

Cheminformatics+ Summer School 2025 (*Ljubljana, 30 june – 4 july*)

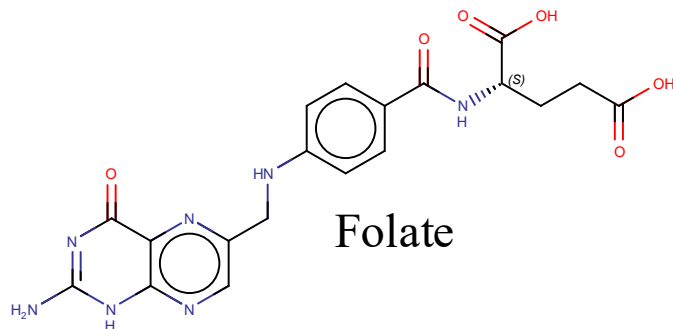
Hackathon results

Lorenzo Marchetti



Group member and goal

- Group member? → Lorenzo Marchetti (University of Modena and Reggio Emilia), André Maio (University of Lisbon) and Gowan Whalley (University of London)
- Goal? → **Design of anti-parasitic agents**
- Strategy? → **Disrupt folate metabolic pathway**



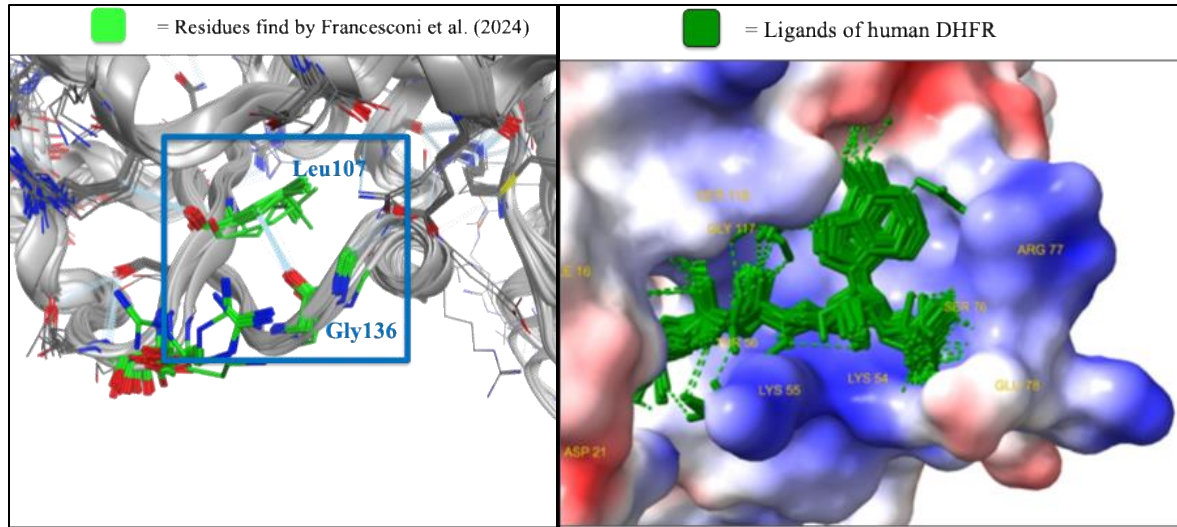
Involved enzymes:

- PTR1/2
- DHFR

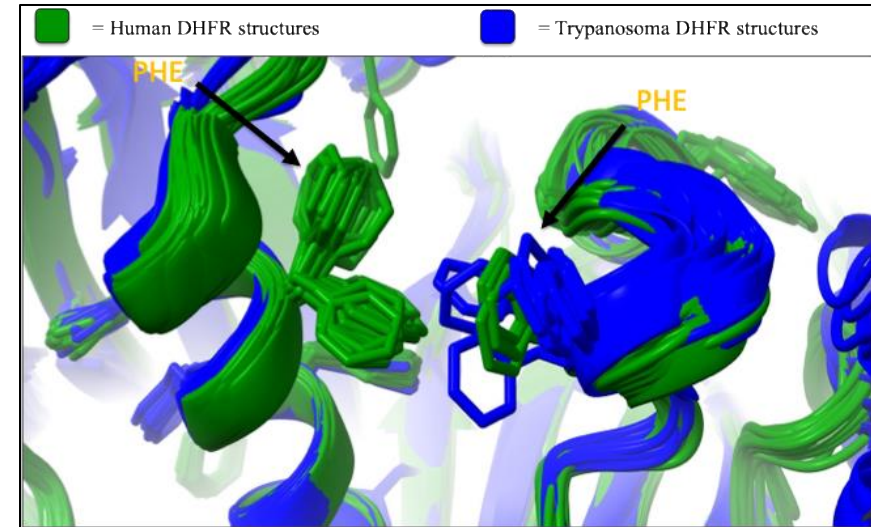
Question to assess: are there any **structural differences** between **human** and **parasites** **DHFR**?

Results - synthesis

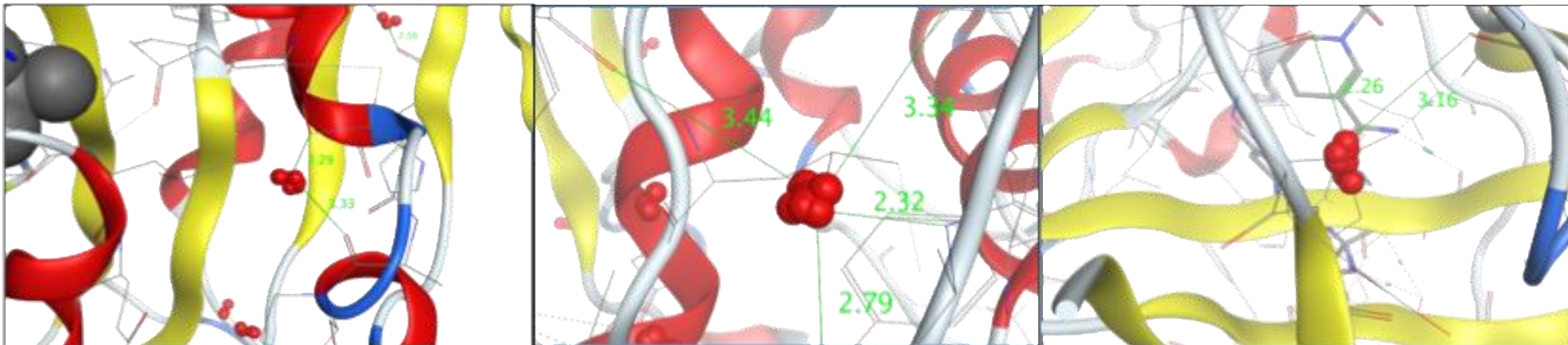
Analysis of Adenine pocket



Analysis of folate pocket

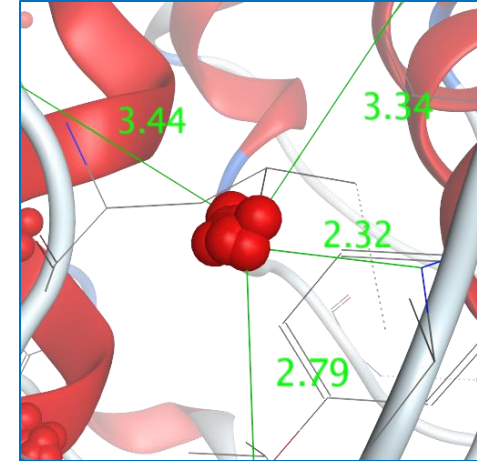
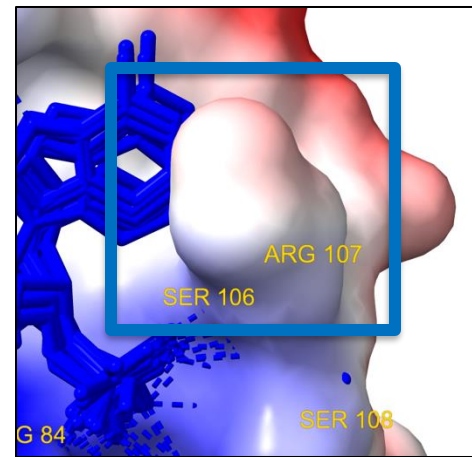
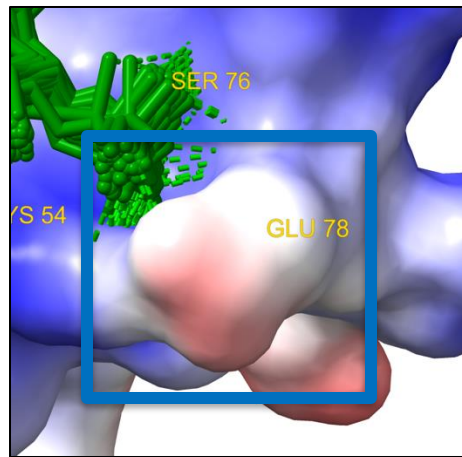
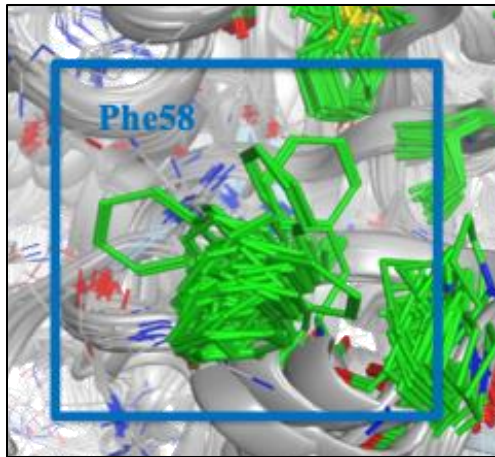


Analysis of crystalized water clusters



Conclusion

Human DHFR and Trypanosoma DHFR provide useful structural information to design new anti-parisitic agents



Further analysis: Homology Modelling? Docking? Molecular Dynamics?