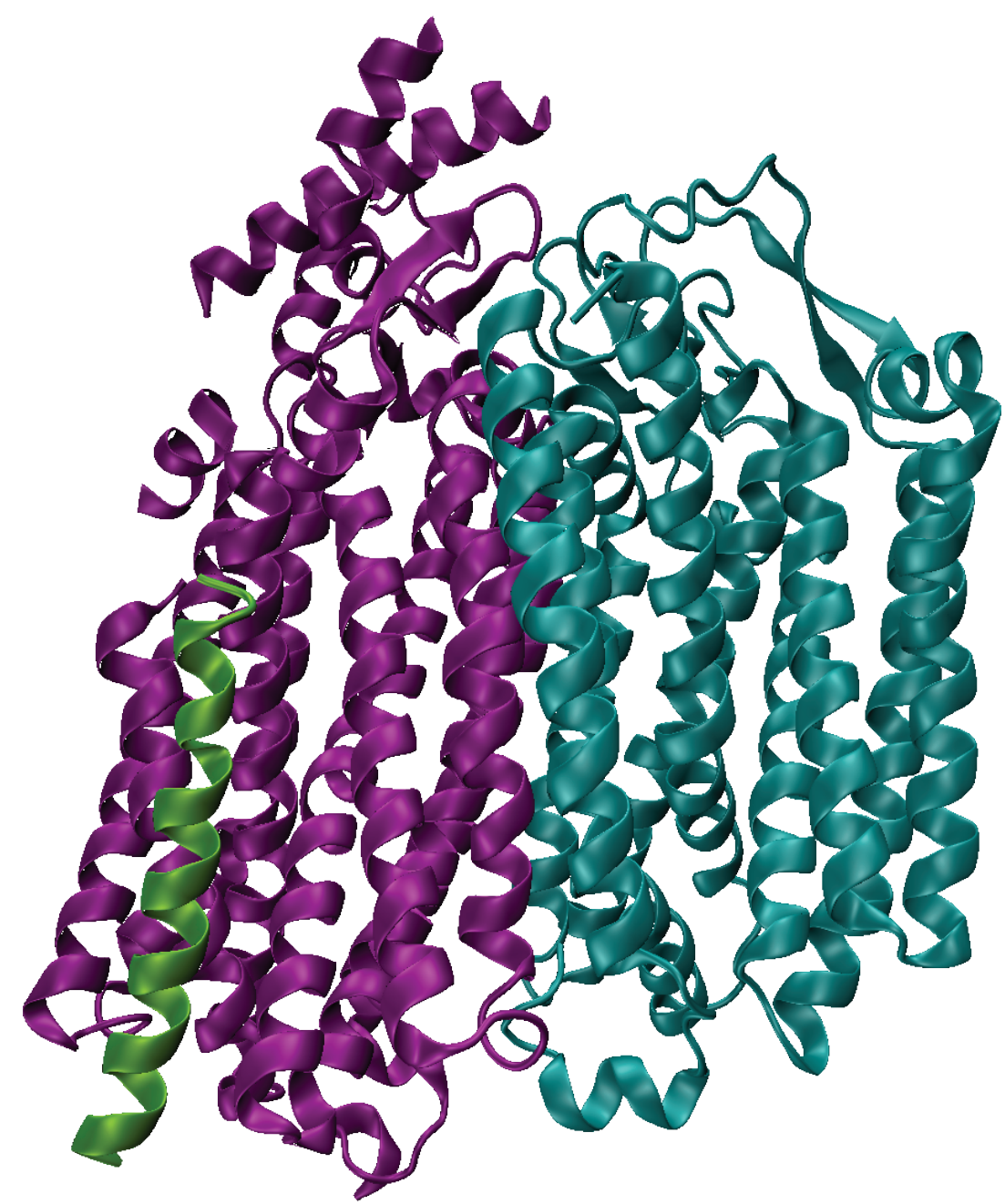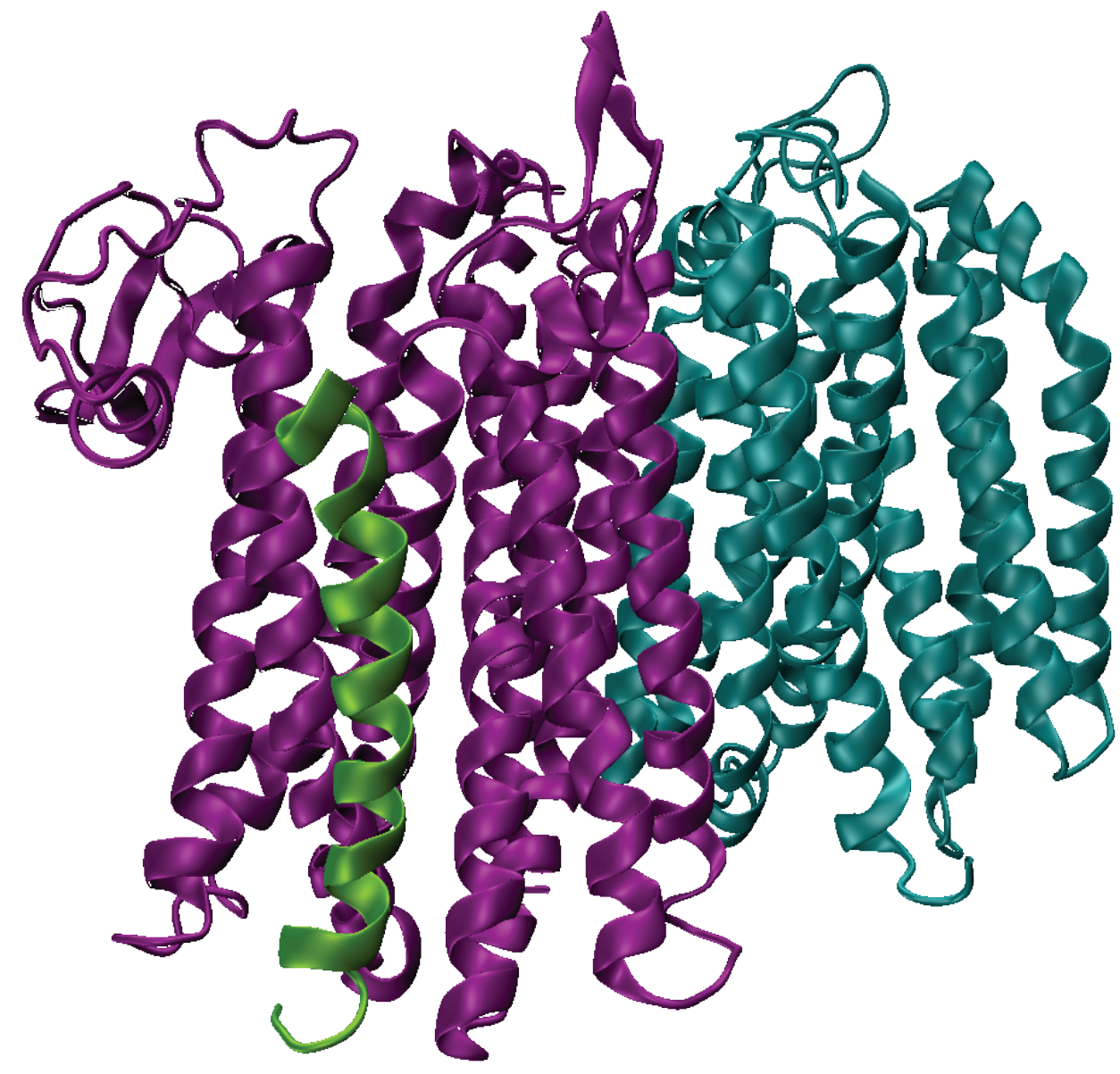# Understanding the redox properties of cytochromes bd in various organisms

Poster by Côme Cattin, École Normale Supérieure de Lyon,
under the supervision of Fabien Cailliez and Aurélien de la Lande , Institut de Chimie Physique, UMR 8000, Université Paris-Saclay and CNRS

Cytochrome bd proteins are involved in the **respiratory chains** in many organisms.
They catalyze the reduction of O₂ in water. *Escherichia coli* (*E. Coli*)
and *Geobacillus thermodenitrificans* (*G. Th.*)
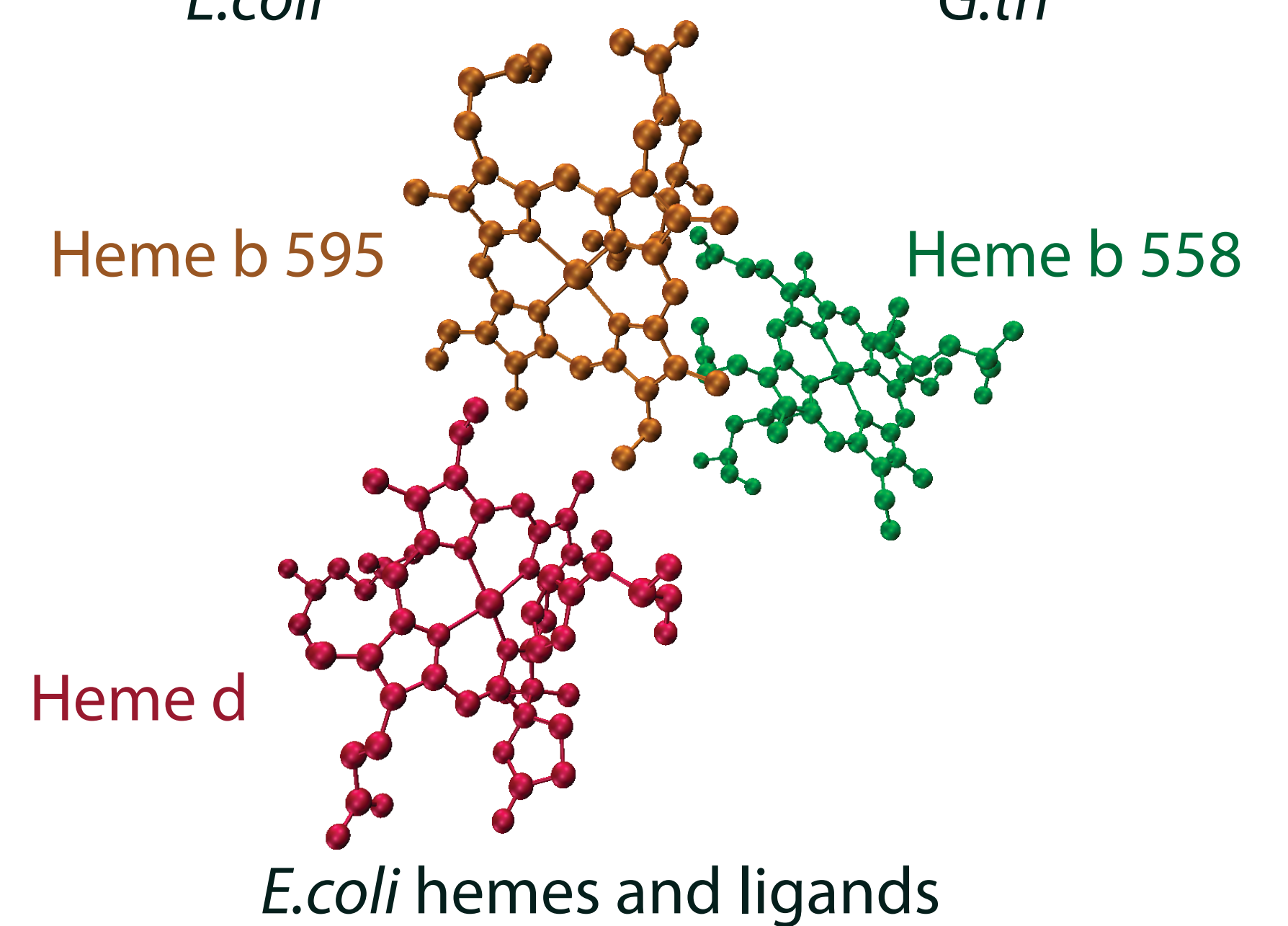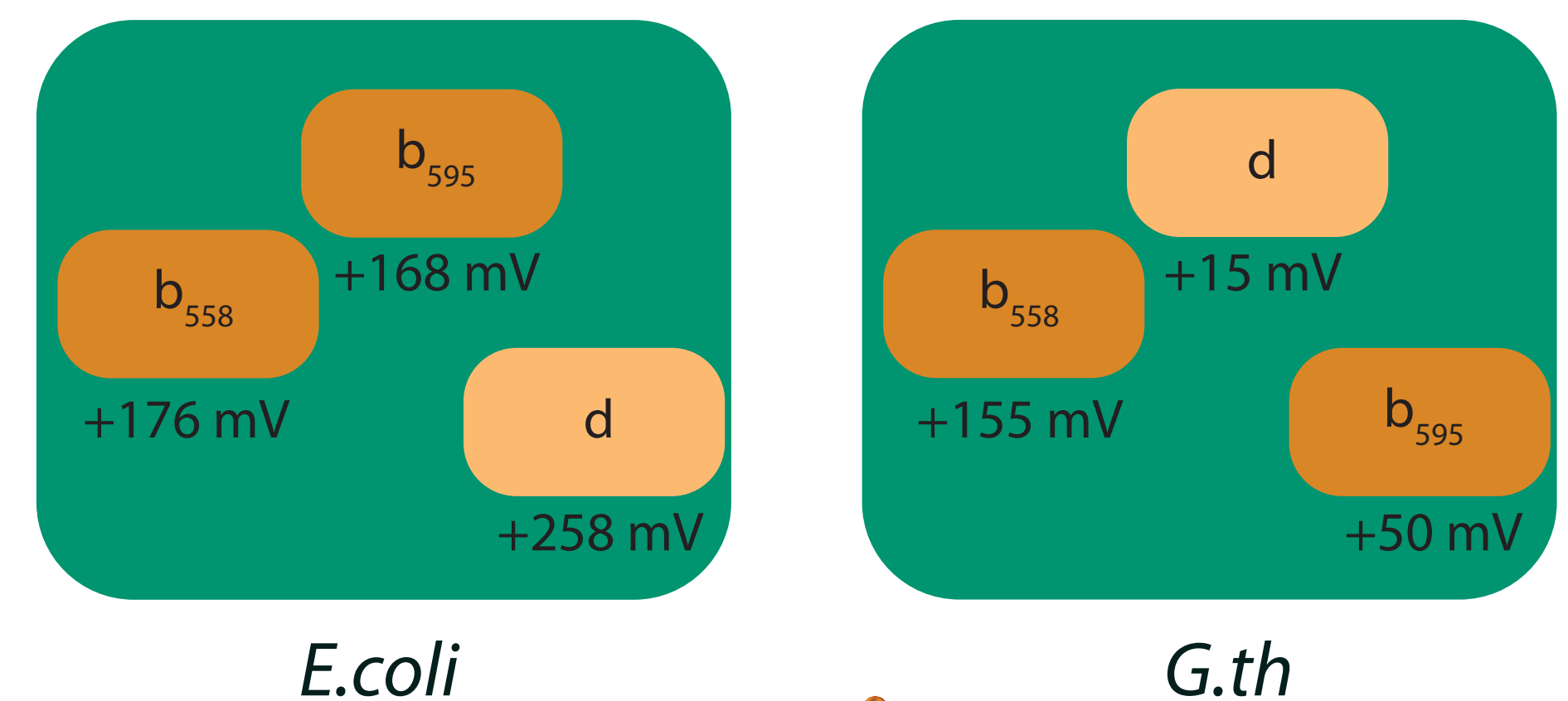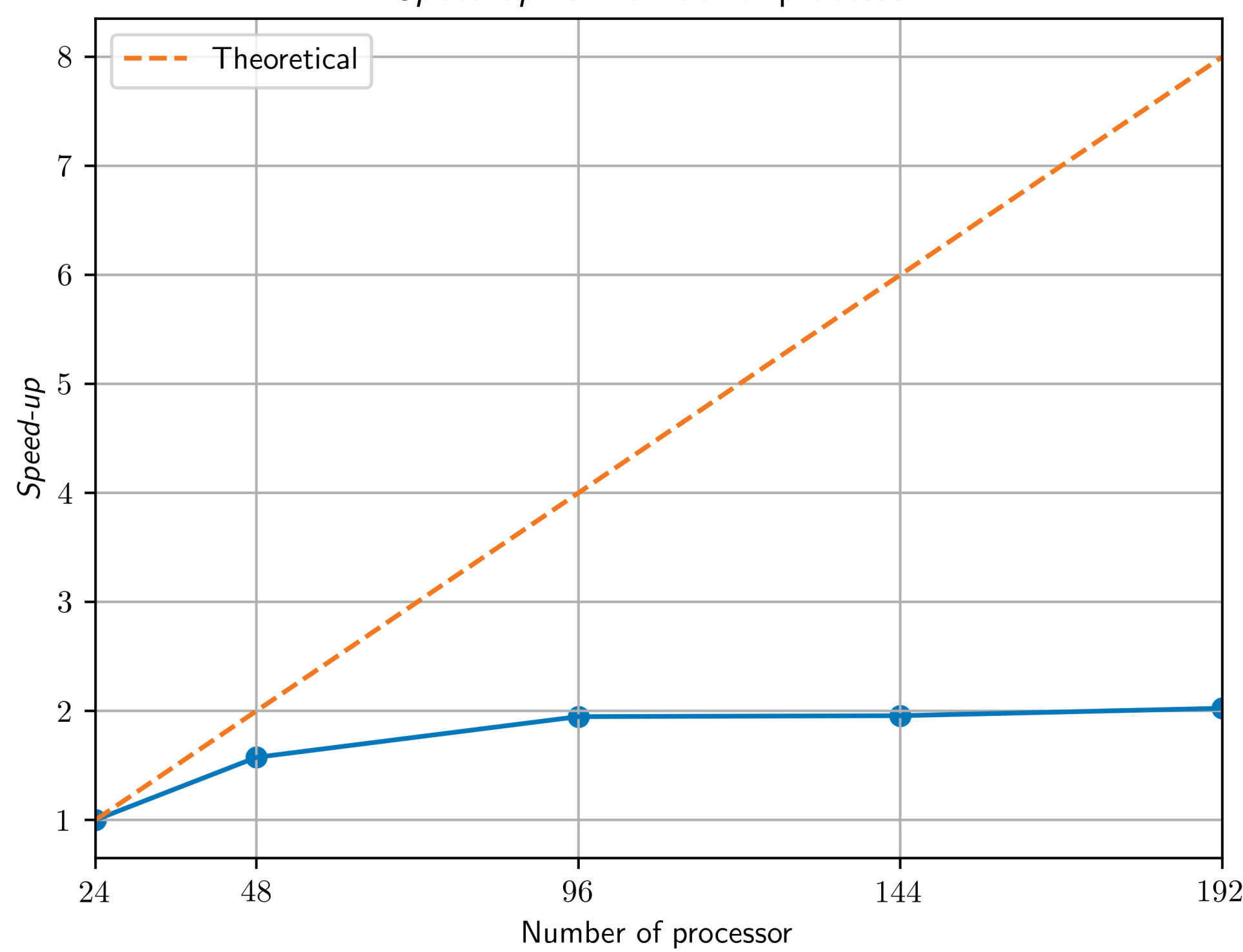cyctochromes bd share a **similar 3D structure**

The two proteins differ mainly from
the **space arragement**
and the **mid point potentials** of hemes [5]

E.coli cytochrome bd

G.th cytochrome bd

E.coli		G.th	
b₅₉₅		d	
b₅₅₈	+168 mV	b₅₅₈	+15 mV
+176 mV		+155 mV	
	d		b₅₉₅
	+258 mV		+50 mV

E.coli   *G.th*

Heme b 595   Heme b 558

Heme d

E.coli hemes and ligands

On **Occigen**

Speed-up vs. number of processor

Using **48 processors**

Using

deMon2k
density of Montréal

DFT (Density Functional Theory)

Optimize geometry

Calculate redox properties
(**ionisation potential, electron affinity**)

A better knowledge of **redox properties**
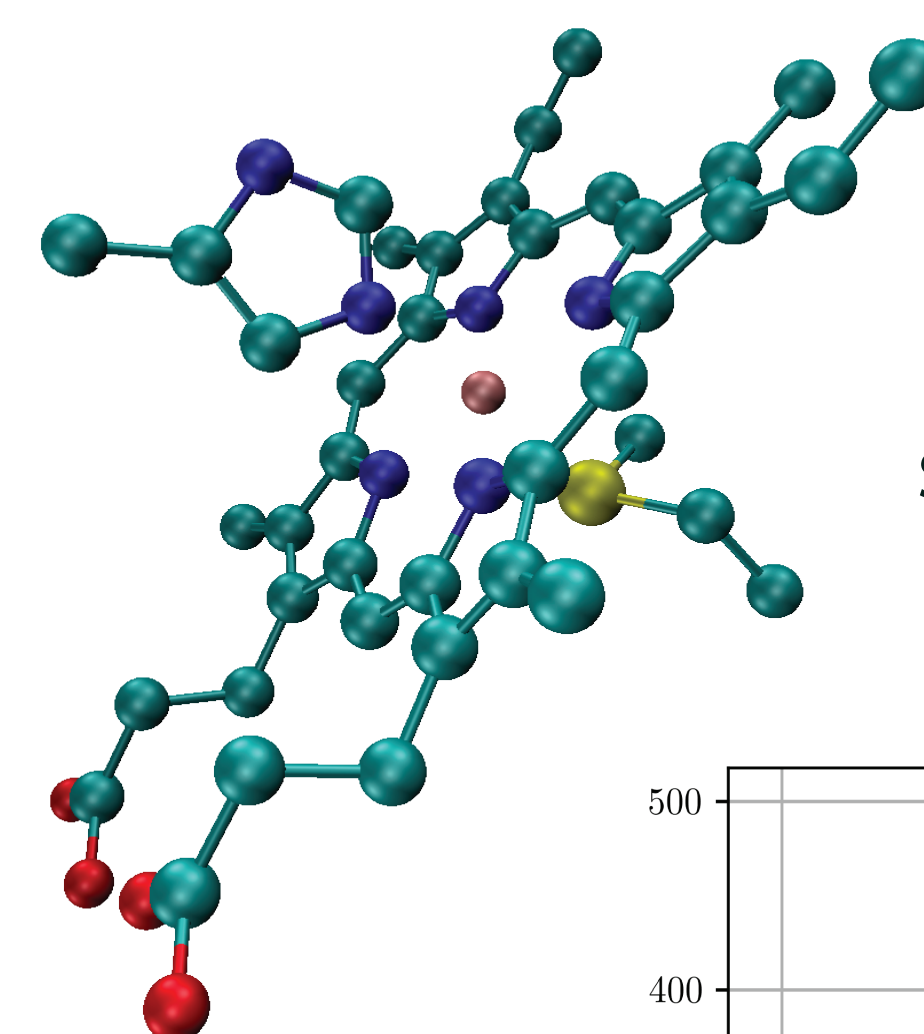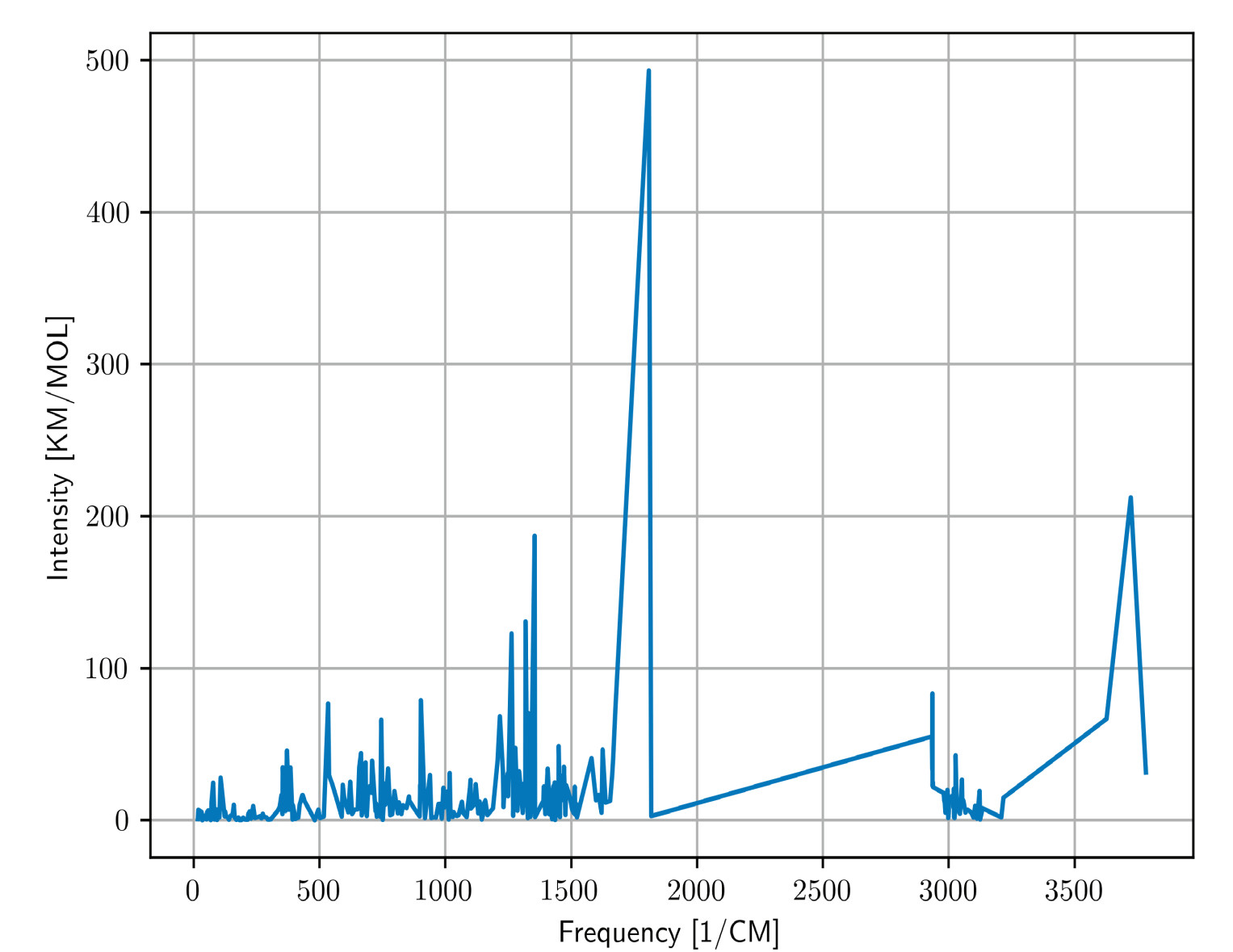for a better understanding of the **molecules functioning**

G.th   **E.coli**

Optimized geometry and its
spectra for heme b 558 in *E.coli*

Now

Optimizing geometry in gaz phase
starting geometries :
• extracted from experimental structure (cryo-EM)
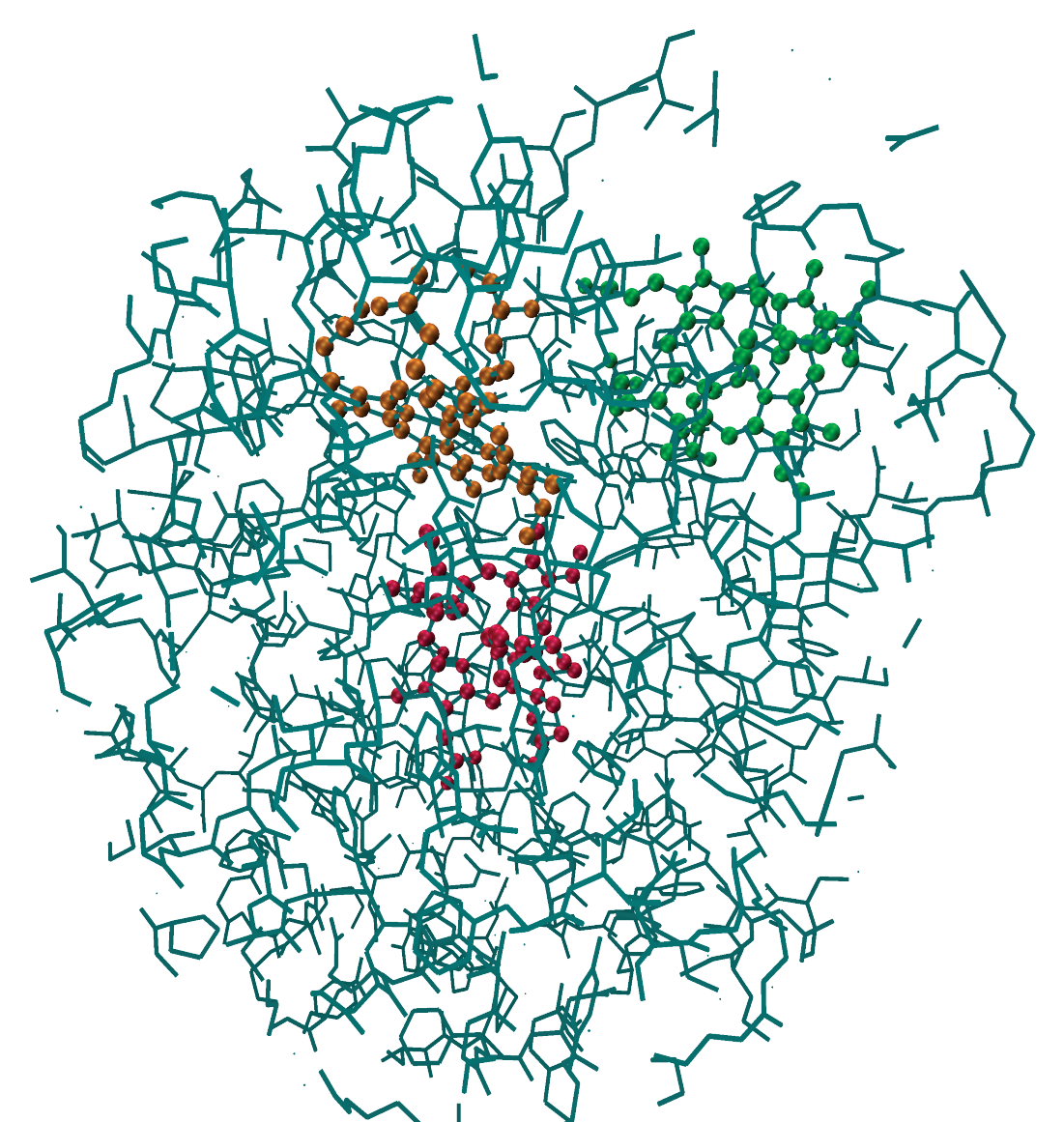• build from scratch

Then

References

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        Tomoichirou Kusumoto, Junshi Sakamoto, and Hartmut Michel.
        'Structure of a Bd Oxidase Indicates Similar Mechanisms for Membrane-Integrated Oxygen Reductases'.
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[7] Theßeling, Alexander, Tim Rasmussen, Sabrina Burschel, Daniel Wohlwend, Jan Kägi, Rolf Müller, Bettina Böttcher, and Thorsten Friedrich
        'Homologous Bd Oxidases Share the Same Architecture but Differ in Mechanism'.
        Nature Communications 10, no. 1 (December 2019): 5138. https://doi.org/10.1038/s41467-019-13122-4.

• Calculate

$$X_g + e^- = X_g^-, \quad \Delta E = {}^e A$$
$$X_g^- = X_g + e^-, \quad \Delta E = IP$$

• Use **QM-MM** to take nearby atoms into account

Hemes in their proteic environment
in *E.coli*