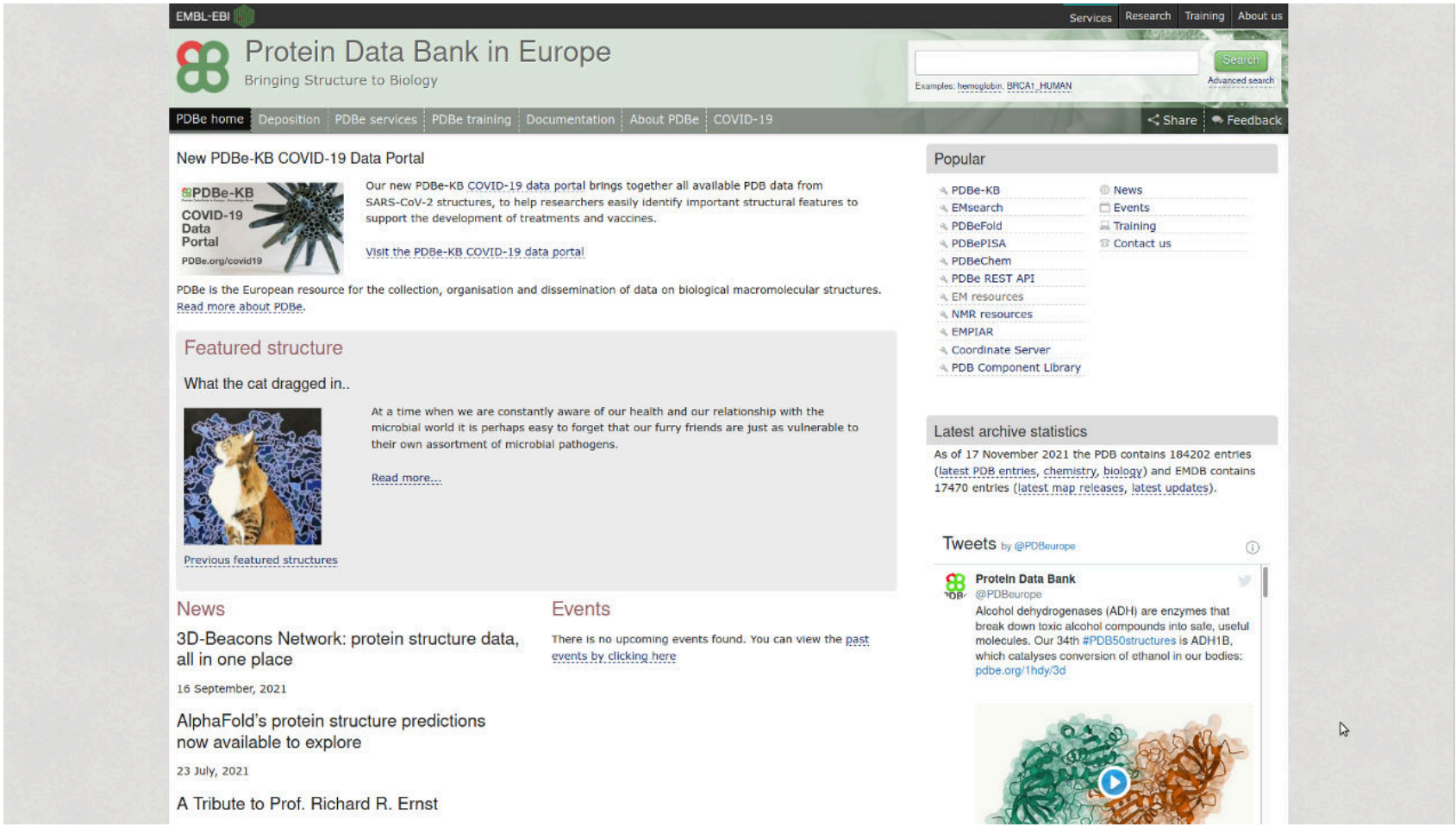
Atviri straipsniai cituojami daugiau!



Journal of Applied Crystallography, IUCr
https://journals.iucr.org/j/services/openaccess.html

Atviros duomenų bazės pasaulyje: PDB

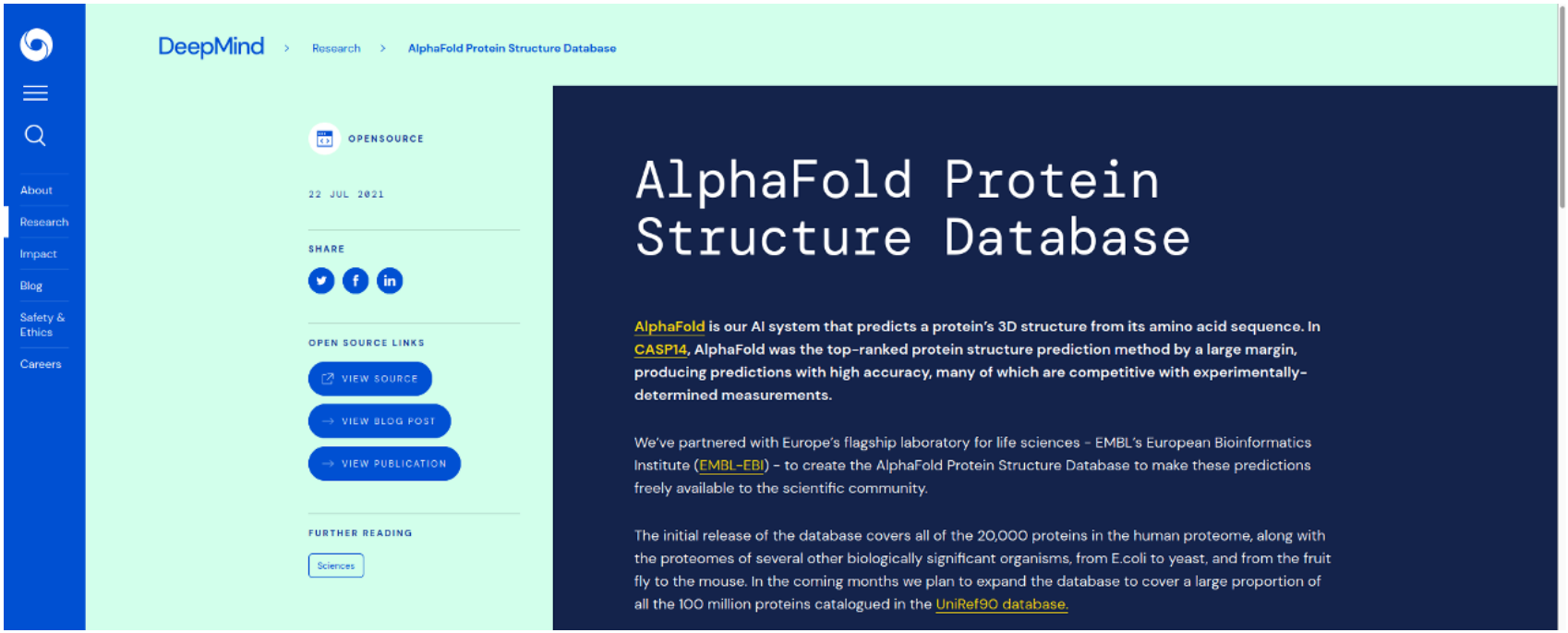
https://www.ebi.ac.uk/pdbe/



(žiūrėta 2021-11-23)

Atviros duomenų bazės pasaulyje: AplhaFold

https://deepmind.com/research/open-source/alphafold-protein-structure-database[2]

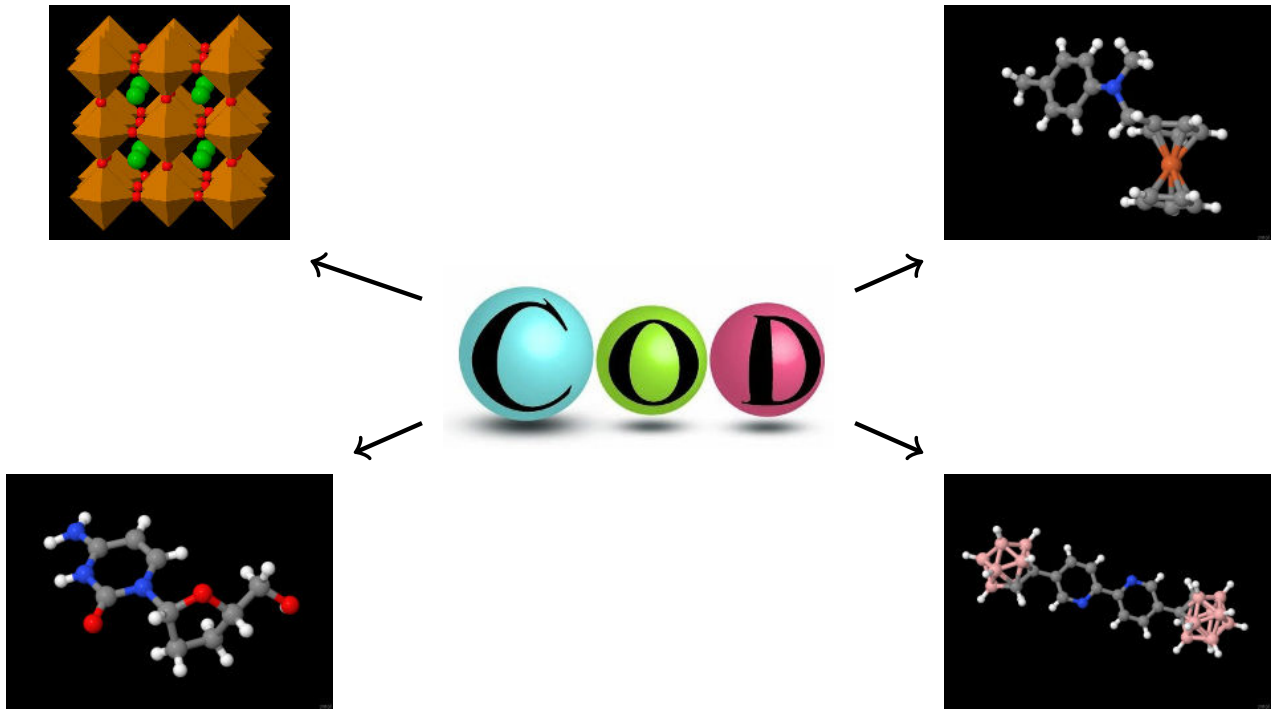


"Our models are trained on structures extracted from the PDB" [Senior et al. (2020)].

[2] (žiūrėta 2021-11-23)

Atviros duomenų bazės pasaulyje ir VU: COD

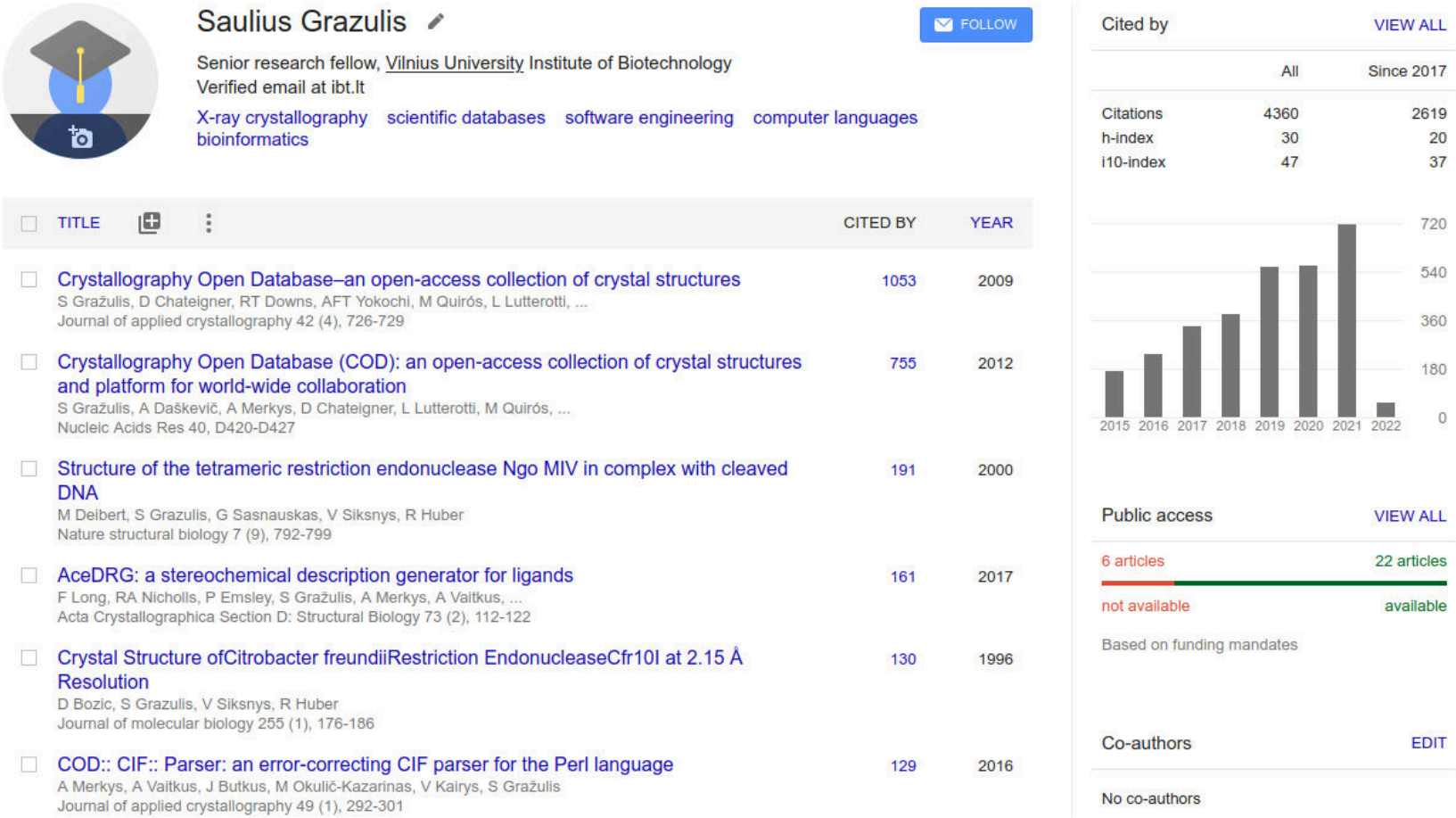
The Crystallography Open Database (COD)
https://www.crystallography.net



483350 įrašų 2022-01-13, platinami pagal CC0 Licenciją

COD duomenų bazės populiarumas

Atviri duomenys gerai cituojami![3]



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FOLLOW

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Verified email at ibt.lt

X-ray crystallography scientific databases software engineering computer languages bioinformatics

TITLE	CITED BY	YEAR
Crystallography Open Database–an open-access collection of crystal structures S Gražulis, D Chateigner, RT Downs, AFT Yokochi, M Quirós, L Lutterotti, ... Journal of applied crystallography 42 (4), 726-729	1053	2009
Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration S Gražulis, A Daškevič, A Merkys, D Chateigner, L Lutterotti, M Quirós, ... Nucleic Acids Res 40, D420-D427	755	2012
Structure of the tetrameric restriction endonuclease Ngo MIV in complex with cleaved DNA M Deibert, S Grazulis, G Sasnauskas, V Siksnys, R Huber Nature structural biology 7 (9), 792-799	191	2000
AceDRG: a stereochemical description generator for ligands F Long, RA Nicholls, P Emsley, S Gražulis, A Merkys, A Vaitkus, ... Acta Crystallographica Section D: Structural Biology 73 (2), 112-122	161	2017
Crystal Structure ofCitrobacter freundiiRestriction EndonucleaseCfr10I at 2.15 Å Resolution D Bozic, S Grazulis, V Siksnys, R Huber Journal of molecular biology 255 (1), 176-186	130	1996
COD:: CIF:: Parser: an error-correcting CIF parser for the Perl language A Merkys, A Vaitkus, J Butkus, M Okulič-Kazarinas, V Kairys, S Gražulis Journal of applied crystallography 49 (1), 292-301	129	2016

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Citations	4360	2619
h-index	30	20
i10-index	47	37

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6 articles 22 articles
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Based on funding mandates

Co-authors EDIT

No co-authors

[3] https://scholar.google.com/citations?hl=en&user=BswX10sAAAAJ, žiūrėta 2022-01-13

Atviras mokslas ir atkartojamumas

TABLE 31

OUTCOMES OF TESTS OF SIGNIFICANCE FOR FOUR PSYCHOLOGY RESEARCH JOURNALS

Journals: All Issues From January To December	Total Number of Research Reports (1)	Number of Research Reports Using Tests of Significance (2)	Number of Research Reports that Reject H_0 with $Pr(E\|H_0) \leq .05$ (3)	Number of Research Reports that Fail to Reject H_0 (4)	Number of Research Reports That are Replication of Previously Published Experiments (5)
Experimental Psychology (1955)	124	106	105	1	0
Comparative and Physiological Psychology (1956)	118	94	91	3	0
Clinical Psychology (1955)	81	62	59	3	0
Social Psychology (1955)	39	32	31	1	0
Total	362	294	286	8	0

[Sterling(1959)]

Klinikinių tyrimų DB

https://clinicaltrials.gov/

Klinikinių tyrimų DB

https://clinicaltrials.gov/ct2/results?cond=COVID-19

Row	Saved	Status	Study Title	Conditions	Interventions
1	☐	Recruiting	Duvelisib to Combat **COVID-19**	• **COVID-19**	• Drug: Duvelisib • Procedure: Peripheral blood draw • Drug: Placebo
2	☐	Recruiting	Relationship Between CT- Value With Prognosis in **COVID-19** Patients	• **COVID-19**	• Diagnostic Test: Cycle threshold
3	☐	Recruiting	Observational Cohort of **COVID-19** Patients at Raymond-Poincare	• **COVID-19**	
4	☐	Not yet recruiting	**COVID-19** Surveillance Based on Smart Wearable Device	• **COVID-19**	
5	☐	Completed Has Results	A Phase 2 Trial of Infliximab in **Coronavirus Disease 2019** (**COVID-19**).	• **COVID-19**	• Drug: Infliximab

Neperskaitomi straipsniai

Kas minutę – daugiau kaip po straipsnį!
https://www.nlm.nih.gov/bsd/medline_cit_counts_yr_pub.html

Home > MEDLINE/PubMed Resources

MEDLINE® Citation Counts by Year of Publication (as of January 2021)*

MEDLINE consists of completed citations indexed with MeSH® (Medical Subject Headings®).

Year of Publication	Total # Citations	# Citations Published in US	%s Citations Published in US
2020*	362,528	138,112	38%
2019	898,145	345,923	39%
2018	866,977	343,605	40%
2017	848,776	343,947	41%
2016	862,829	351,138	41%
2015	878,403	367,373	43%

PubMed.gov
Go to PubMed

$$898145/(365 \times 24 \times 60) = 1.7$$

Pasiūlymas: Recenzuojamas duomenų bazės įrašas

- Duomenys šiuo metu recenzuojami prastai;
- Duomenys kartais vertingesni už patį straipsnį;
- Kokybiškas, praėjęs kolegų peržiūrą duomenų bazės įrašas turėtų būti užskaitomas kaip mokslo rezultatas („produkcija“);

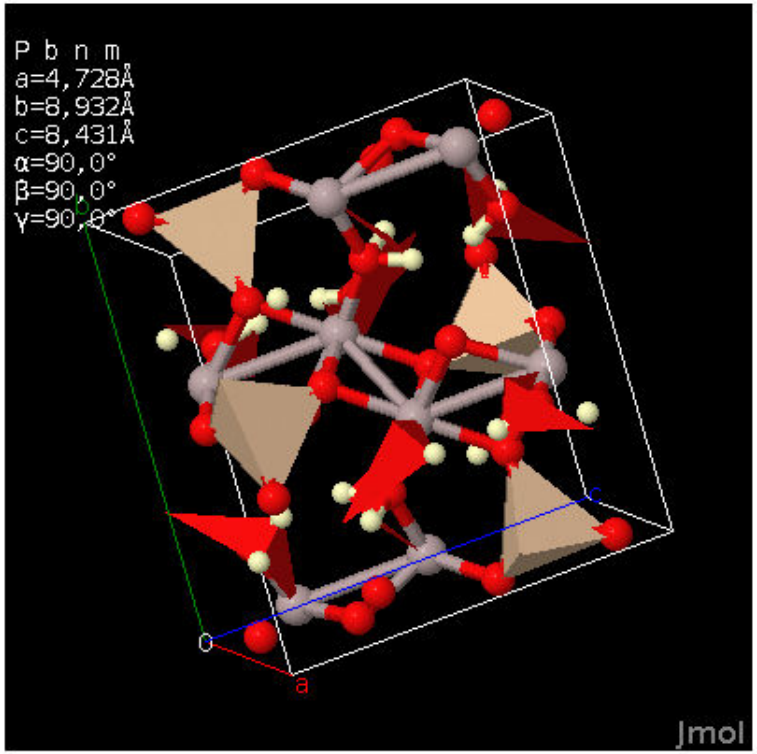
„Gimę skaitmeniniame pavidale“

- Skaitmeninių duomenų kiekis auga (eksponentiškai);
- Duomenų tvarkymas tampa iššūkiu;
- Reikalinga „duomenų tvarkytojų“ (angl. “data stewards”) specialybė ir pareigybės (rolės);

Apibendrinimas

- Mokslas turi būti atviras!
- Atviras mokslas naudingas mums visiems!
- XXIa. iššūkiai be atviro mokslo neišsprendžiami!
- Siūlomas gairių projektas atsižvelgia į šiuos aspektus:
  - kiek galima atvira, kiek reikia uždara;
  - infrastruktūros svarba;
  - duomenų specialistų poreikis;
- **Bet svarbiausia – Jūsų visų palaikymas!**

Ačiū už dėmesį!



Coordinates	2207377.cif
Original IUCr paper	HTML

http://en.wikipedia.org/wiki/Topaz

http://www.crystallography.net/2207377.html

Nuorodos I


Boulton GS (2021) Science as a global public good. DOI 10.24948/2021.09, URL https://council.science/wp-content/uploads/2020/06/Science-as-a-global-public-good_v041021.pdf


Senior AW, Evans R, Jumper J, Kirkpatrick J, Sifre L, Green T, et al. (2020) Improved protein structure prediction using potentials from deep learning. Nature 577(7792):706–710, DOI 10.1038/s41586-019-1923-7, https://doi.org/10.1038/s41586-019-1923-7


Sterling TD (1959) Publication decisions and their possible effects on inferences drawn from tests of significance — or vice versa. Journal of the American Statistical Association 54:30–34, DOI 10.1080/01621459.1959.10501497, http://dx.doi.org/10.1080/01621459.1959.10501497