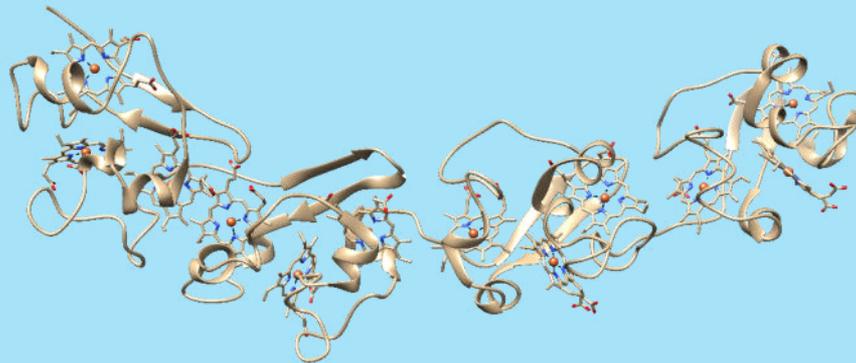


# LIVING CAPACITORS

*Caracterização funcional de um citocromo  
que atua como nanofio*

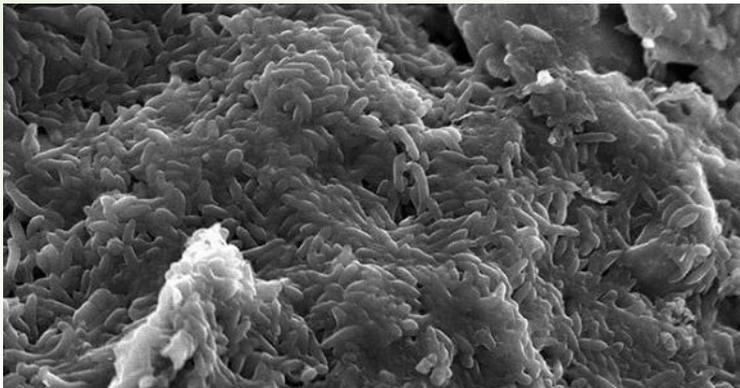


Ana Fernandes

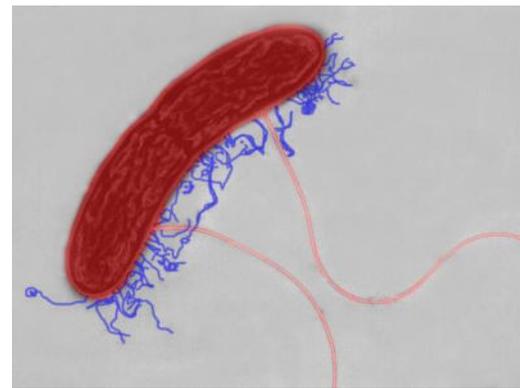
TC Nunes, DL Turner, CM Paquete and CA Salgueiro

# *Geobacter sulfurreducens*

- Bactéria anaeróbia Gram-negativa
- Flexibilidade nas cadeias de transferência de eletrônica
- Genoma sequenciado
  - >100 genes que codificam para citocromos de tipo c



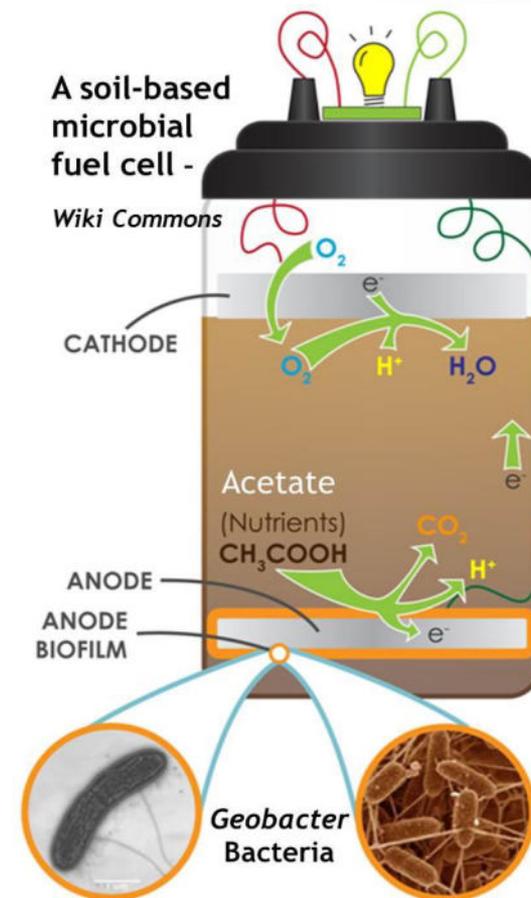
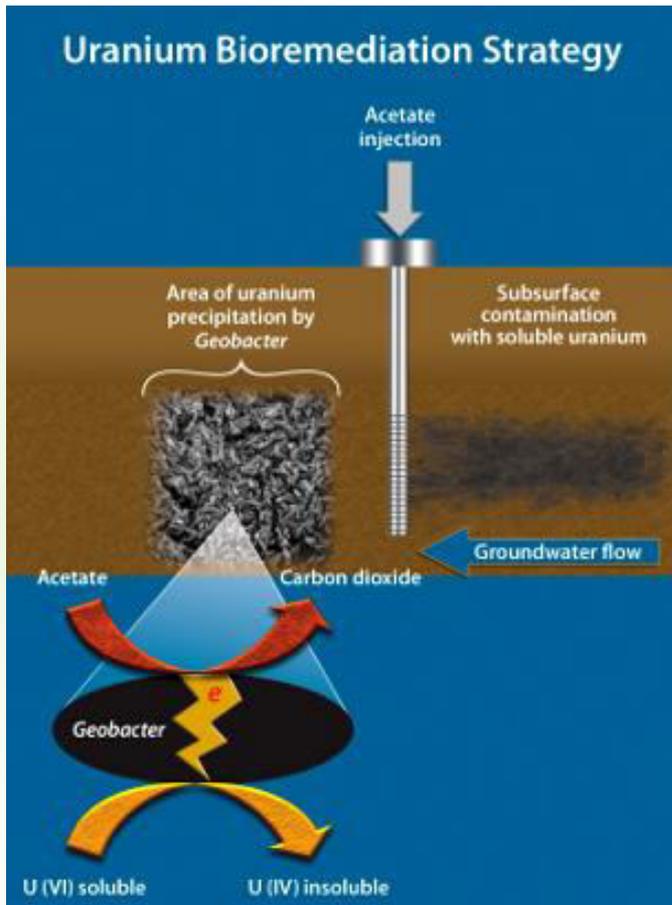
Luciana Robuschi



Derek R. Lovley, Gemma Reguera, Kevin D. McCarthy

# Geobacter sulfurreducens

- Aplicações biotecnológicas

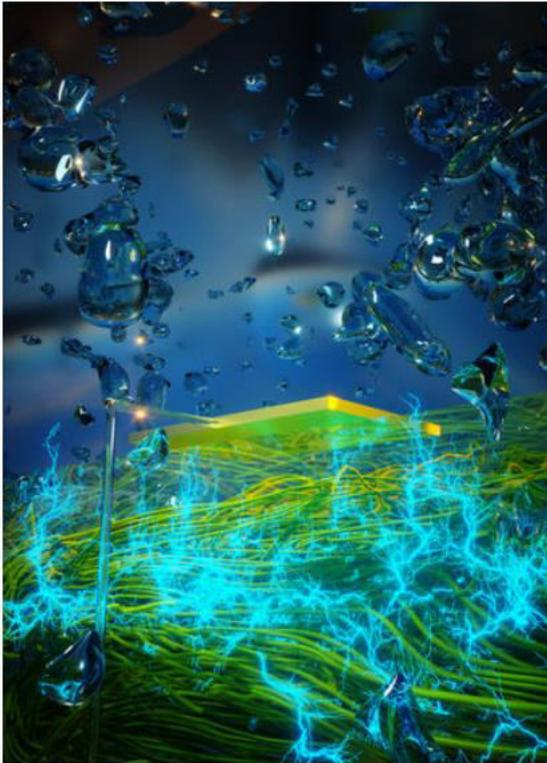


# Geobacter sulfurreducens

- Aplicações biotecnológicas

## NEW GREEN TECHNOLOGY FROM UMASS AMHERST GENERATES ELECTRICITY 'OUT OF THIN AIR'

Renewable device could help mitigate climate change, power medical devices



Xiaomeng Liu<sup>1</sup>, Hongyan Gao<sup>1</sup>, Joy E. Ward<sup>2</sup>, Xiaorong Liu<sup>3</sup>, Bing Yin<sup>1</sup>, Tianda Fu<sup>1</sup>, Jianhan Chen<sup>3,4,5</sup>, Derek R. Lovley<sup>2,4</sup> & Jun Yao<sup>1,4</sup>✉

As reported today in *Nature*, the laboratories of electrical engineer Jun Yao and microbiologist Derek Lovley at UMass Amherst have created a device they call an “Air-gen.” or air-powered generator, with electrically conductive protein nanowires produced by the microbe *Geobacter*. The Air-gen connects electrodes to the protein nanowires in such a way that electrical current is generated from the water vapor naturally present in the atmosphere.

“We are literally making electricity out of thin air,” says Yao. “The Air-gen generates clean energy 24/7.”

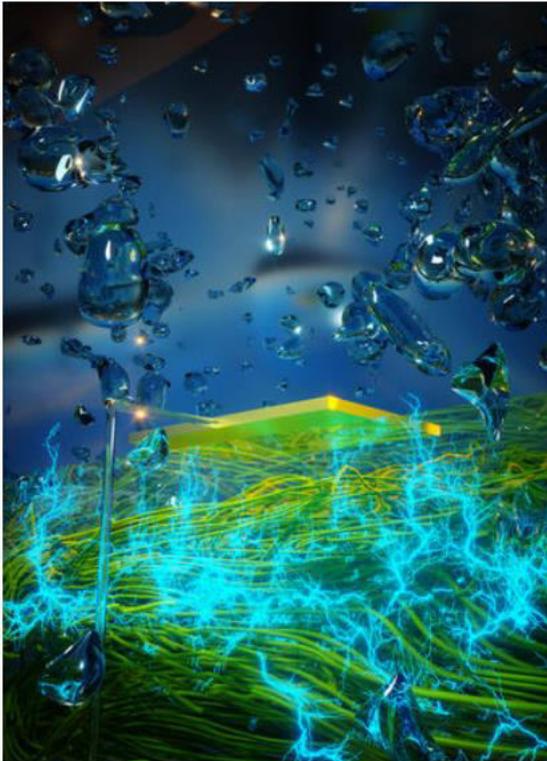
Graphic image of a thin film of protein nanowires generating electricity from atmospheric humidity.

# Geobacter sulfurreducens

- Aplicações biotecnológicas

## NEW GREEN TECHNOLOGY FROM UMASS AMHERST GENERATES ELECTRICITY 'OUT OF THIN AIR'

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The new technology developed in Yao's lab is non-polluting, renewable and low-cost. It can generate power even in areas with extremely low humidity such as the Sahara Desert. It has significant advantages over other forms of renewable energy including solar and wind, Lovley says, because unlike these other renewable energy sources, the Air-gen does not require sunlight or wind, and "it even works indoors."

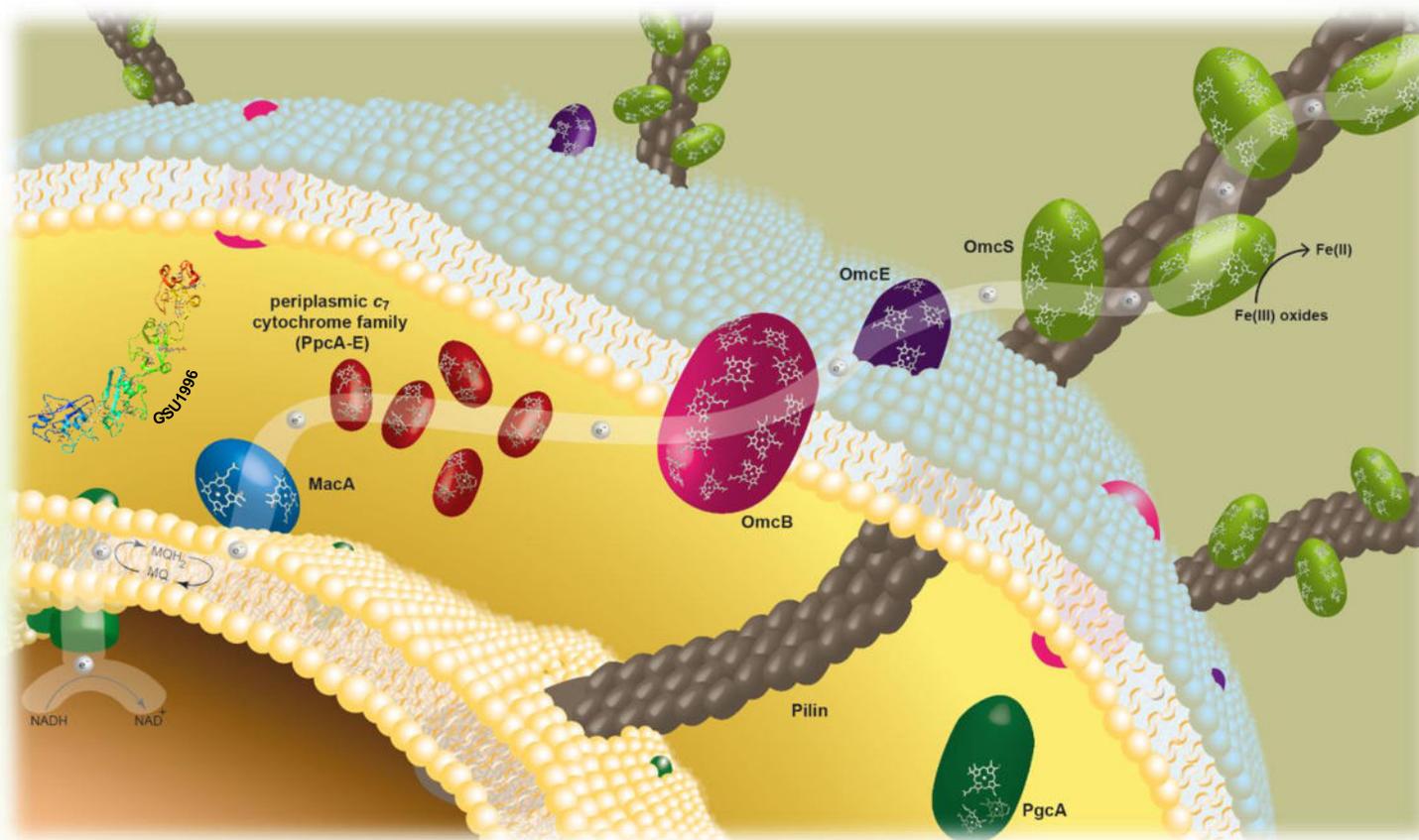
The Air-gen device requires only a thin film of protein nanowires less than 10 microns thick, the researchers explain. The bottom of the film rests on an electrode, while a smaller electrode that covers only part of the nanowire film sits on top. The film adsorbs water vapor from the atmosphere. A combination of the electrical conductivity and surface chemistry of the protein nanowires, coupled with the fine pores between the nanowires within the film, establishes the conditions that generate an electrical current between the two electrodes.

The researchers say that the current generation of Air-gen devices are able to power small electronics, and they expect to bring the invention to commercial scale soon. |

Graphic image of a thin film of protein nanowires generating electricity from atmospheric humidity.

# *Geobacter sulfurreducens*

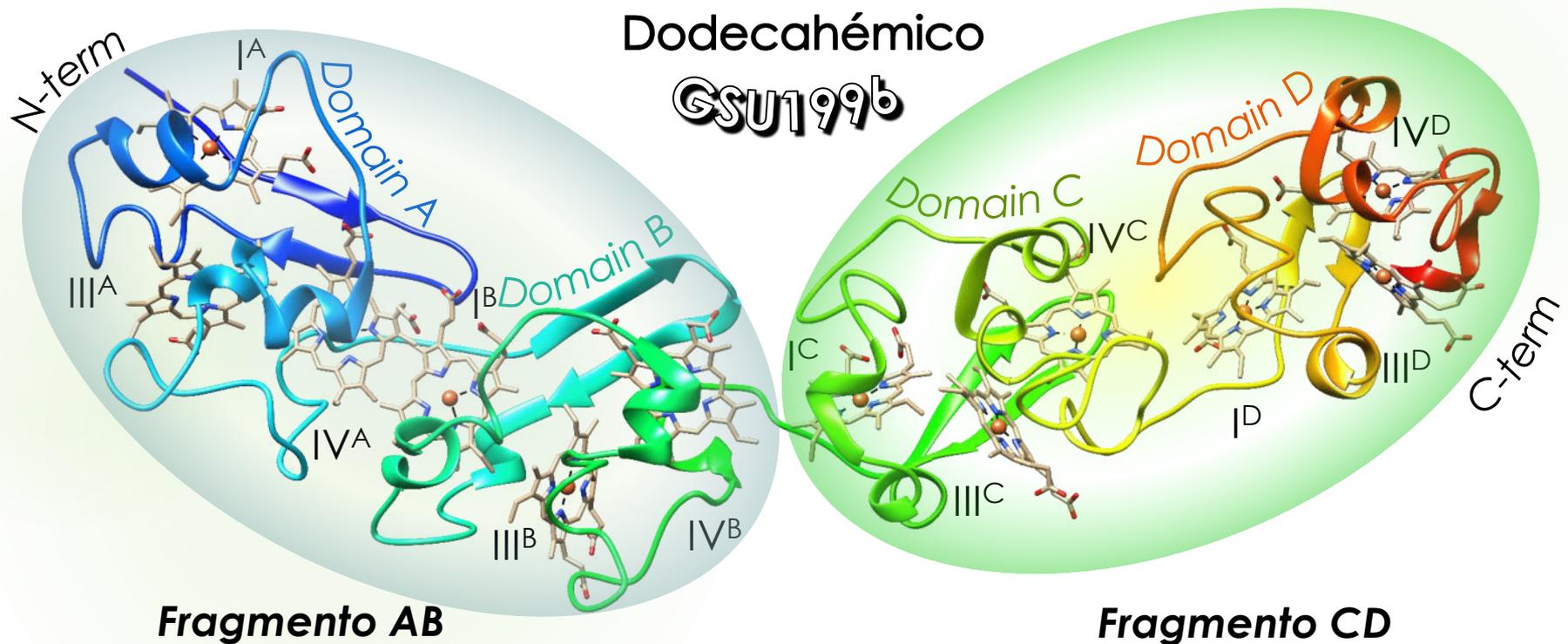
- Transferência eletrônica extracelular



# *Geobacter sulfurreducens*

- Citocromos tipo nanofio

Citocromo  
Dodecahémico  
**GSU1996**

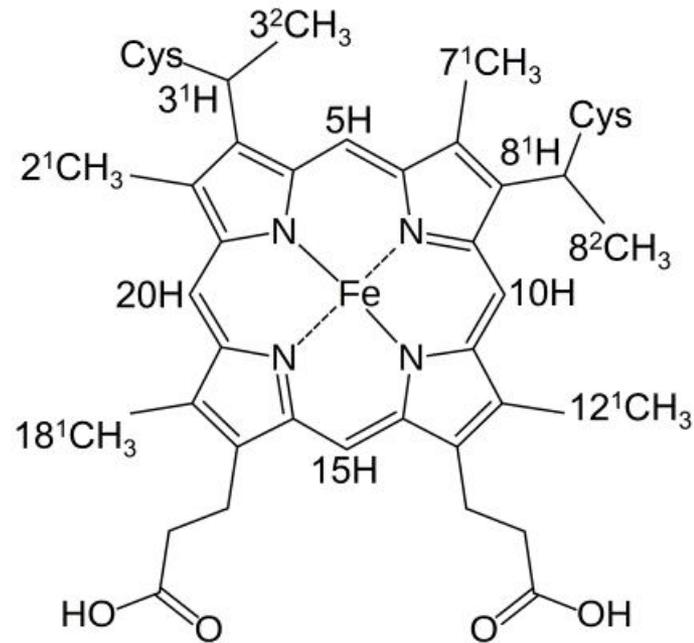


PDB ID: 3OV0

Pokkuluri et al, J Struct Biol 2011, 174(1): p 223-33.

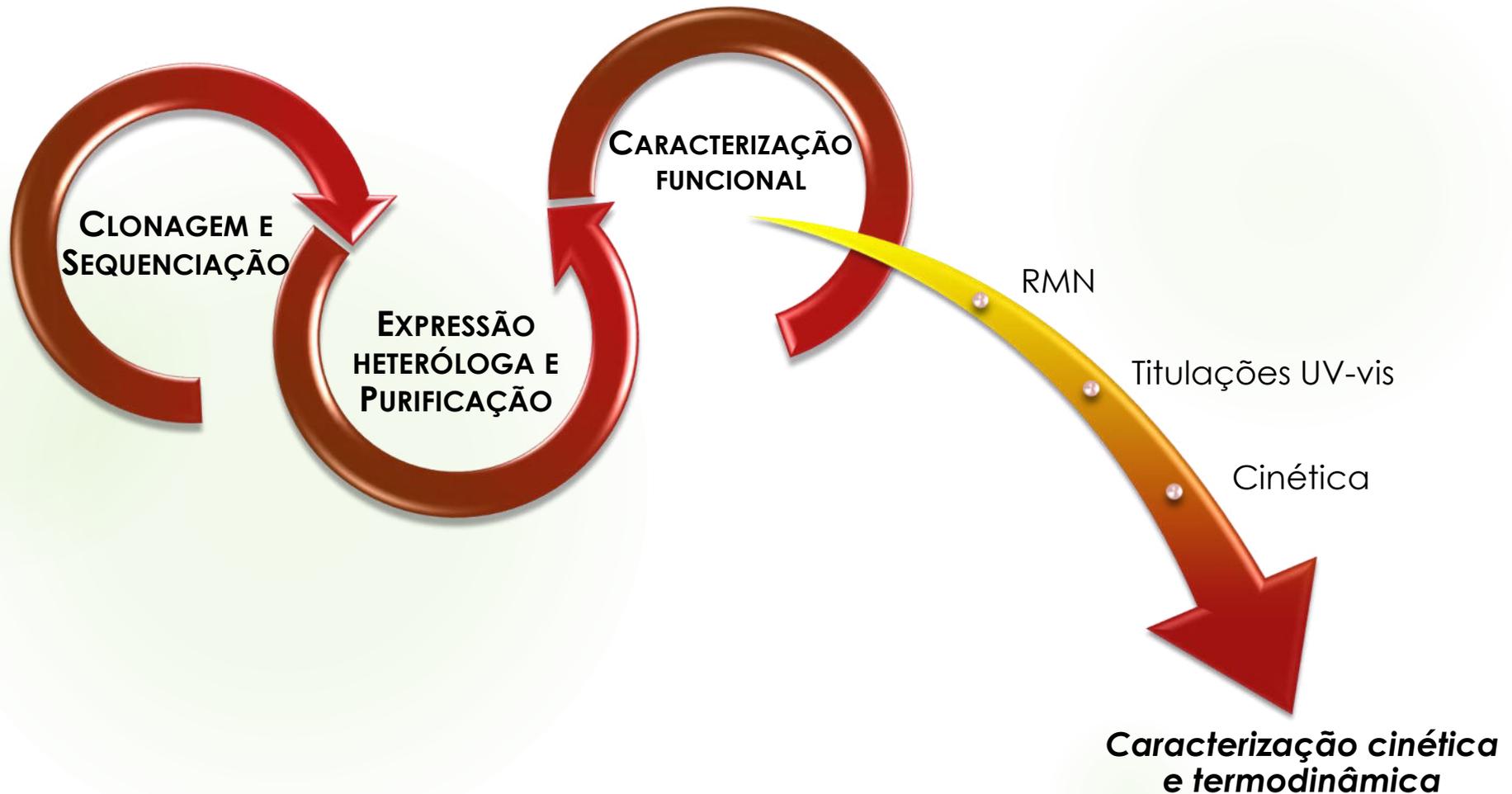
# *Geobacter sulfurreducens*

- Grupo Heme



# Caracterização funcional

- Citocromos c multihêmicos



# Caracterização funcional

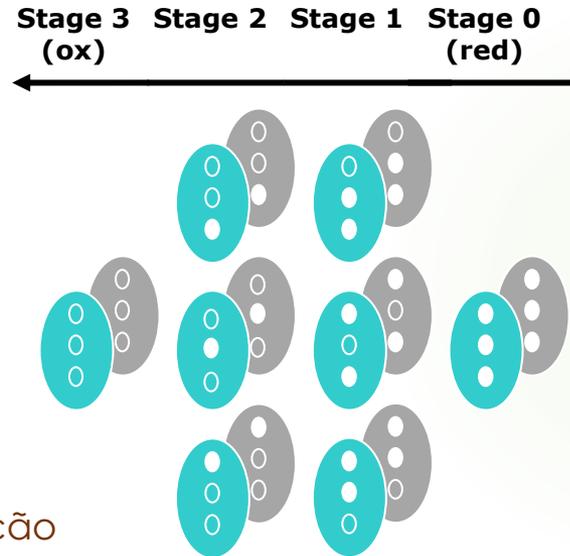
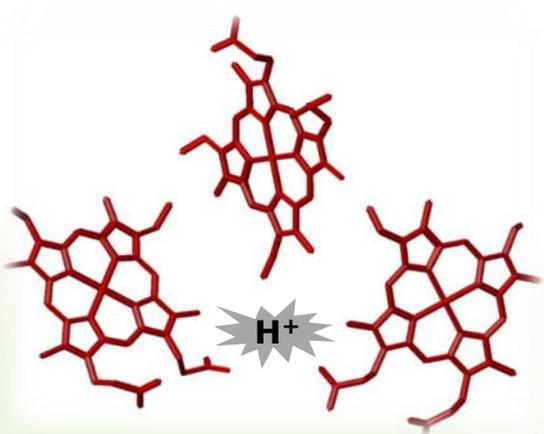
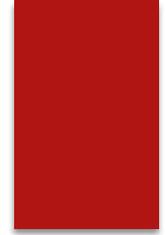
- Aproximação modular

Desenvolvimento de estratégias para a caracterização funcional do citocromo dodecahémico GSU1996



Caracterização funcional de cada domínio e de cada fragmento de dois domínios do GSU1996

# Caracterização termodinâmica



3 potenciais hémicos microscópicos de redução

3 energias de interação oxidação-redução entre grupos heme

3 energias de interação redox-Bohr hemo-centro protonável

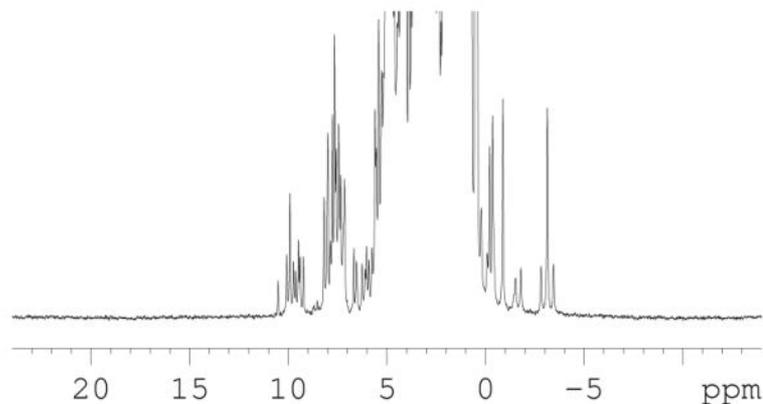
1  $pK_a$  do centro protonável

**10 parâmetros termodinâmicos**

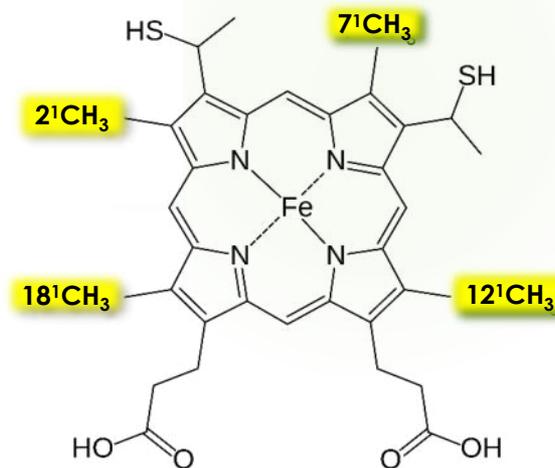
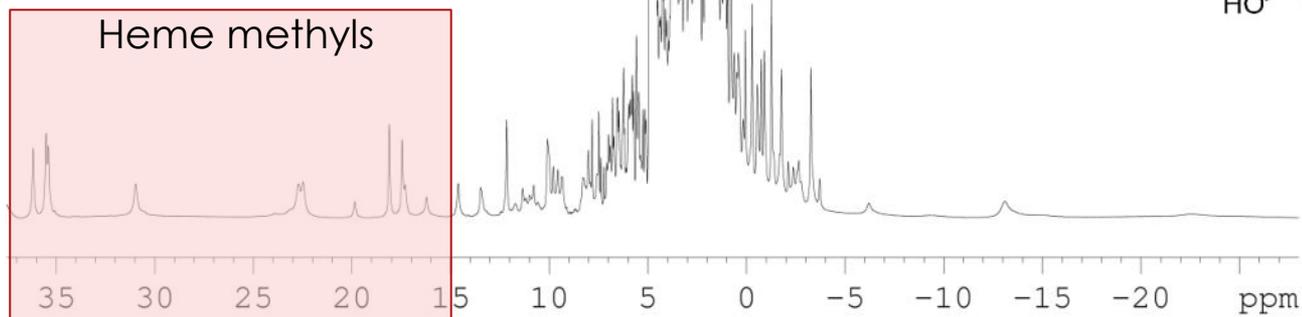
# Caracterização termodinâmica

- Domínio C

Reduced

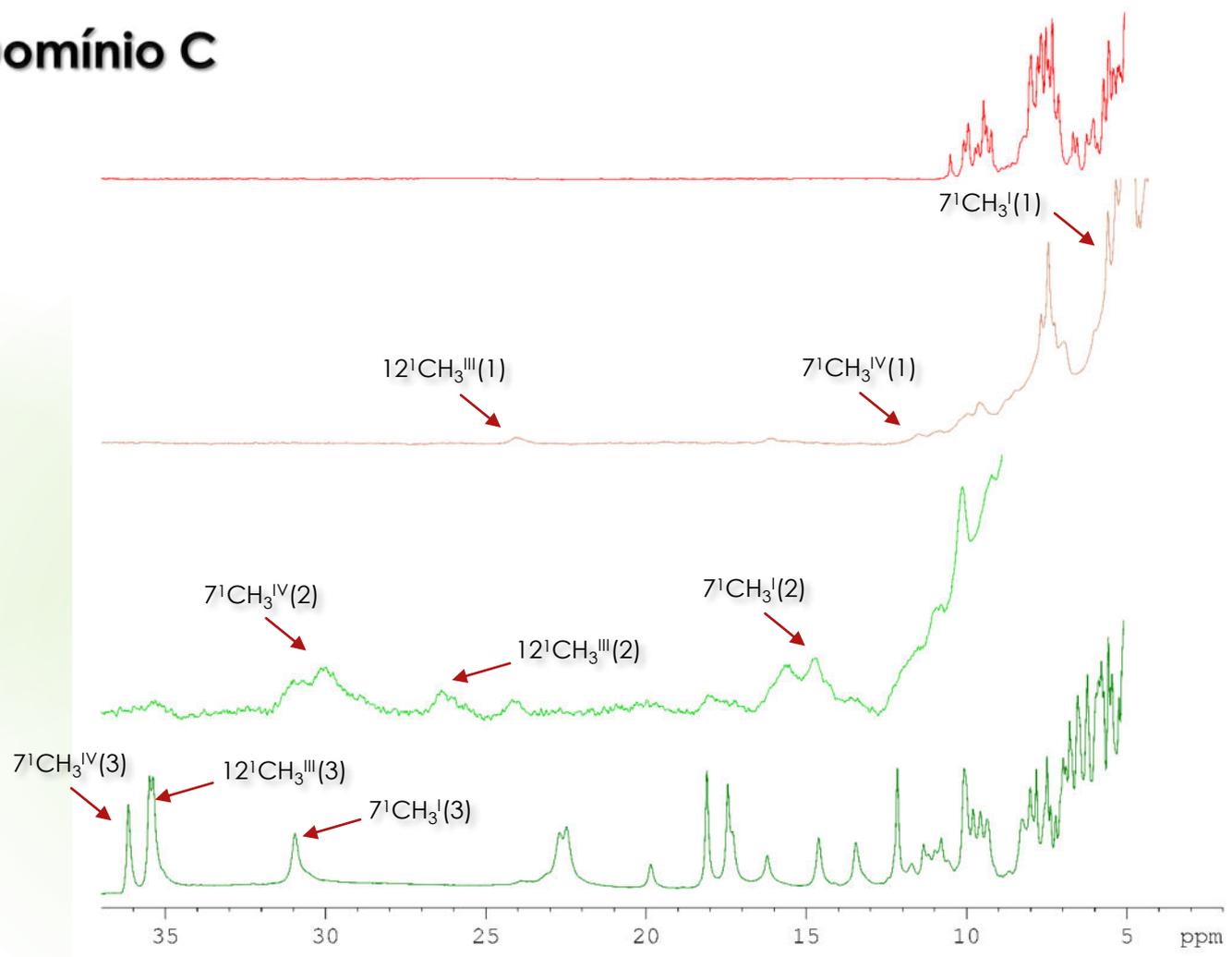


Oxidized



# Caracterização termodinâmica

- Domínio C

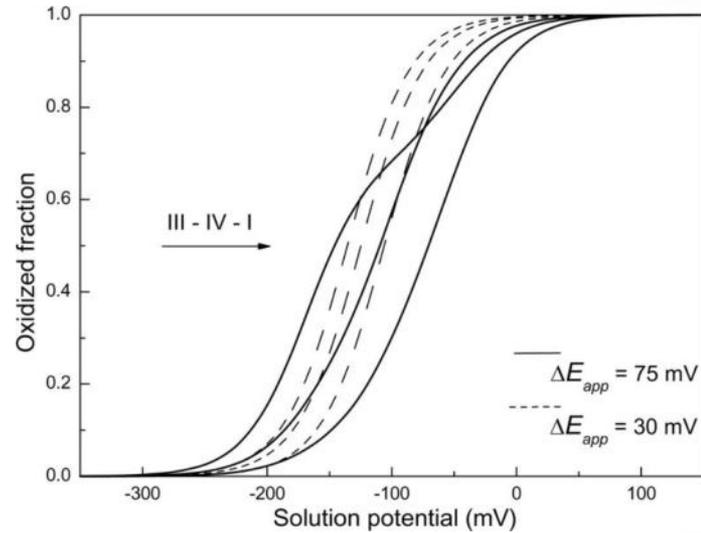
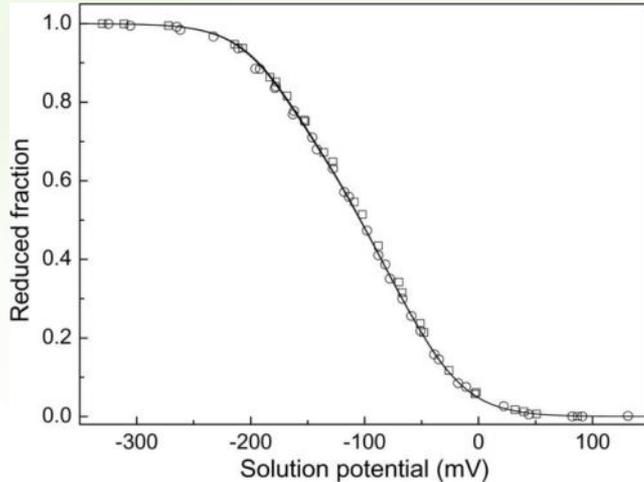


Oxidação



# Caracterização termodinâmica

- Domínio C



	Energies (meV)			
	Haem I	Haem III	Haem IV	Protonatable centre
Haem I	<b>-106 (2)</b>	44 (2)	7 (2)	-4 (6)
Haem III		<b>-136 (2)</b>	40 (2)	-25 (6)
Haem IV			<b>-125 (2)</b>	-13 (7)
Protonatable centre				<b>340 (11)</b>

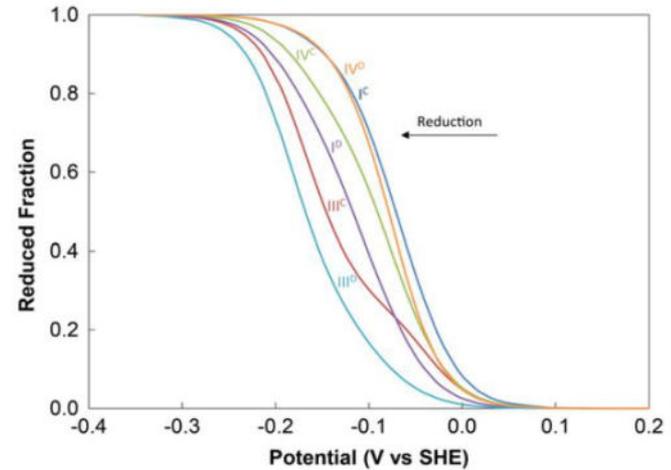
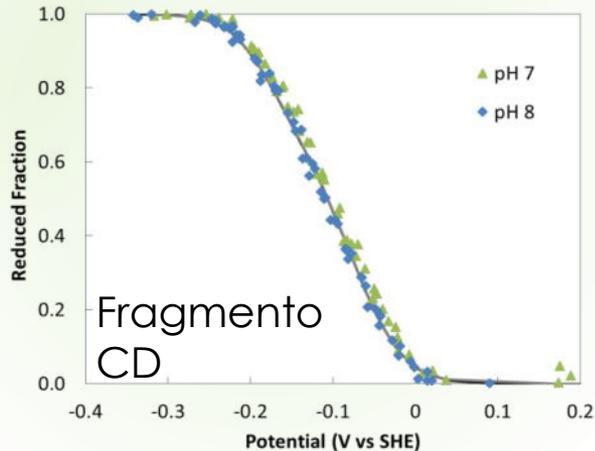
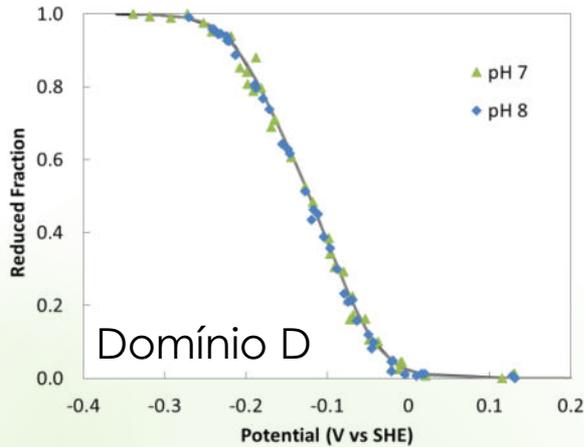
# Caracterização termodinâmica

- Domínio D

	Heme pairs	Distance (Å)	Interaction energies (meV)
Fragment CD	I <sup>D</sup> -III <sup>D</sup>	11.3	34
	I <sup>D</sup> -IV <sup>D</sup>	18.0	9
	III <sup>D</sup> -IV <sup>D</sup>	12.1	29
	I <sup>C</sup> -I <sup>D</sup>	30.7	1
	I <sup>C</sup> -III <sup>D</sup>	40.6	0
	I <sup>C</sup> -IV <sup>D</sup>	48.3	0
	III <sup>C</sup> -I <sup>D</sup>	21.8	5
	III <sup>C</sup> -III <sup>D</sup>	30.4	1
	III <sup>C</sup> -IV <sup>D</sup>	39.5	0
	IV <sup>C</sup> -I <sup>D</sup>	14.7	17
	IV <sup>C</sup> -III <sup>D</sup>	25.3	3
	IV <sup>C</sup> -IV <sup>D</sup>	32.3	1

# Caracterização termodinâmica

## • Fragmento CD



Hemes	Energies (meV)						Ionizable center
	I <sup>C</sup>	III <sup>C</sup>	IV <sup>C</sup>	I <sup>D</sup>	III <sup>D</sup>	IV <sup>D</sup>	
I <sup>C</sup>	-106	44	7	1	0	0	-4
III <sup>C</sup>		-136	40	5	1	0	-25
IV <sup>C</sup>			-125	17	3	1	-13
I <sup>D</sup>				-155 (7)	34	9	-
III <sup>D</sup>					-178 (5)	29	-
IV <sup>D</sup>						-113(4)	-
Ionizable center							340

# Caracterização cinética

- Fragmento CD



$$k_i^j = k_i^0 \exp \left[ \frac{e_i^j F}{2RT} \left( 1 + \frac{e_o F}{\lambda} - \frac{e_i^j F}{2\lambda} \right) \right]$$

Intrinsic to each individual redox centre

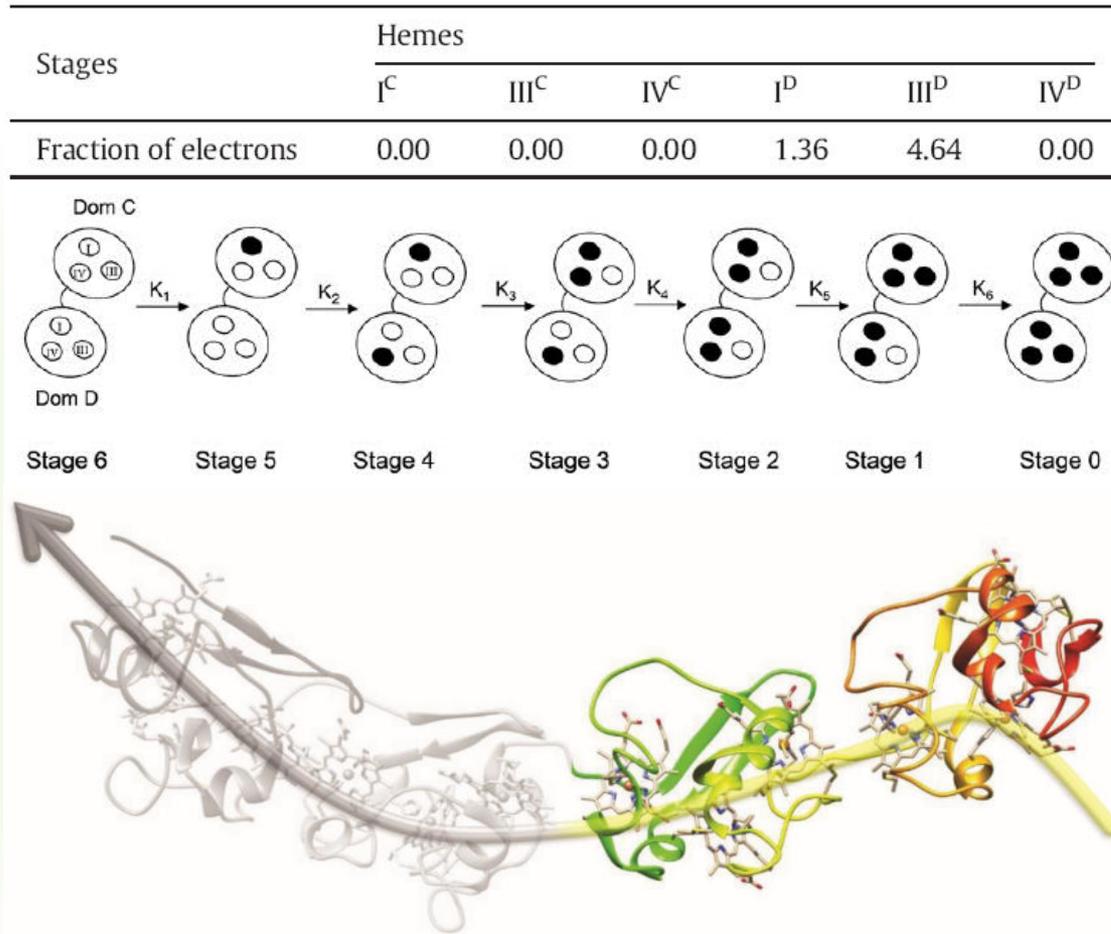
Dependent on the driving force (thermodynamic parameters)

Constantes de velocidade de cada hemo no processo de redução com ditonito de sódio ( $k_i^0$ ) do fragmento CD de GSU1996

		$k_i^0 (\times 10^6 \text{ s}^{-1} \text{ M}^{-1})$
Domain C	Heme I	0.0 (5.7)
	Heme III	0.0 (2.4)
	Heme IV	0.0 (5.2)
Domain D	Heme I	74.0 (2.2)
	Heme III	274.3 (1.2)
	Heme IV	0.0 (2.1)

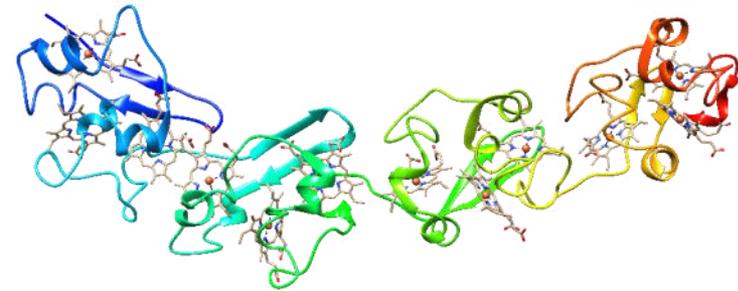
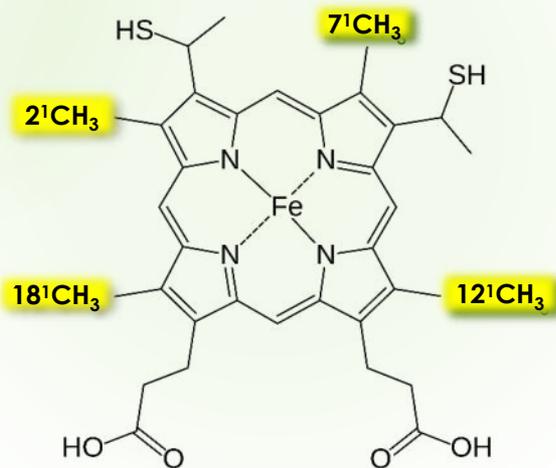
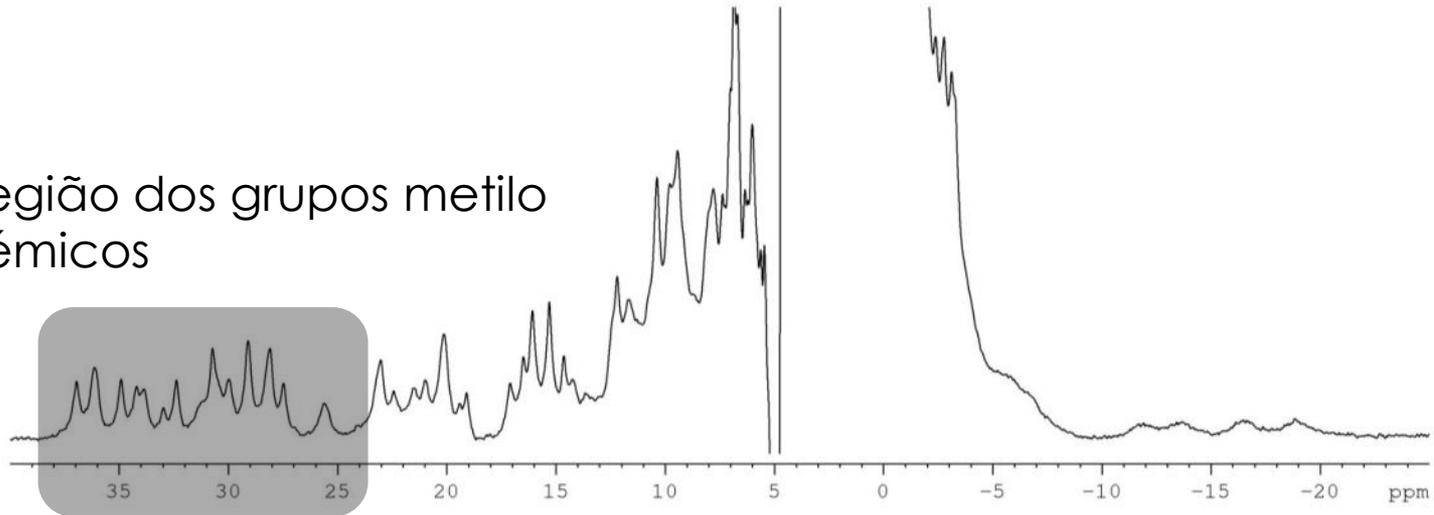
# Caracterização funcional

- Fragmento CD



# Vias de transferência eletrônica

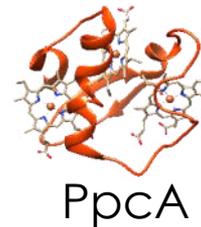
Região dos grupos metilo  
hêmicos



GSU1996

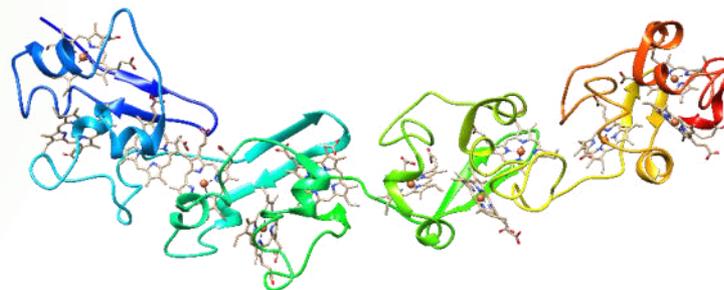
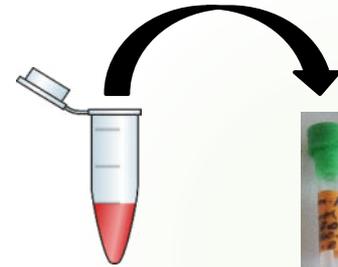
# Vias de transferência eletrônica

- Perturbação nos desvios químicos – 1D  $^1\text{H}$  RMN



PpcA

PDB ID: 2mz9



GSU1996

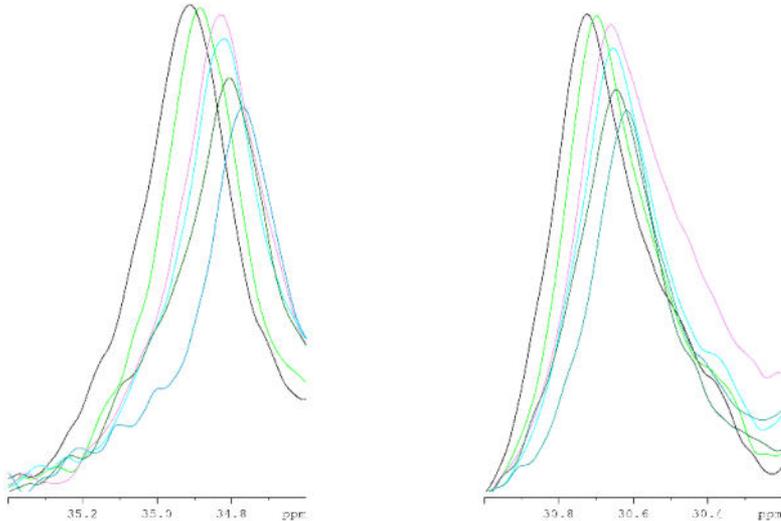
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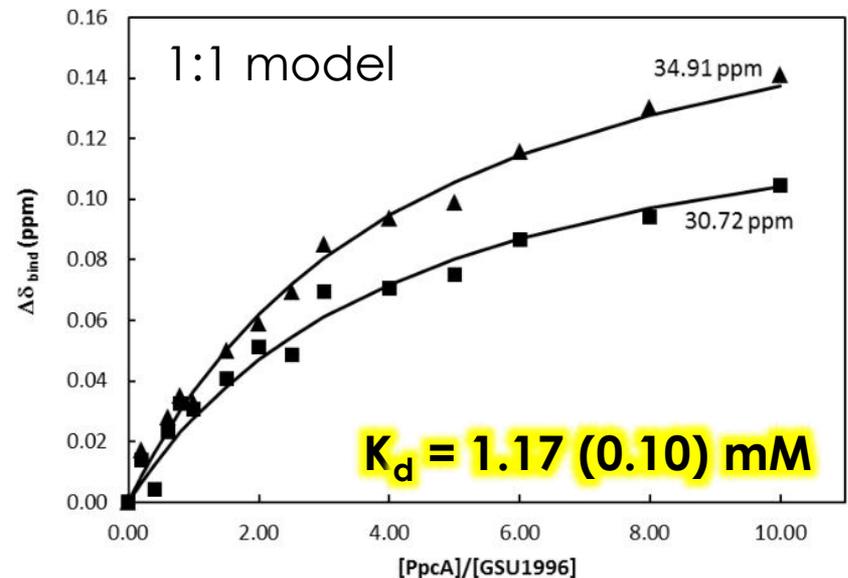
# Vias de transferência eletrônica

- Constante de dissociação

GSU1996:PpcA

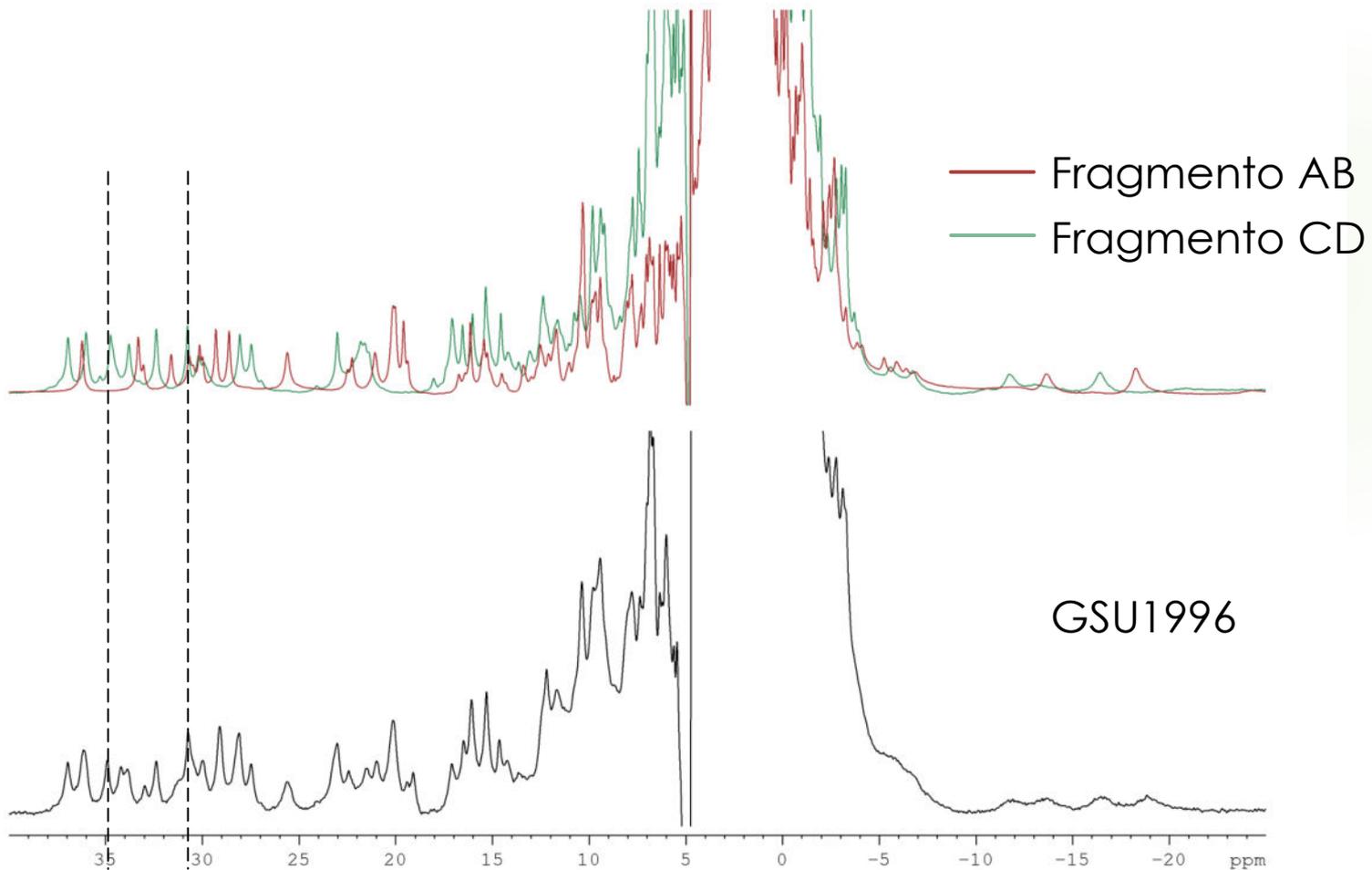


Alterações ao espectro de 1D <sup>1</sup>H RMN do GSU1996 na presença de quantidades crescentes de PpcA

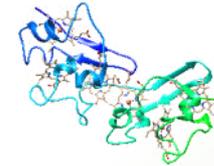
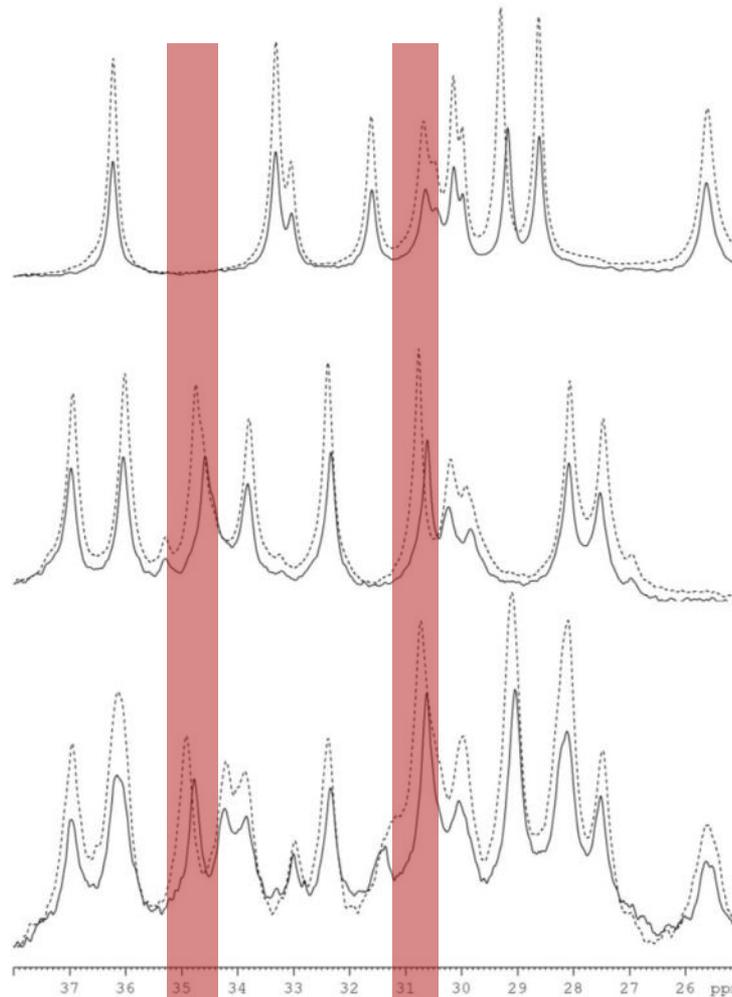


Curvas de ligação do GSU1996 com o PpcA que apresentam interações

# Vias de transferência eletrônica

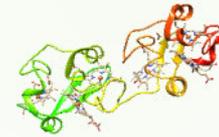


# Vias de transferência eletrônica



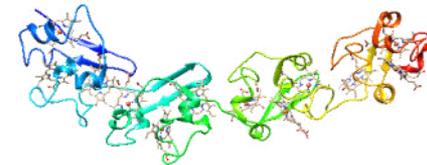
--- Fragmento AB

— Fragmento AB + PpcA



--- Fragmento CD

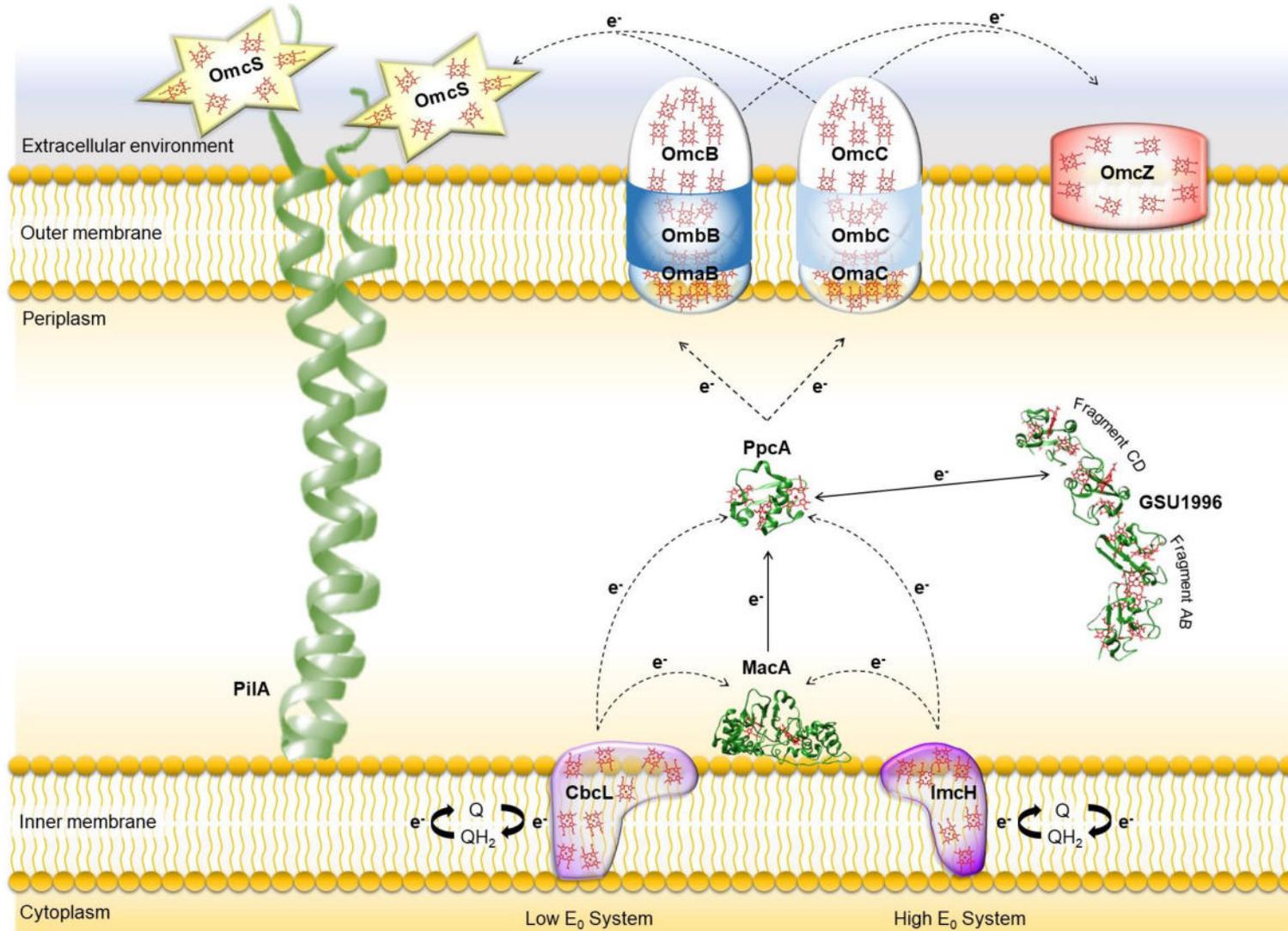
— Fragmento CD + PpcA



--- GSU1996

— GSU1996 + PpcA

# Extracellular electron transfer proposal



# Agradecimentos



**Tiago C. Nunes**  
**Carlos A. Salgueiro**



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**Mónica Alves**  
**Catarina M. Paquete**  
**Ricardo Louro**  
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# Agradecimentos



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