#### Open Science Week

16.-20. 10. 2023



# Open Science v praxi: Show and tell

Open Science v živých vědách a chemii Karel Berka





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International
Open Access Week

### Open Science - flavours



















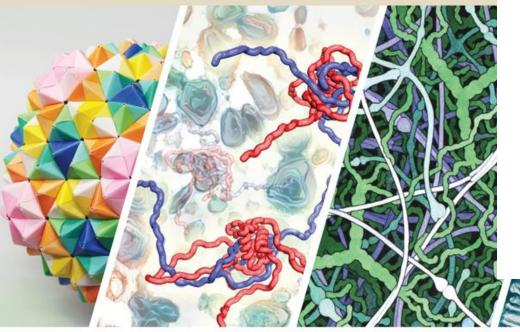


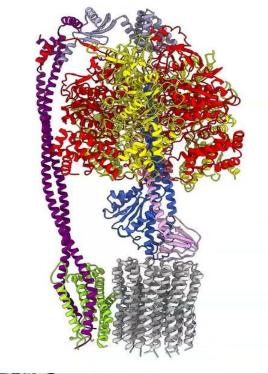
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#### Open Science ve strukturní biologii

• PDB (1971) ->





Guo et al., 2019

#### AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

ples: Free fatty acid receptor 2 At1g58602 Q5VSL9 E. coli Help: AlphaFold DB search help pack on structure: Contact DeepMind

aFold DB provides open access to over 200 million protein structure predictions to accelerate scientific research.

#### :kground

AlphaFold Protein Structure Database

Fold is an AI system developed pMind that predicts a



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2021 Calendar

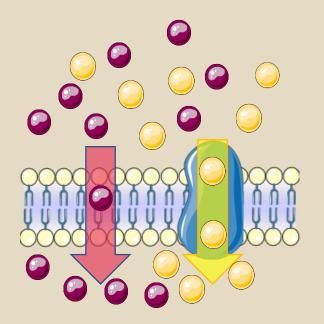
Celebrating 50 Years of Protein Data Bank

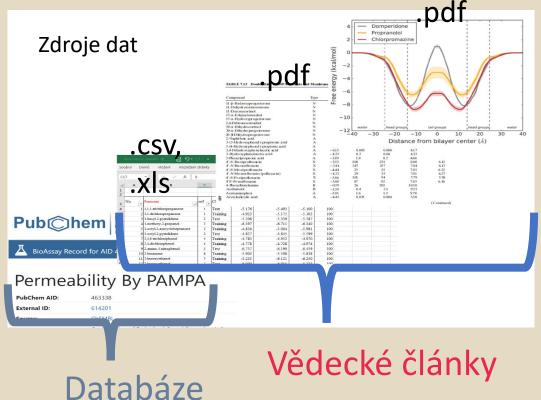


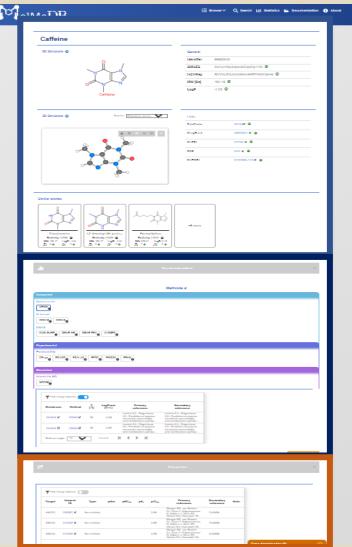
## Open Science - olMeDB



• Molecules on Membranes database







#### Open Science - ChannelsDB





Search Methods

API

Documentation

CAVER

MOLE

Contribute

About

**8PDBe** 

Search ChannelsDB 2.0 for experimental structures using name or IDs (e.g. cytochrome P450, 5ebl, KcsA, P08686)

αfill

Search ChannelsDB 2.0 for AlphaFill structures via Uniprot ID (e.g. P08686, P10635)

ChannelsDB last update on 12/09/2023 contains: 71353 protein entries Show details

ChannelsDB database is located at https://channelsdb.ncbr.muni.cz/.

ChannelsDB 2.0 is a comprehensive and regularly updated resource of channels, pores and tunnels found in biomacromolecules deposited in the Protein Data Bank and AlphaFill / AlphaFold databases. As such, it is a unique service for channel-related analyses. Pathways were calculated using an algorithms CAVER and MOLE.



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https://channelsdb2.biodata.ceitec.cz/

#### Děkuji za pozornost – otázky na Slido

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Melanie Imming, & Jon Tennant. (2018, June 8). Sticker open science: just science done right. Zenodo. <a href="http://doi.org/10.5281/zenodo.128557">http://doi.org/10.5281/zenodo.128557</a>