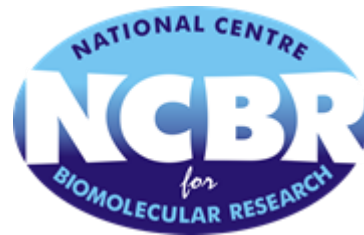
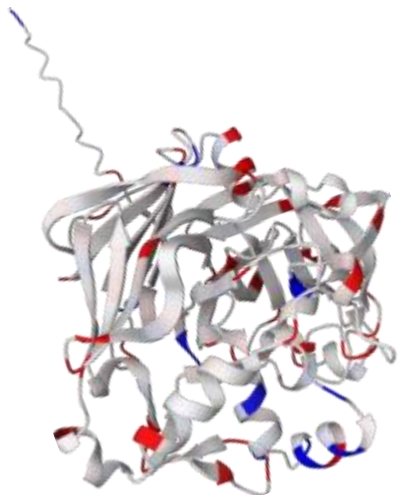


# $\alpha$ Charges

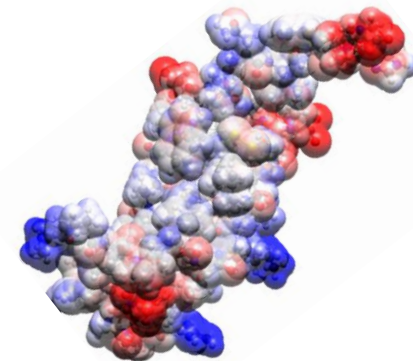
## Partial atomic charges for AlphaFold structures

Ondřej Schindler, Karel Berka, Alessio Cantara, Aleš Křenek,  
Dominik Tichý, Tomáš Raček, Radka Svobodová

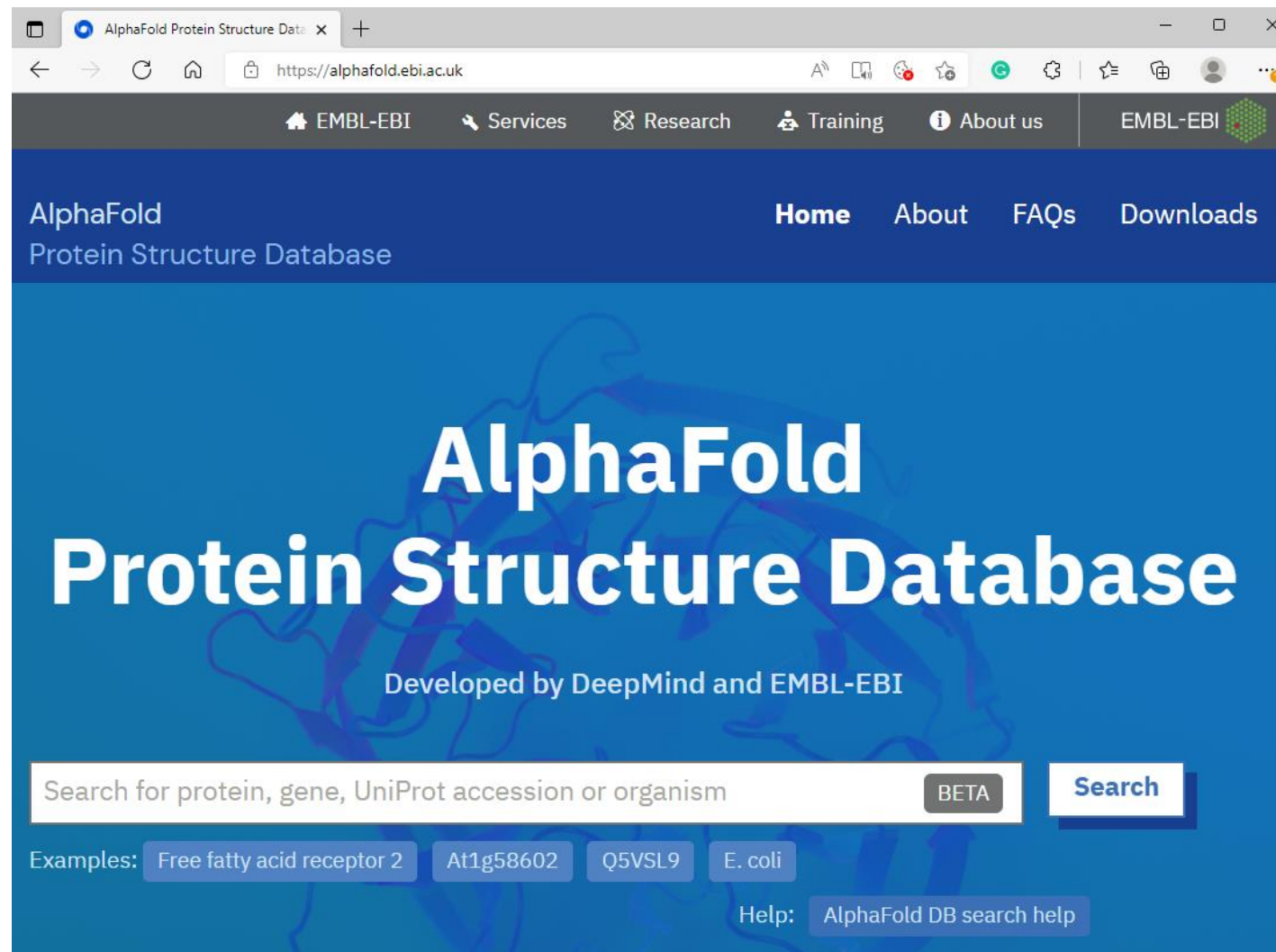


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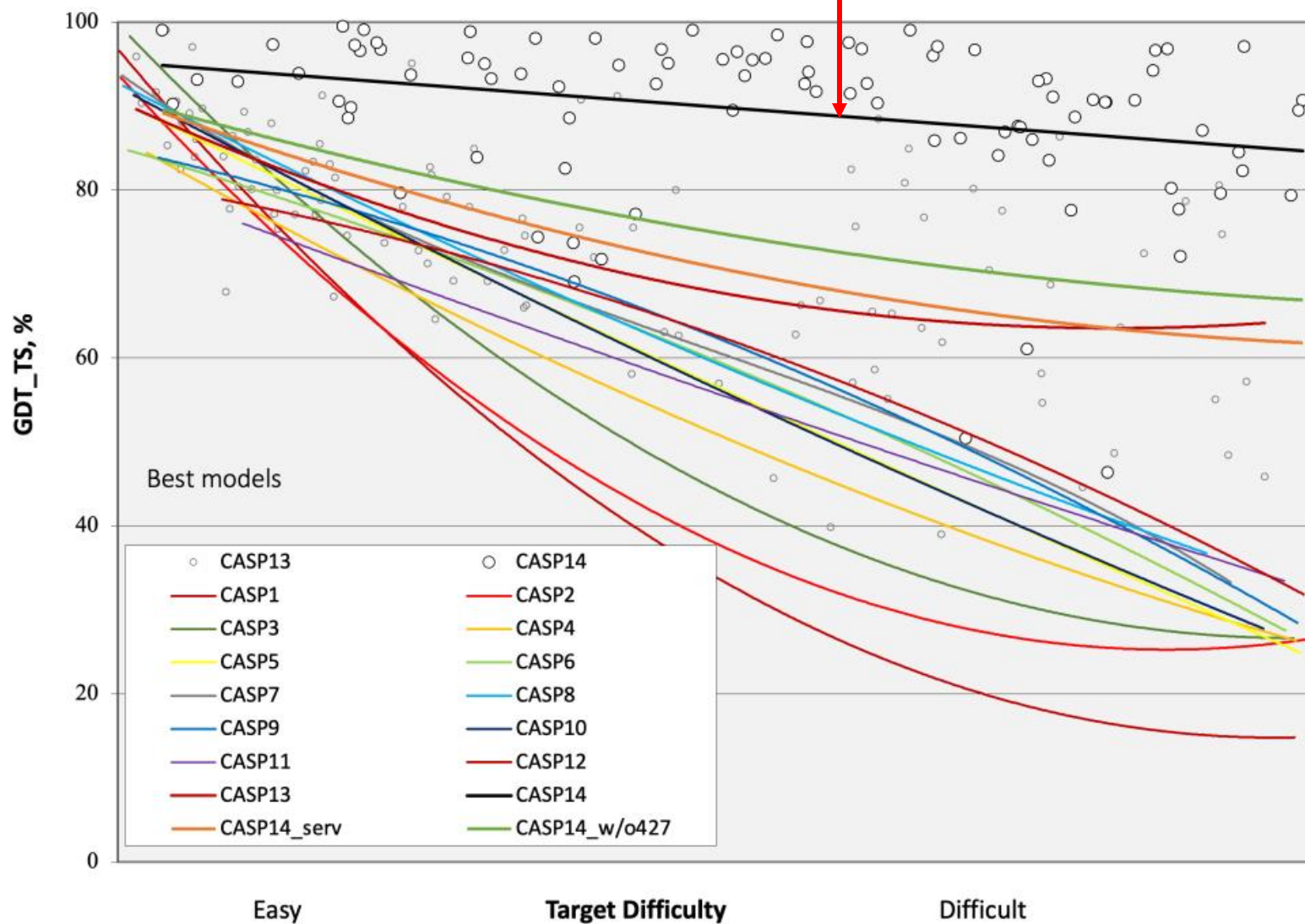
# AlphaFoldDB – predicted protein structures



**~ 200 M protein structures**

# AlphaFoldDB

Structure prediction challenge 2020: AlphaFold2 wins



[https://predictioncenter.org/casp14/doc/presentations/2020\\_11\\_30\\_CASP14\\_Introduction\\_Moult.pdf](https://predictioncenter.org/casp14/doc/presentations/2020_11_30_CASP14_Introduction_Moult.pdf)

AlphaFoldDB

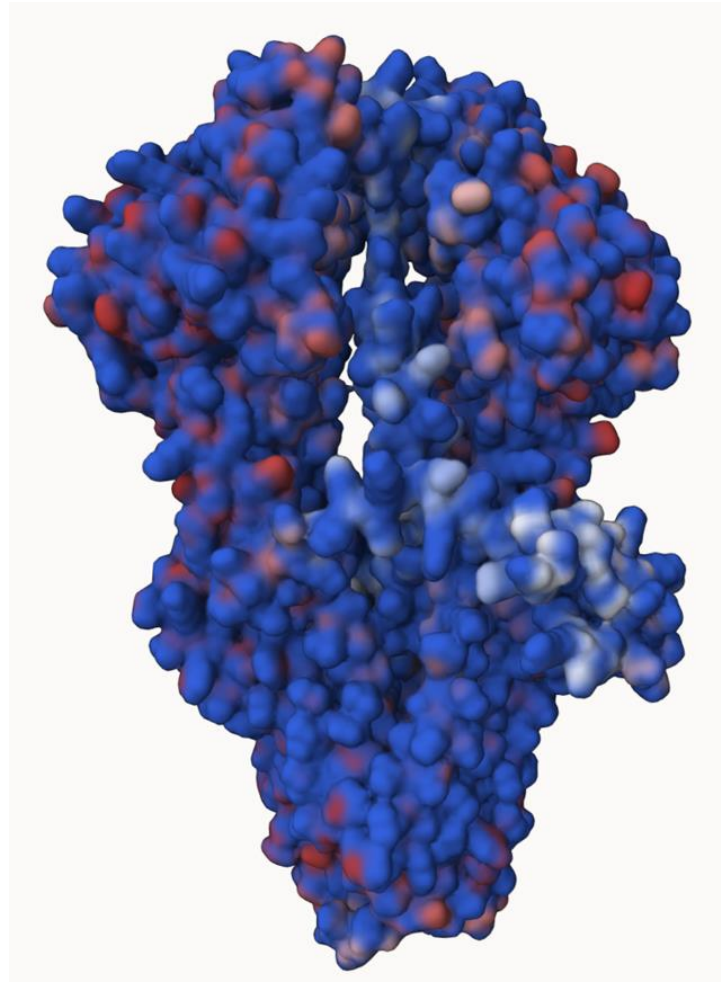
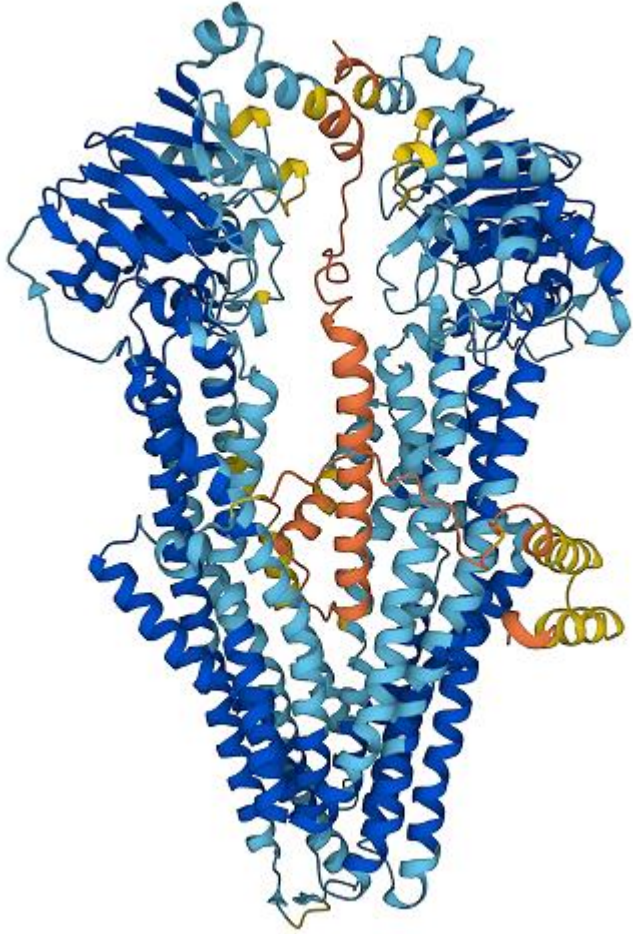
## **Structural Biology Seminar**

Today (2.3.) 14:00

## **AlphaFold and AlphaPulldown**

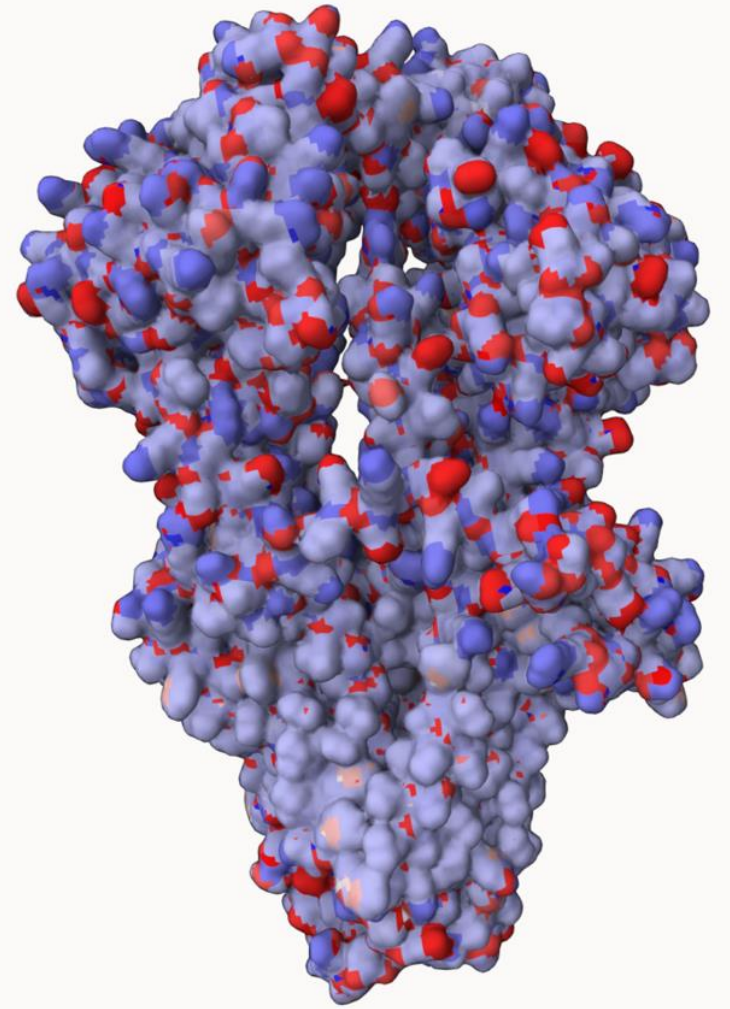
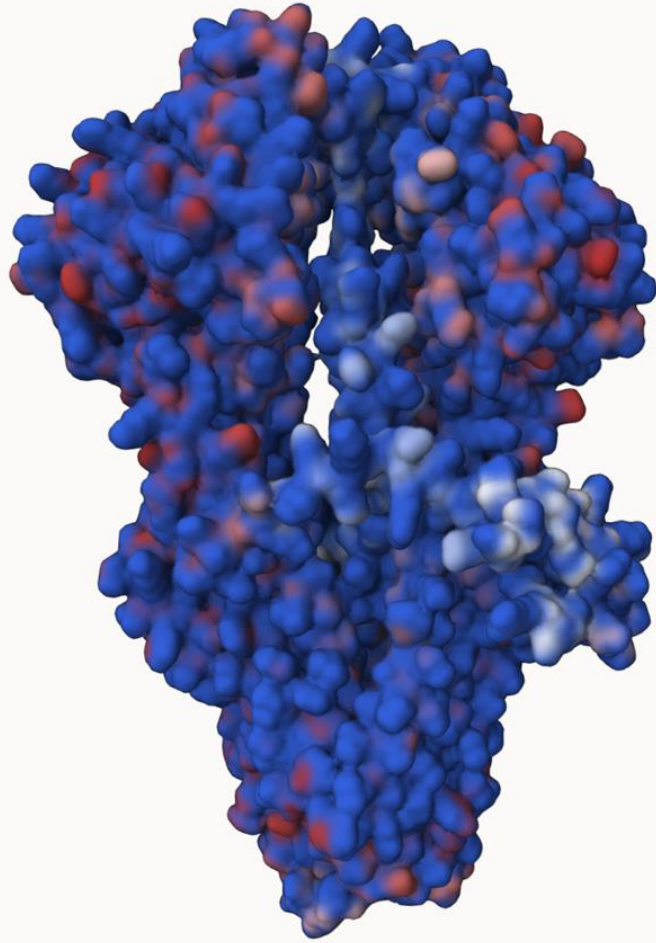
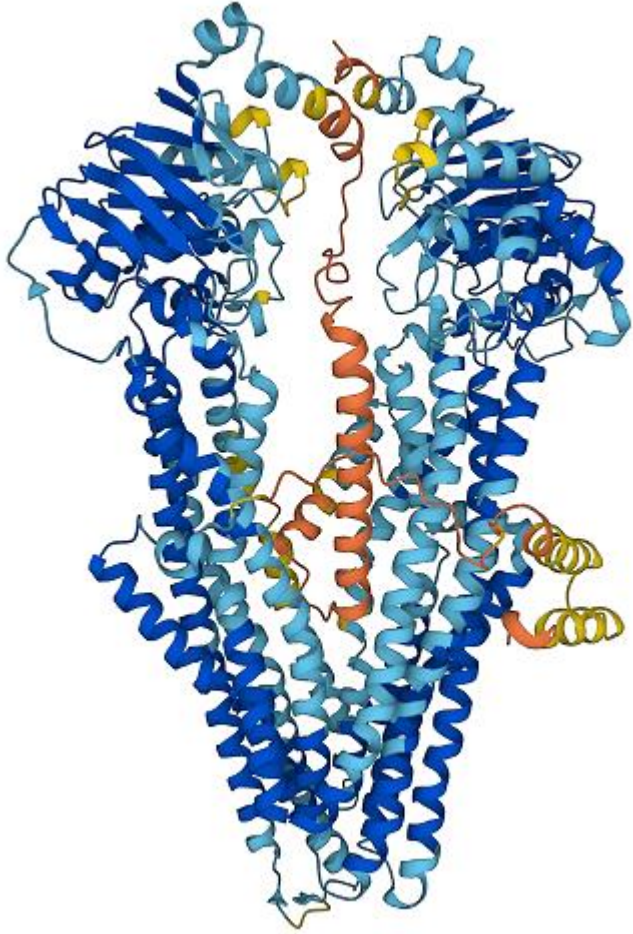
Petr Kulhánek

# P-glycoprotein

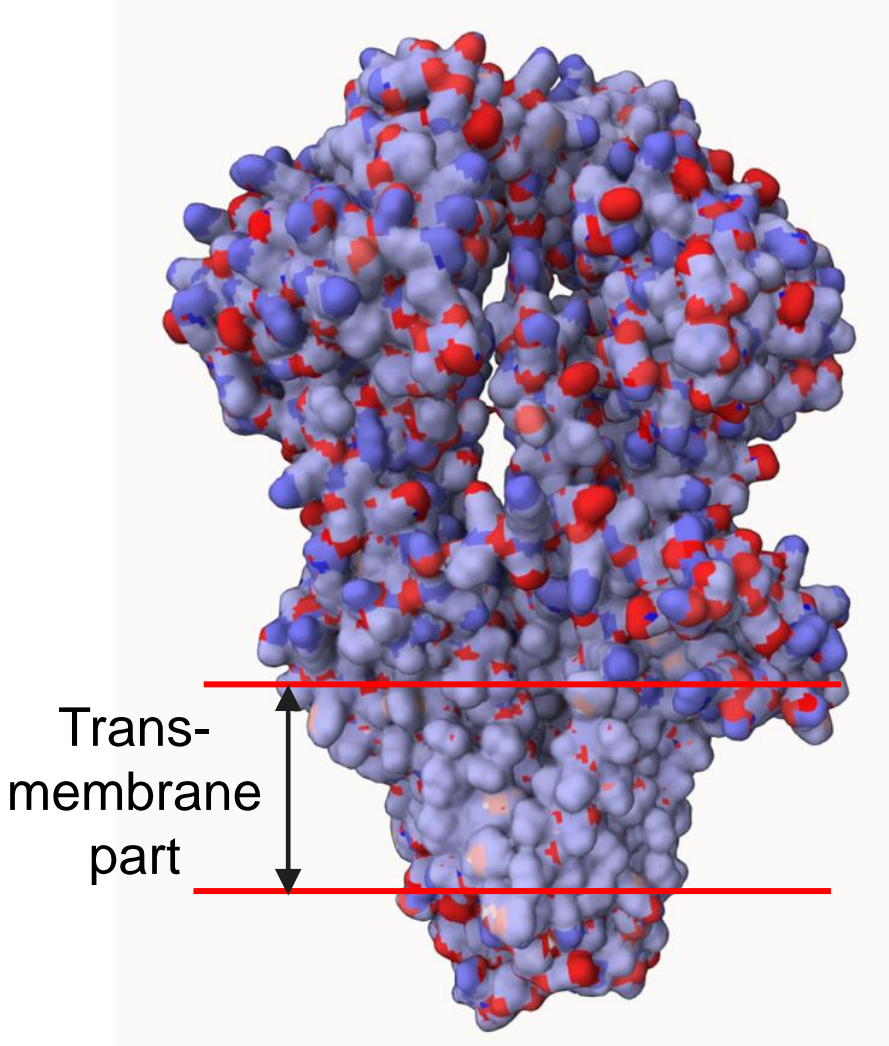
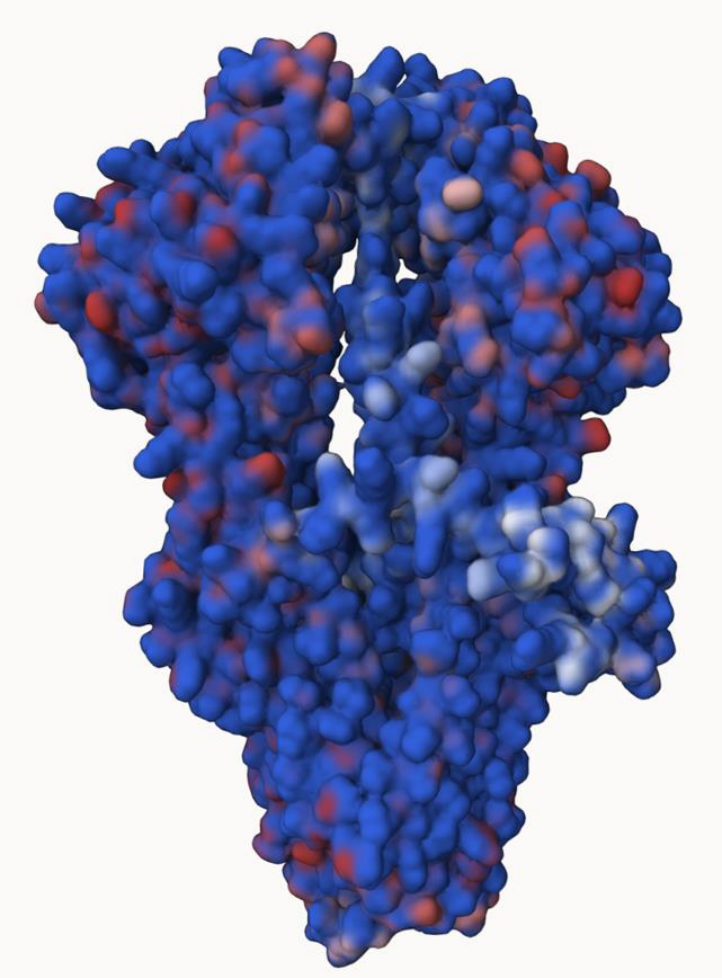
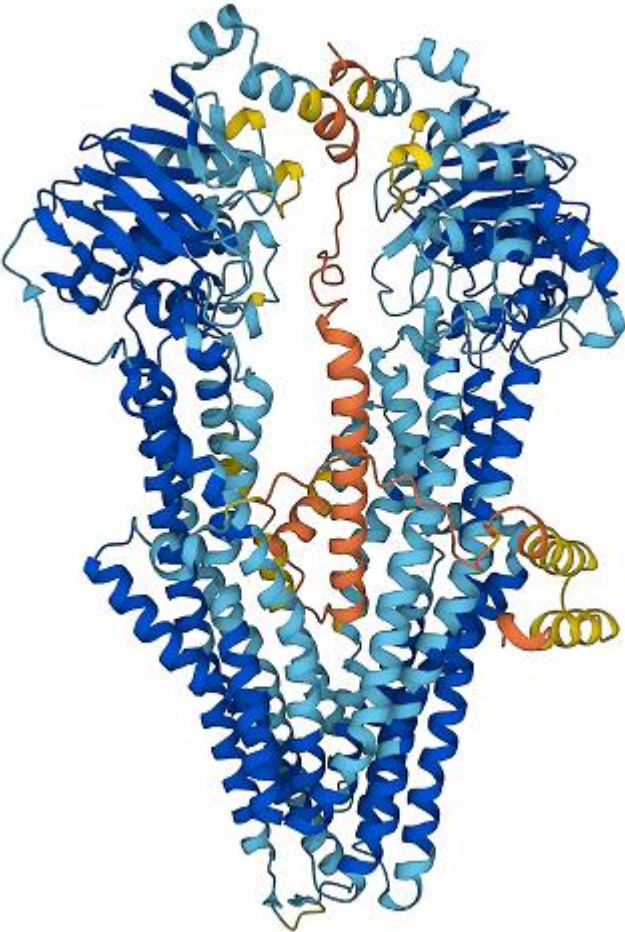




# P-glycoprotein



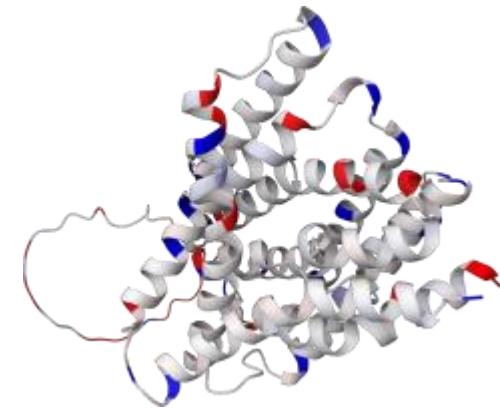
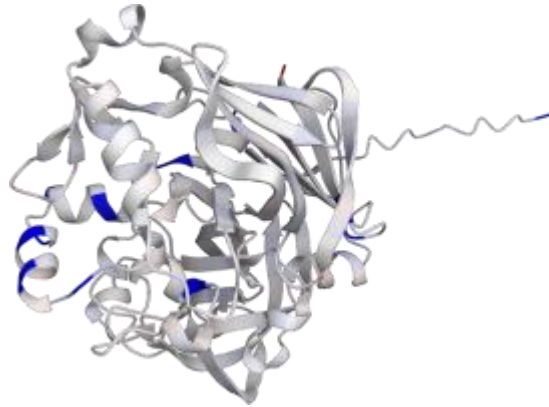
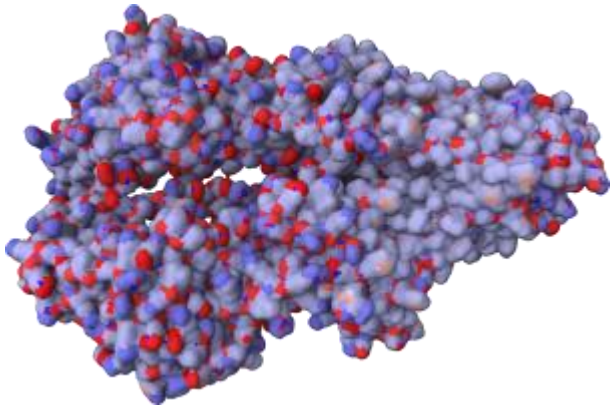
# P-glycoprotein





# $\alpha$ Charges: Partial atomic charges for AlphaFold structures

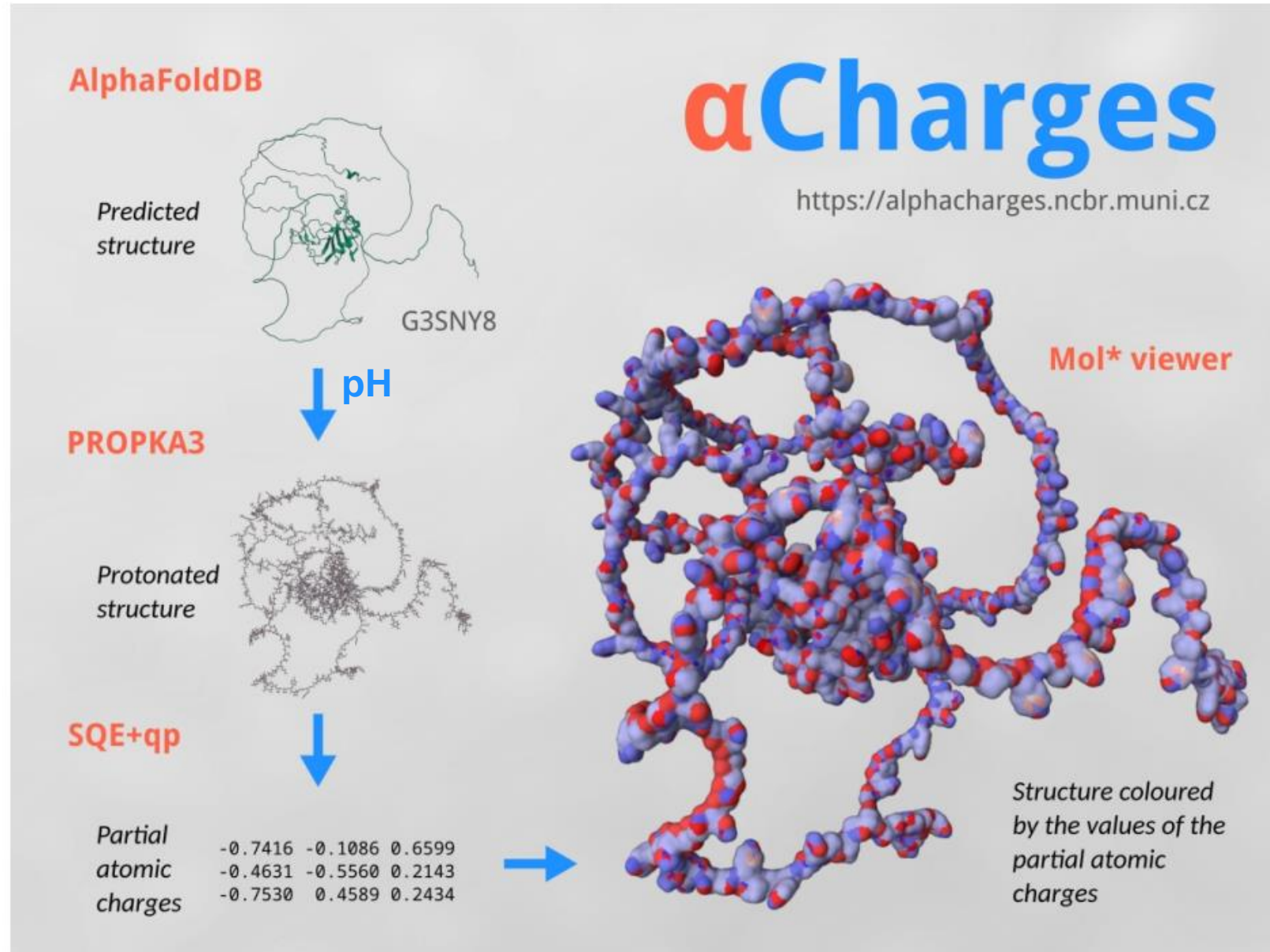
- **Computes charges for AlphaFold2 structures from AlphaFoldDB**
- **Method:** SQE+qp, parameterized for (B3LYP/6-31G\*/NPA)
- **Inputs:** UniProt ID of AlphaFoldDB molecules
- **Outputs:** plain text, mmCIF, PQR
- **Visualization:** Mol\*
- **Web page:** <https://alphacharges.ncbr.muni.cz/>



Schindler O., Berka K., Cantara A., Křenek A., Tichý D., Raček T., Svobodová R,  
2023.  *$\alpha$ Charges: Partial atomic charges for AlphaFold structures in high  
quality.* **Nucleic acids research** ?, submitted 18.2.2023



# $\alpha$ Charges: Partial atomic charges for AlphaFold structures



# $\alpha$ Charges

**AlphaCharges** ( $\alpha$ Charges) is a web application for the calculation of partial atomic charges on protein structures predicted by the [AlphaFold2 algorithm](#) and deposited in the [AlphaFoldDB](#) database. The charges are computed by the [SQE+qp empirical method](#), which quality is comparable to quantum mechanical charge calculation approaches (specifically, it is parameterized using B3LYP/6-31G\*/NPA quantum mechanical charges). Before computation of the charges,  $\alpha$ Charges protonates the input protein structures by [PROPKA3](#). The details about the methodology and usage are described in the [manual](#). This website is free and open to all users and there is no login requirement. Source codes are freely available at [GitHub](#).

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## UniProt code:

e.g., P34712, L8BU87

Calculate charges

Setup calculation

# $\alpha$ Charges – Calculation settings

UniProt code: [P34712](#)

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**Protonate in pH:**

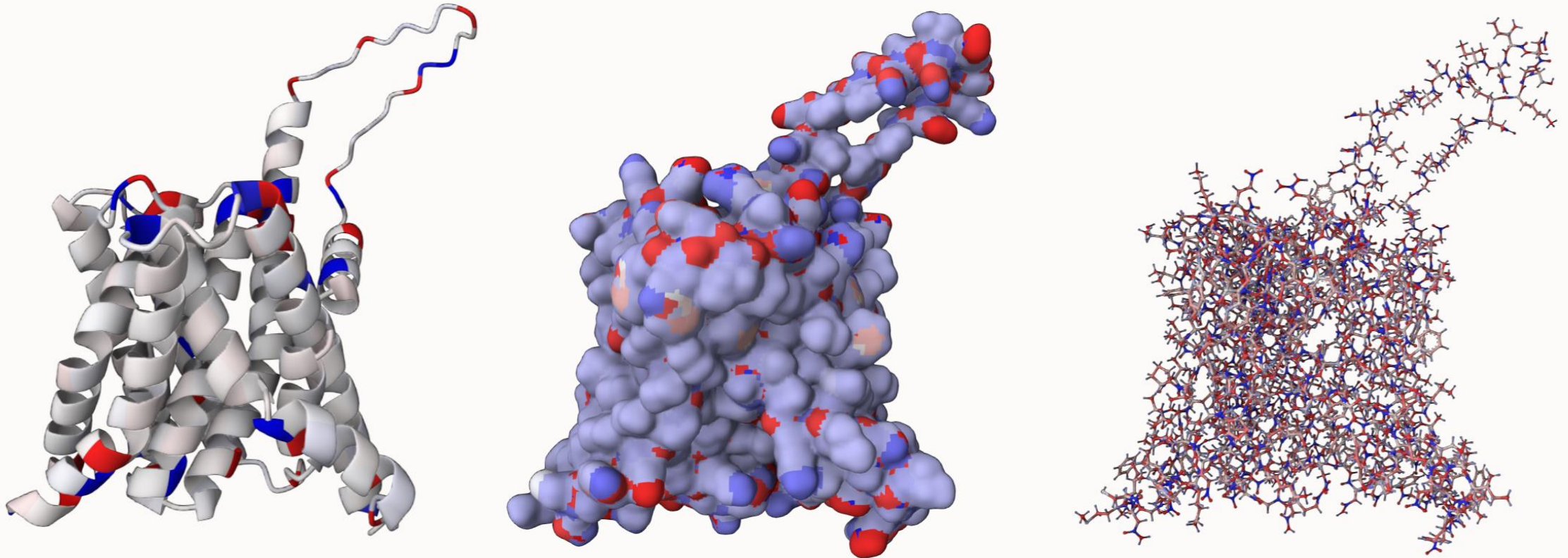
**AlphaFold  
prediction  
version:**

Calculate charges

Back to main page

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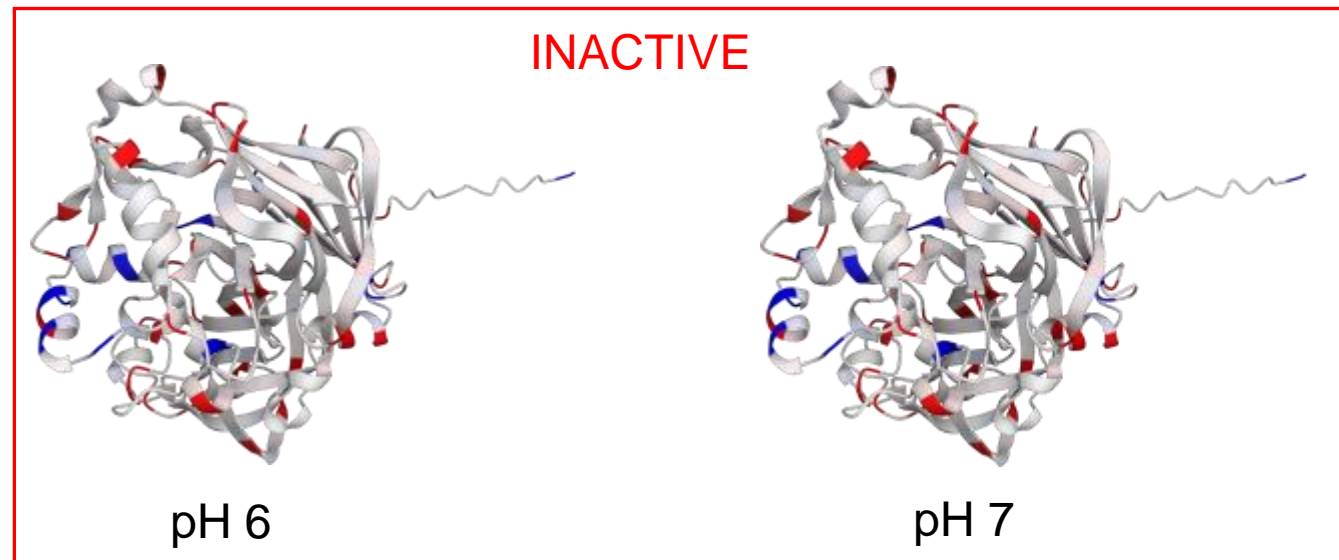
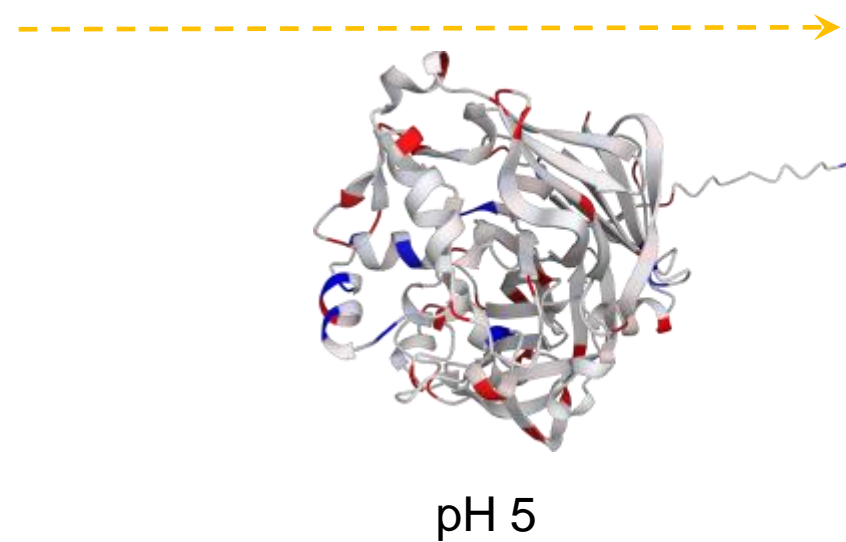
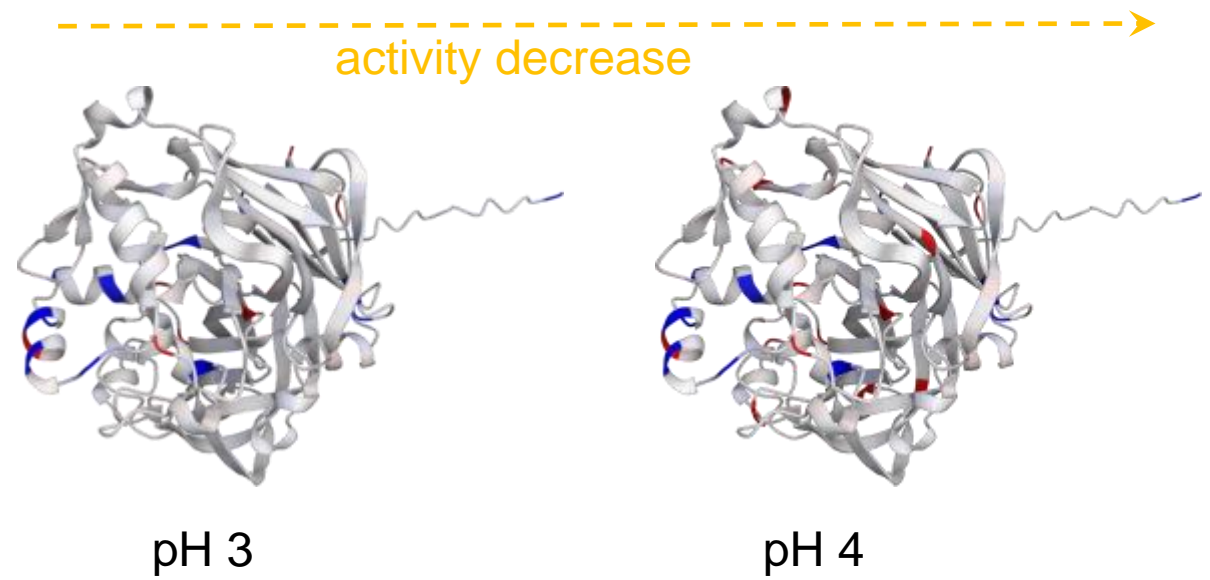
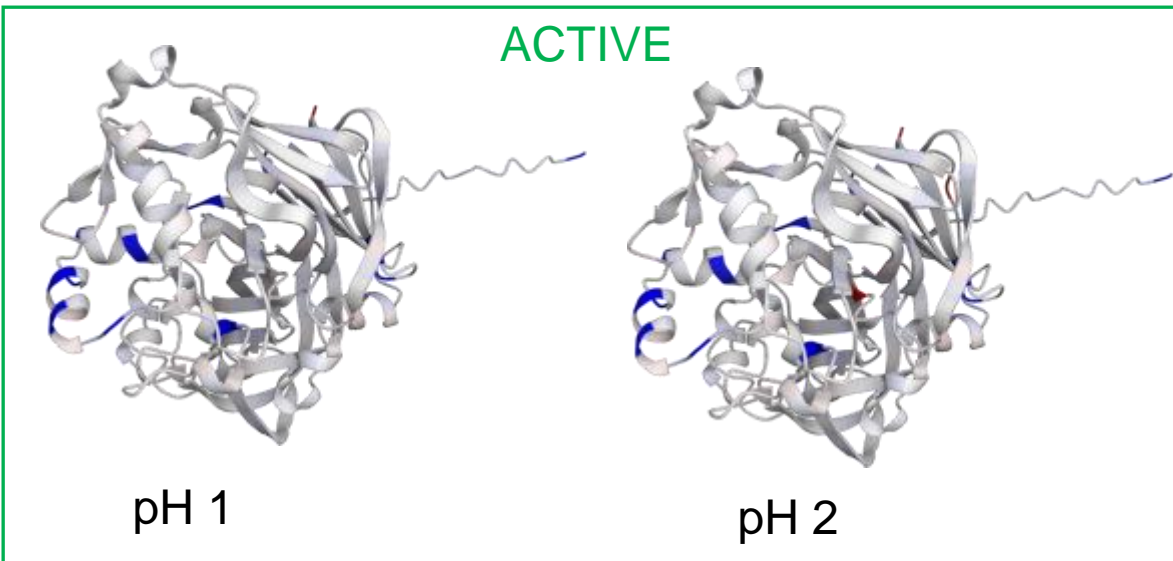




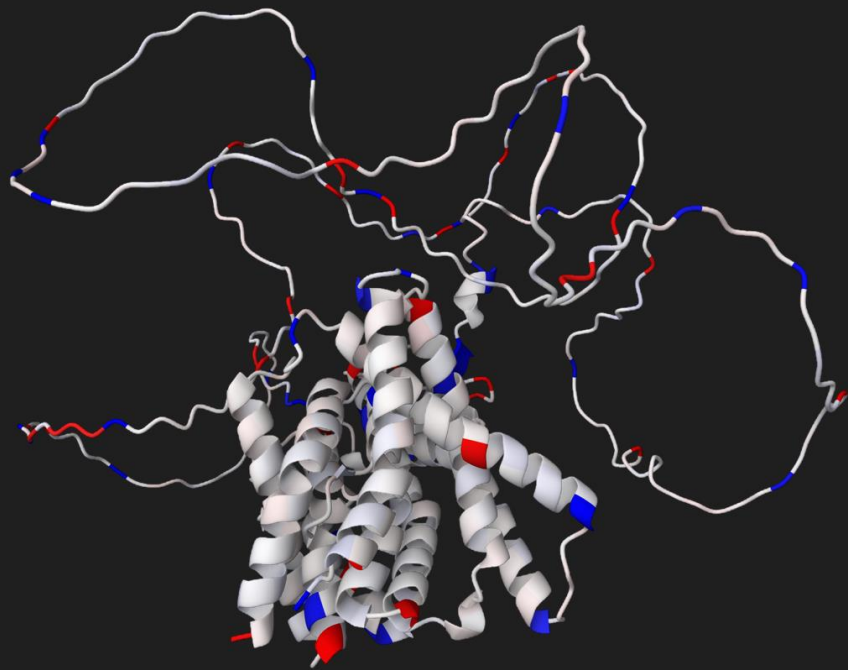
Sehna D., Bittrich S., Deshpande M., Svobodová R., Berka K., Bazgier V., ... & Rose A. S. (2021). *Mol\* Viewer: modern web app for 3D visualization and analysis of large biomolecular structures*. **Nucleic Acids Research**, 49(W1), W431-W437.

# Examples: Pepsin in different pH values

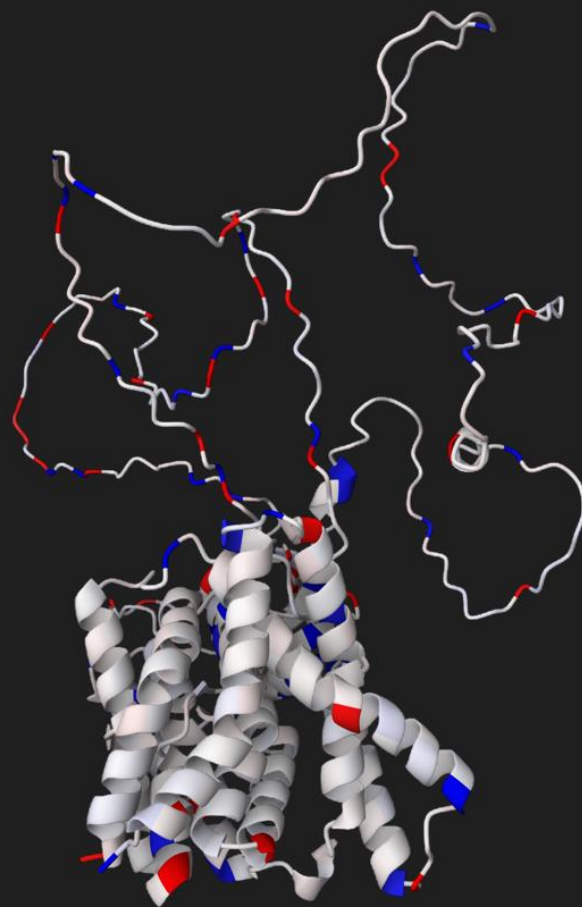
Alessio Cantara



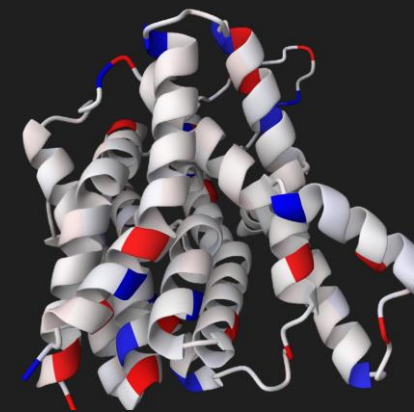
# Examples: PIN proteins



PIN3



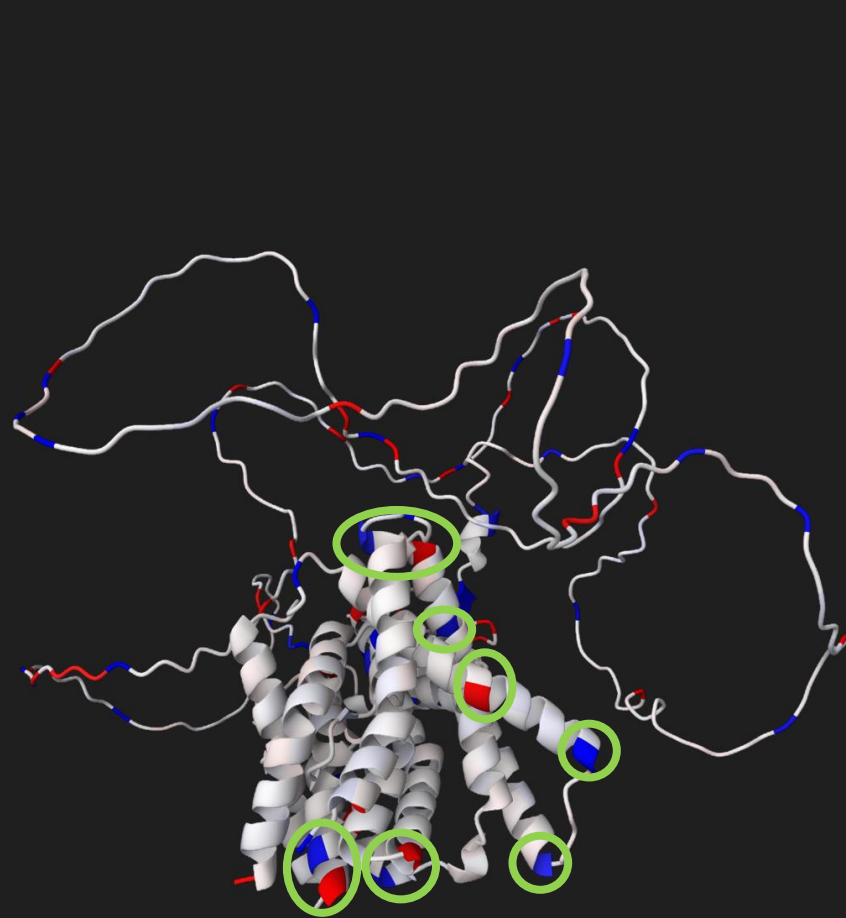
PIN7



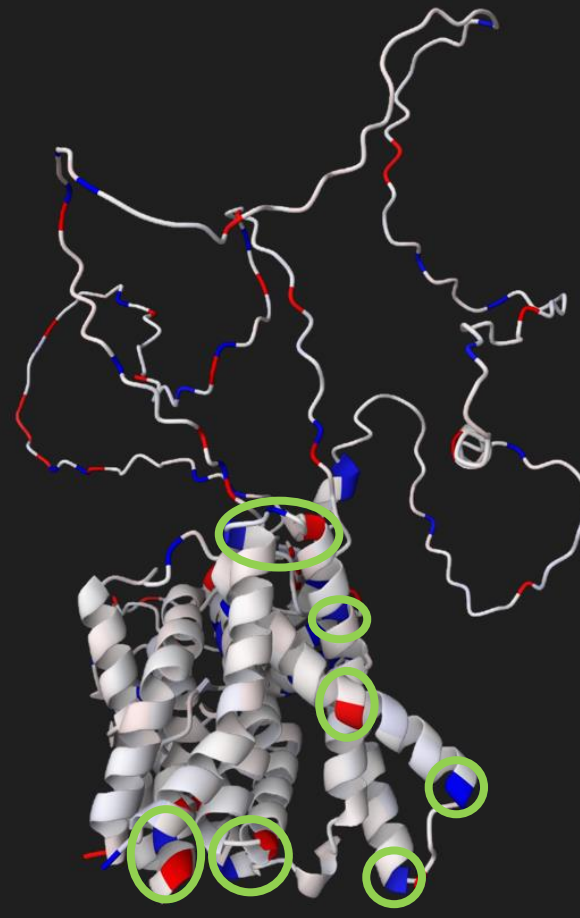
PIN5



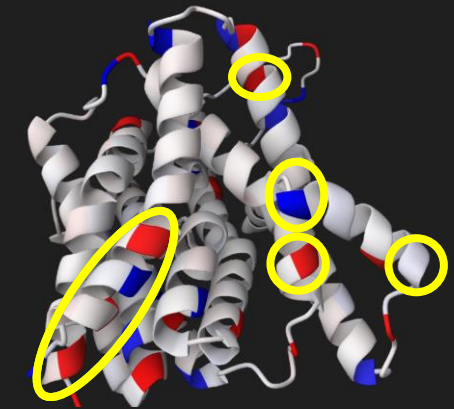
# Examples: PIN proteins



PIN3



PIN7



PIN5

Legend:  
Similar charges  
Different charges