

# EXTRACTIVE BIOCONVERSION OF 3-HYDROXYPROPIONIC ACID: INSIGHTS IN EXTRACTION AND MASS TRANSFER MECHANISMS

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UMR 782 INRA/AgroParisTech « Génie et Microbiologie des Procédés Alimentaires »



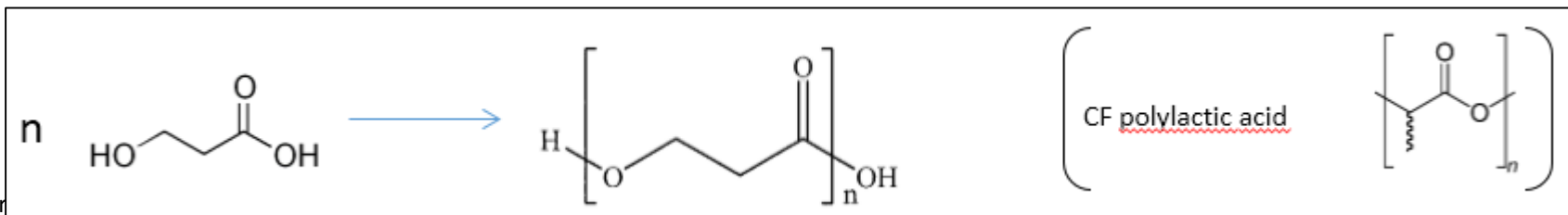
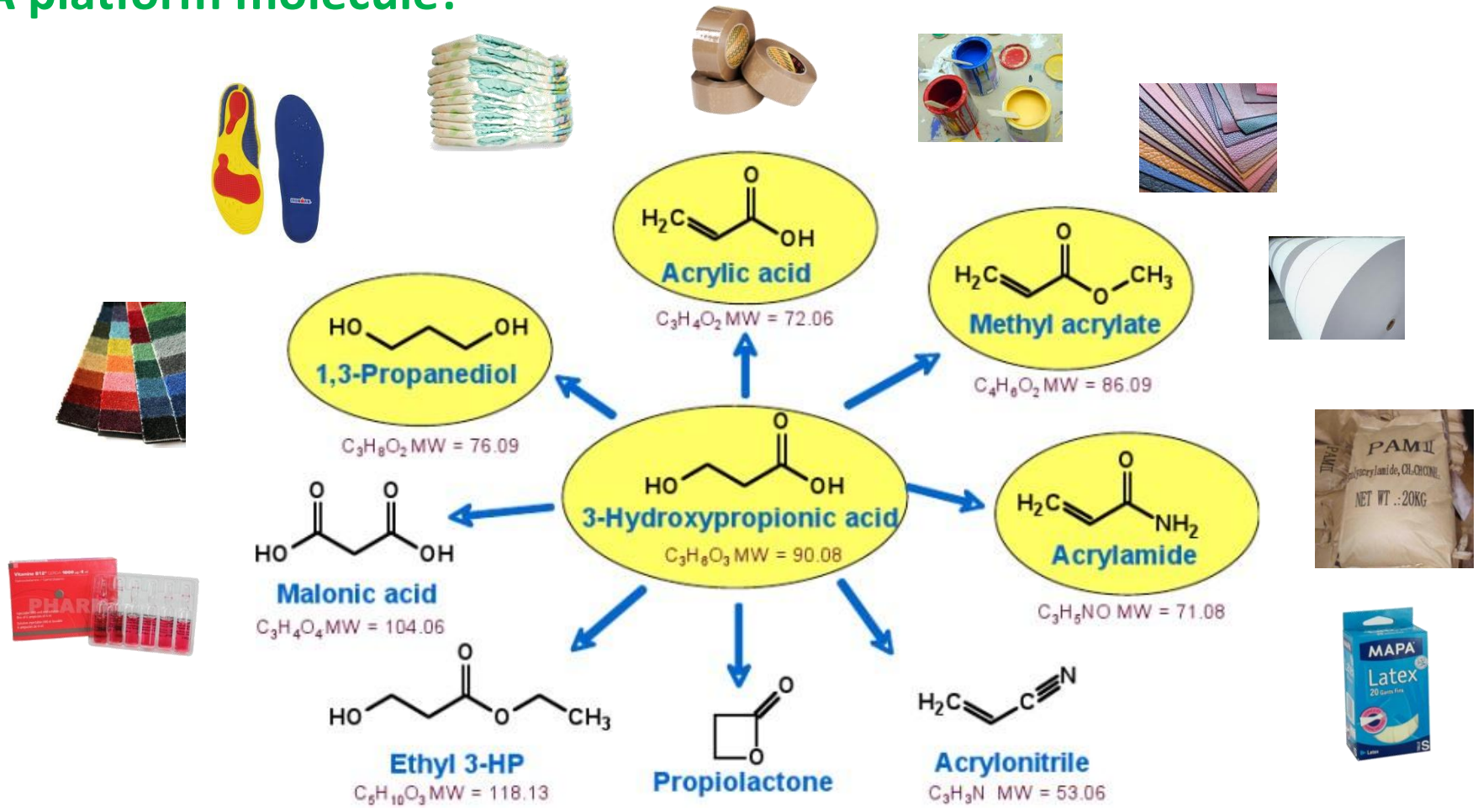
WasteEng 2016, Albi

May, 25<sup>th</sup> 2016



# 3-HYDROXYPROPIONIC ACID

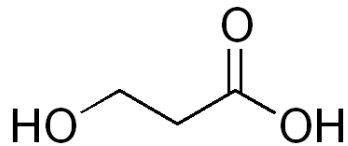
A platform molecule!



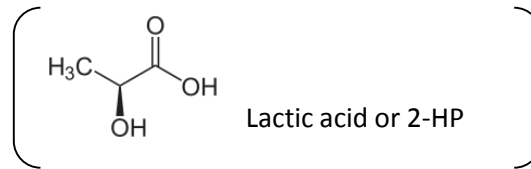
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# 3-HYDROXYPROPIONIC ACID

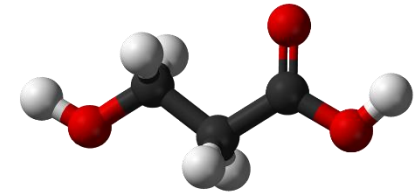
→ What is 3-hydroxypropionic acid ?



3-HP



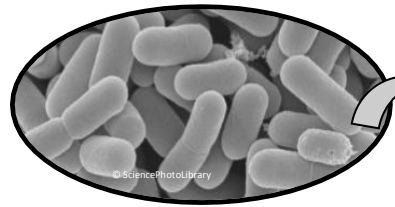
Lactic acid or 2-HP



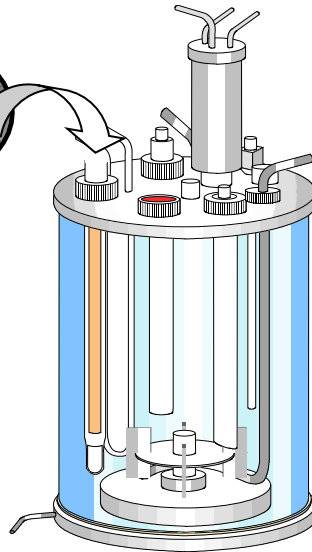
→ What are its properties?

- Chemical formula:  $C_3H_6O_3$
- Molecular weight: 90 g/mol
- Polar
- Hydrophilic:  $\log K_{ow} = -0,89$  (EPI suite)
- Weak acid:  $pK_a = 4.51$

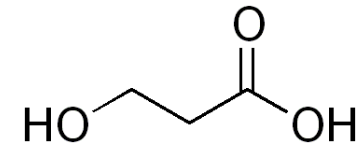
# BIOCONVERSION PROCESS



Bacteria or yeasts  
Modified or not

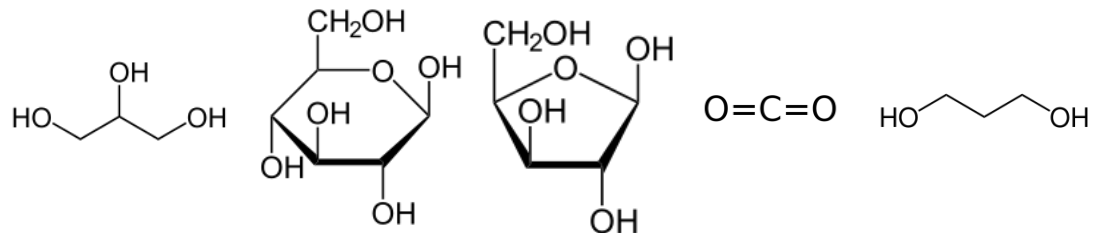


**Bioconversion**

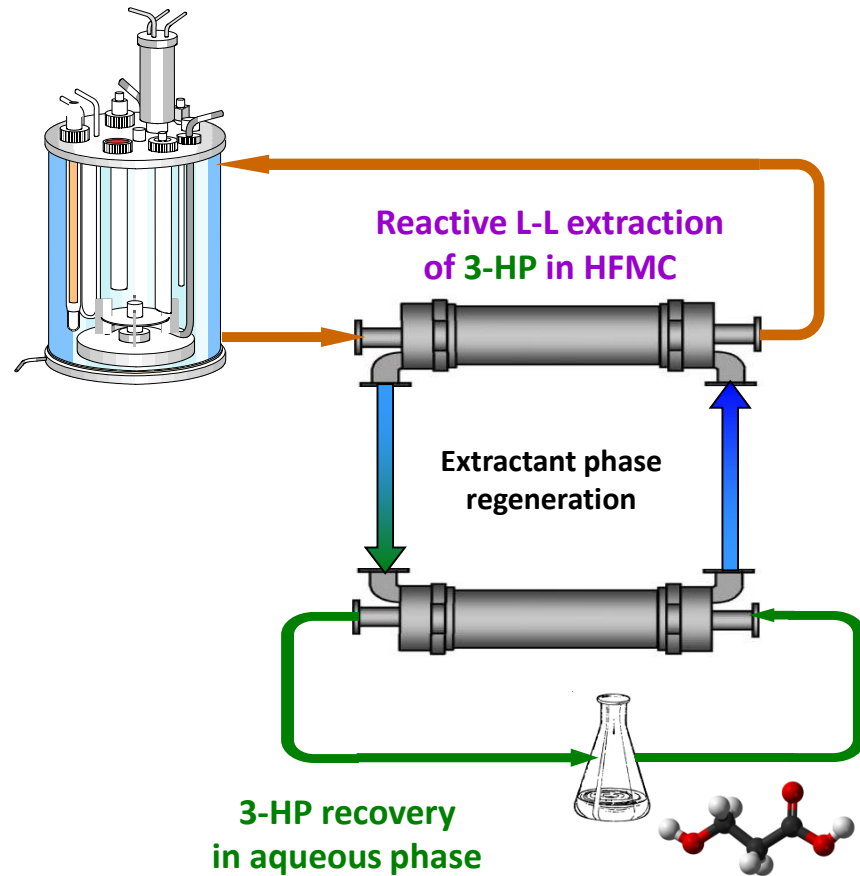


**Microbial  
inhibition**

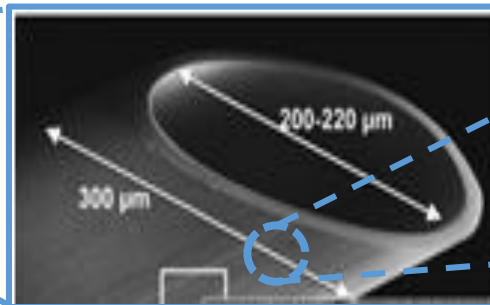
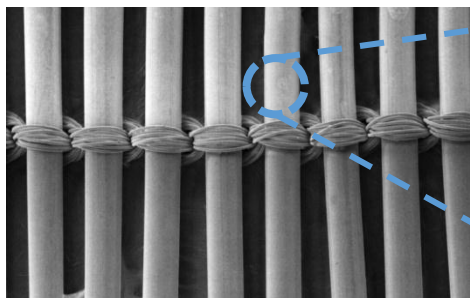
*Dishisha et al, 2014;*  
*Chu et al, 2015;*  
*Kildegaard et al, 2015;*  
*Wang et al, 2016;*  
*Zhao et al, 2015*



# REACTIVE LIQUID-LIQUID EXTRACTION PROCESS INTEGRATED TO THE BIOCONVERSION



Hydrophobic membrane  
(porosity = 30-40 %  
pore diameter = 30 nm)



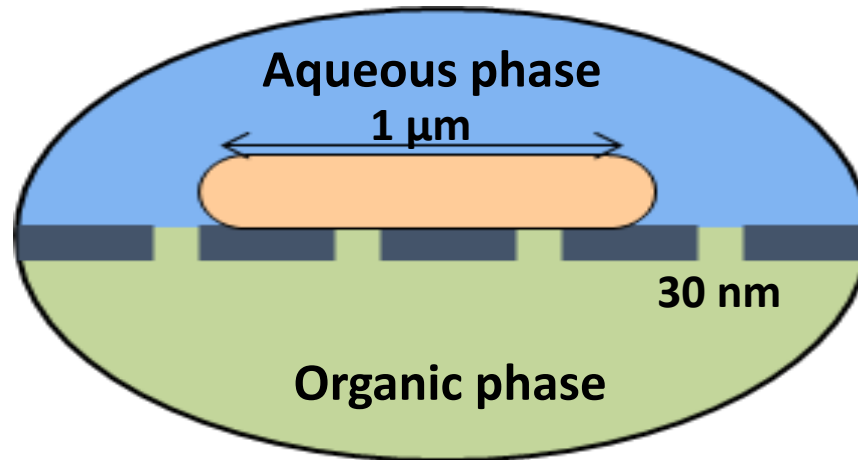
# WHY USING A MEMBRANE CONTACTOR IN OUR CASE?

High specific surface area without dispersion

→ No emulsion

Prevents cells from contacting the organic phase

→ Potentially avoids contact toxicity with solvents



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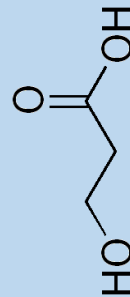
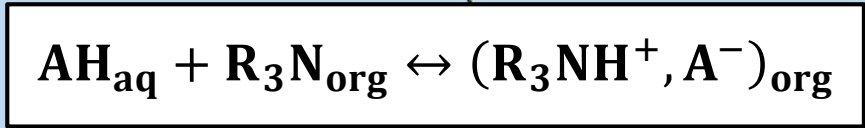
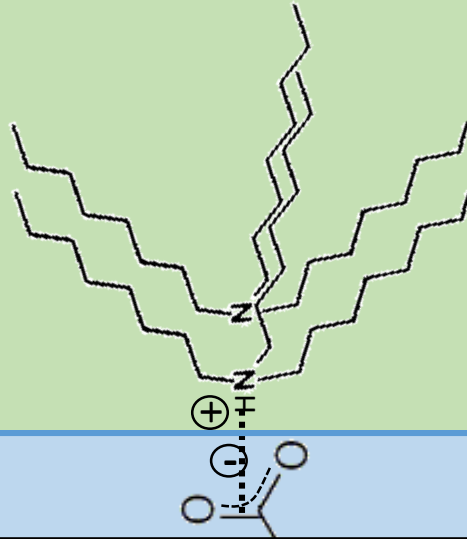
**What are the mechanisms implied in this extraction process and can we easily predict the results?**

**Finally, does a complex bioconversion medium have an impact on our extraction efficiency?**

# 3-HP REACTIVE EXTRACTION BY TRIOCTYLAMINE

Organic phase

Aqueous phase



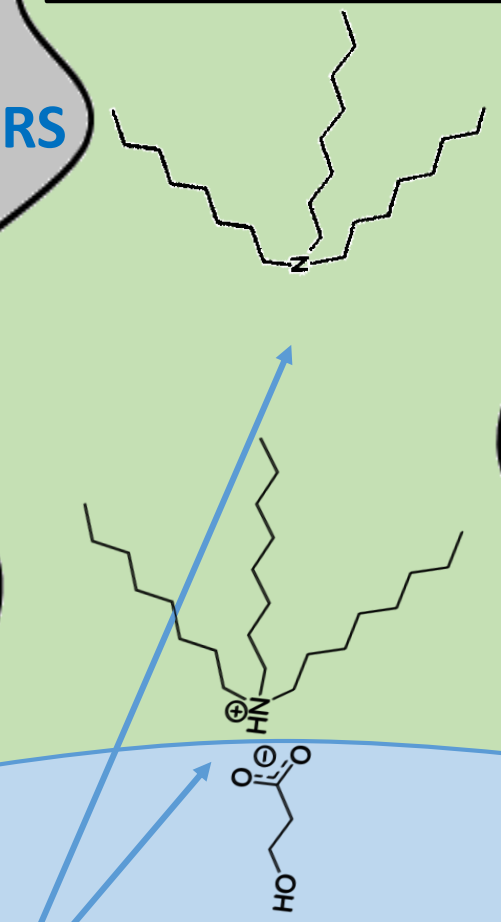


# MASS TRANSFER IN MEMBRANE CONTACTORS

Membrane pore filled with the organic phase

Hydrophobic membrane material

Aqueous phase



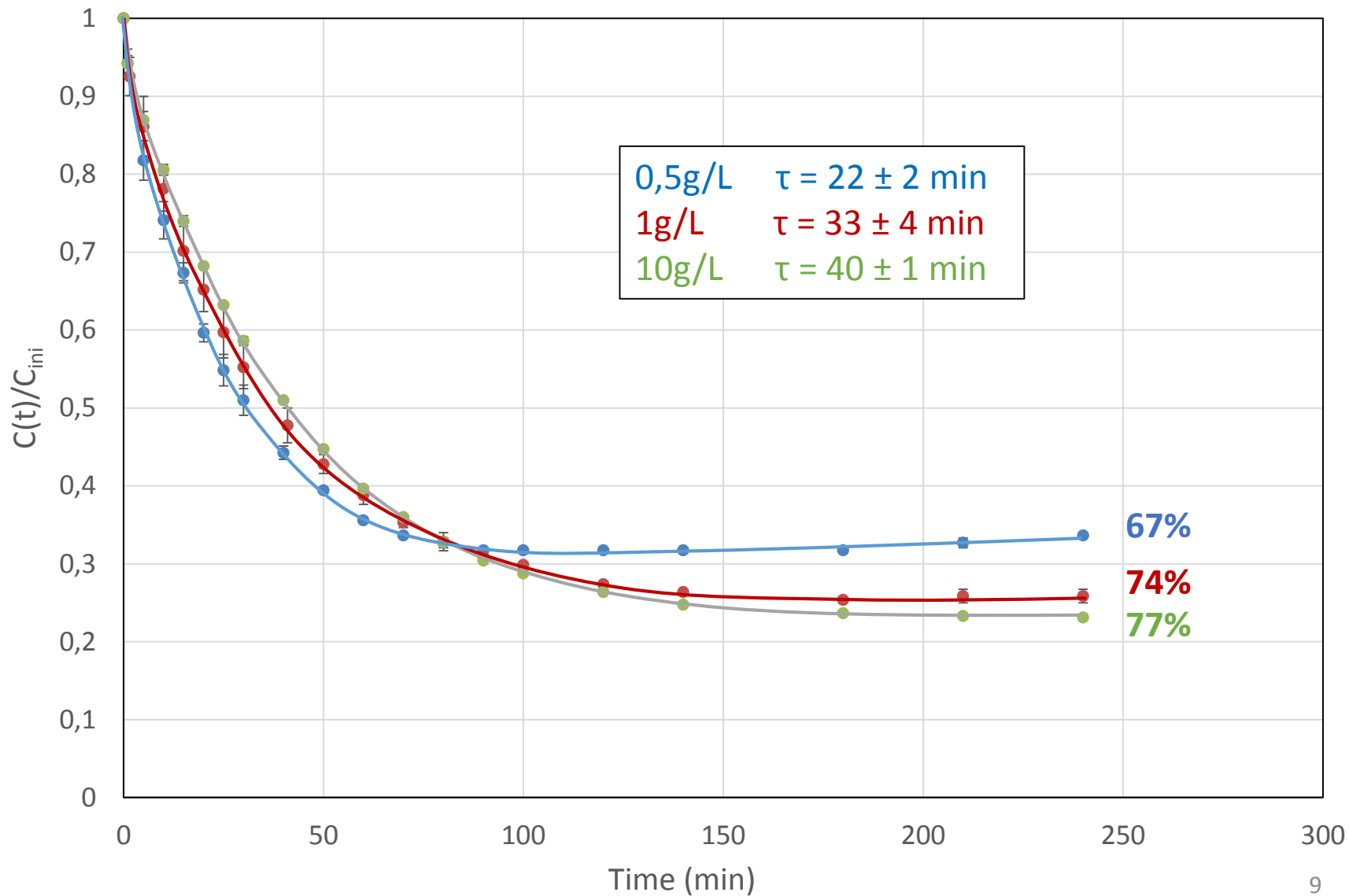
- Diffusion limiting step in membrane pores
- Major role of chemical reactions



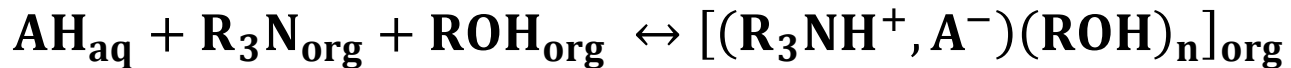


# INFLUENCE OF INITIAL CONCENTRATION

Yield over time for different initial concentrations of 3-HP

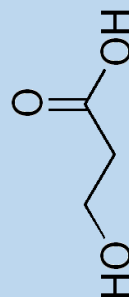
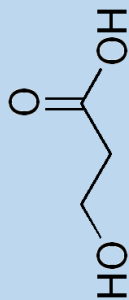
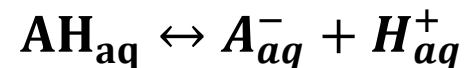
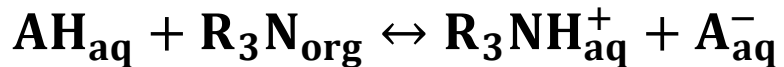


# ACTUALLY, NOT AS SIMPLE AS IT SEEMS...



Organic phase

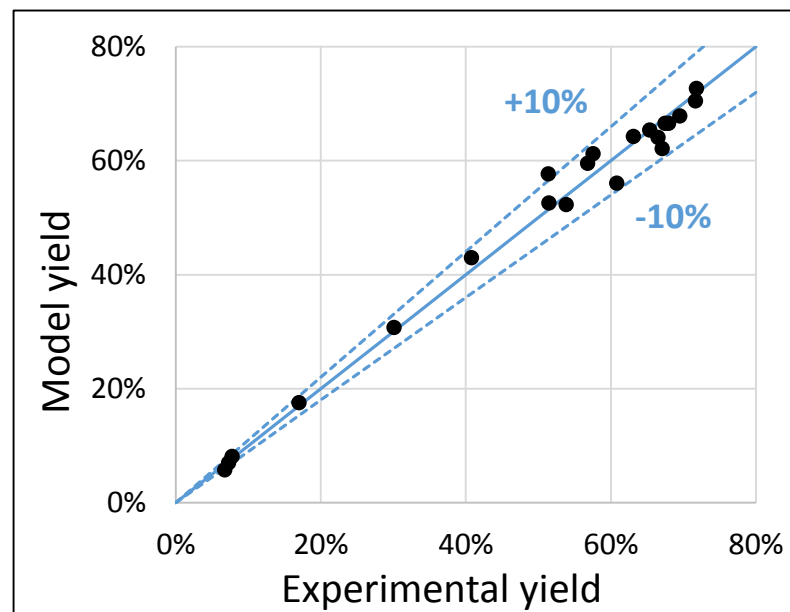
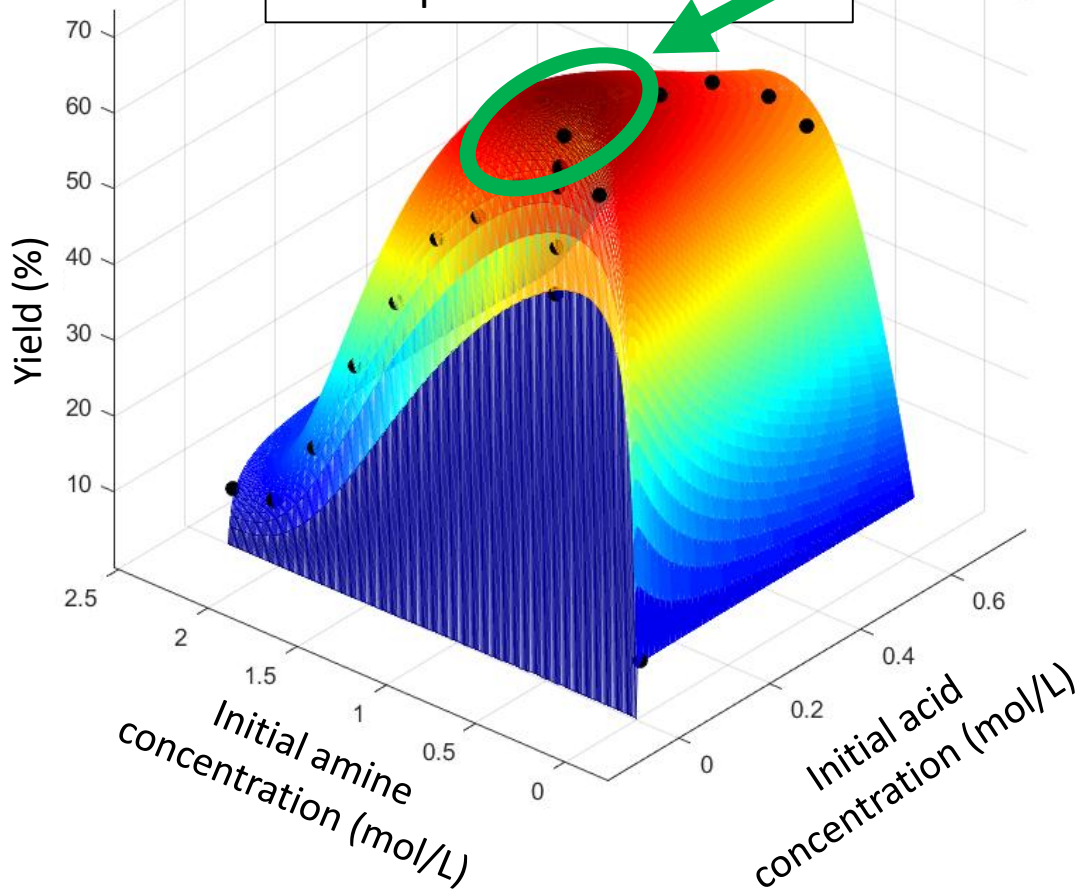
Aqueous phase



# EQUILIBRIUM MODELING

~ 20% amine / ~ 80% decanol (v/v)

Color surface: model results  
• : experimental results



$R^2 = 0,99$

Mean Absolute Percentage Error = 4%

Maximum error = 14% (low yield)

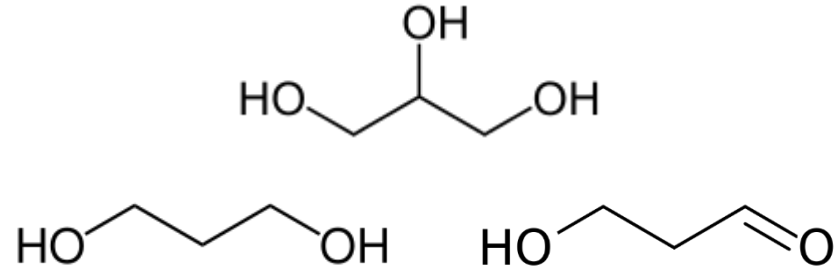
# WHAT ARE THE IMPACTS OF BIOCONVERSION MEDIA?

Until now: “binary” aqueous phase

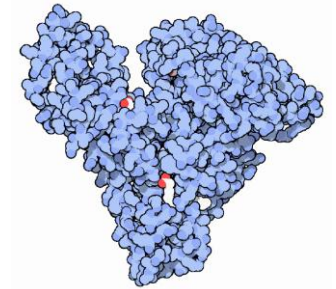
What about the bioconversion medium?



A complex medium

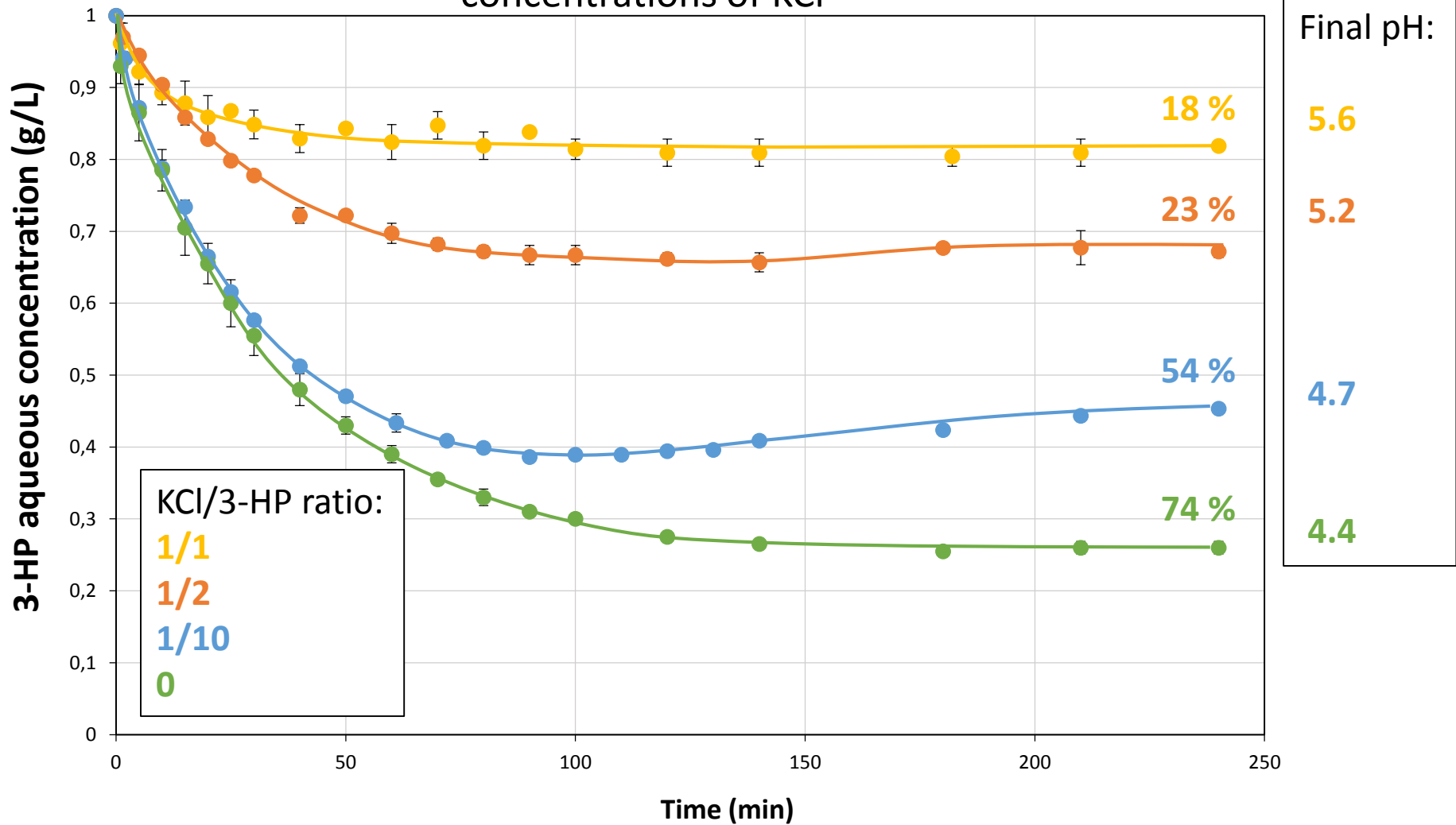


- Substrates
- Co-products
- Biomolecules
- Salts
- pH
- Cellular compounds
- ...



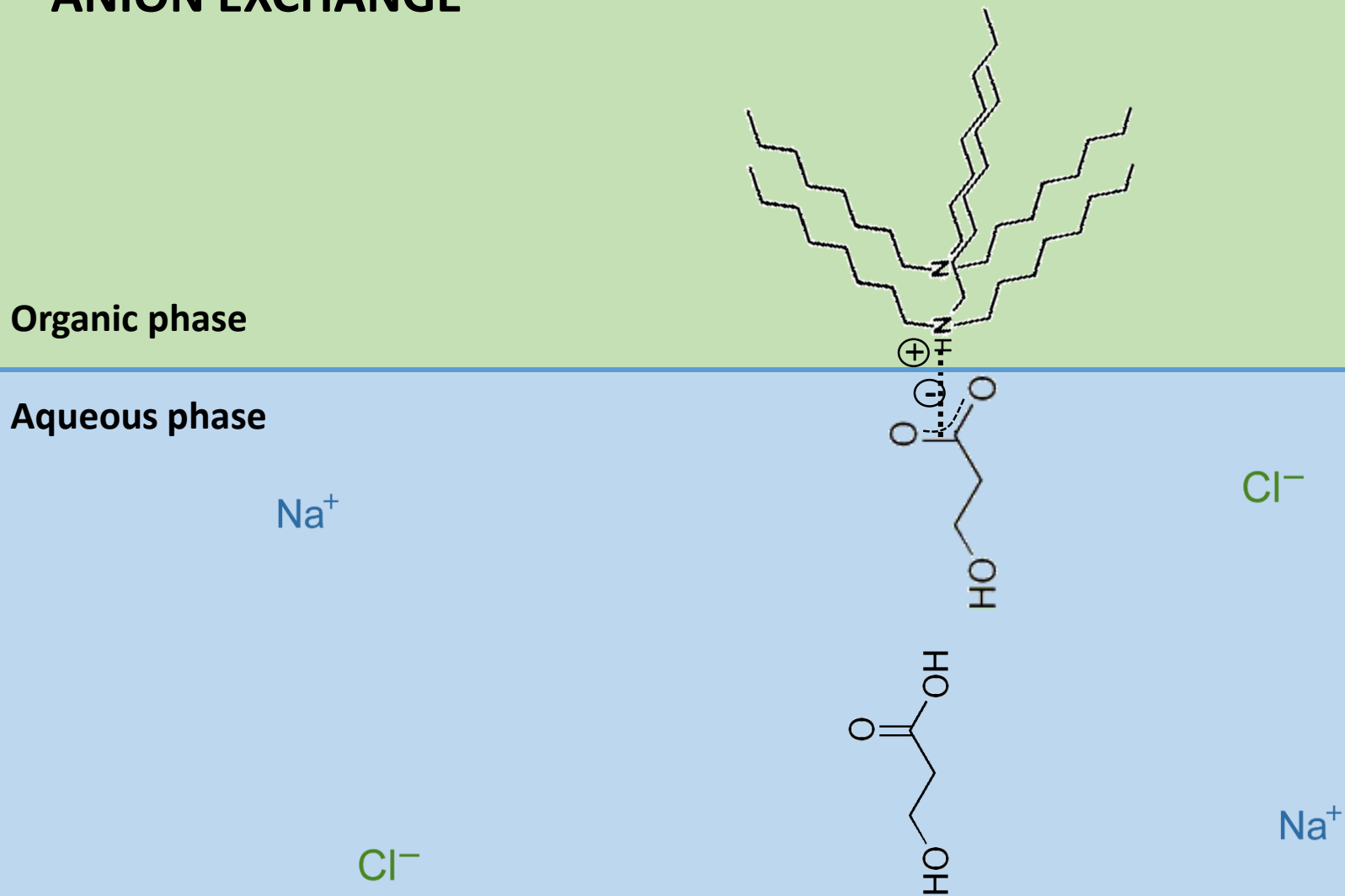
# WHAT ARE THE IMPACTS OF BIOCONVERSION MEDIA?

3-HP Concentration over time for different initial concentrations of KCl



# PRESENCE OF SALTS

## ANION EXCHANGE



# CONCLUSION

What are the mechanisms implied in this extraction process and can we easily predict the results?

- **Yields can be described thanks to a small set of chemical reactions**
- **Good prediction of process yields for a wide range of initial conditions**

Finally, does the complex bioconversion medium have an impact on extraction efficiency?

- **Real systems are complex (bioconversion broth)**
  - Strong influence of the anions present in the broth
  - High influence of pH (dissociated 3-HP is not extracted at all)
  - No influence of neutral organic compounds (substrates or metabolites)

Current and future work...

- **Valuable results to understand and predict kinetics in membrane contactor to finally be able to couple both processes successfully**



**THANK YOU FOR YOUR ATTENTION**

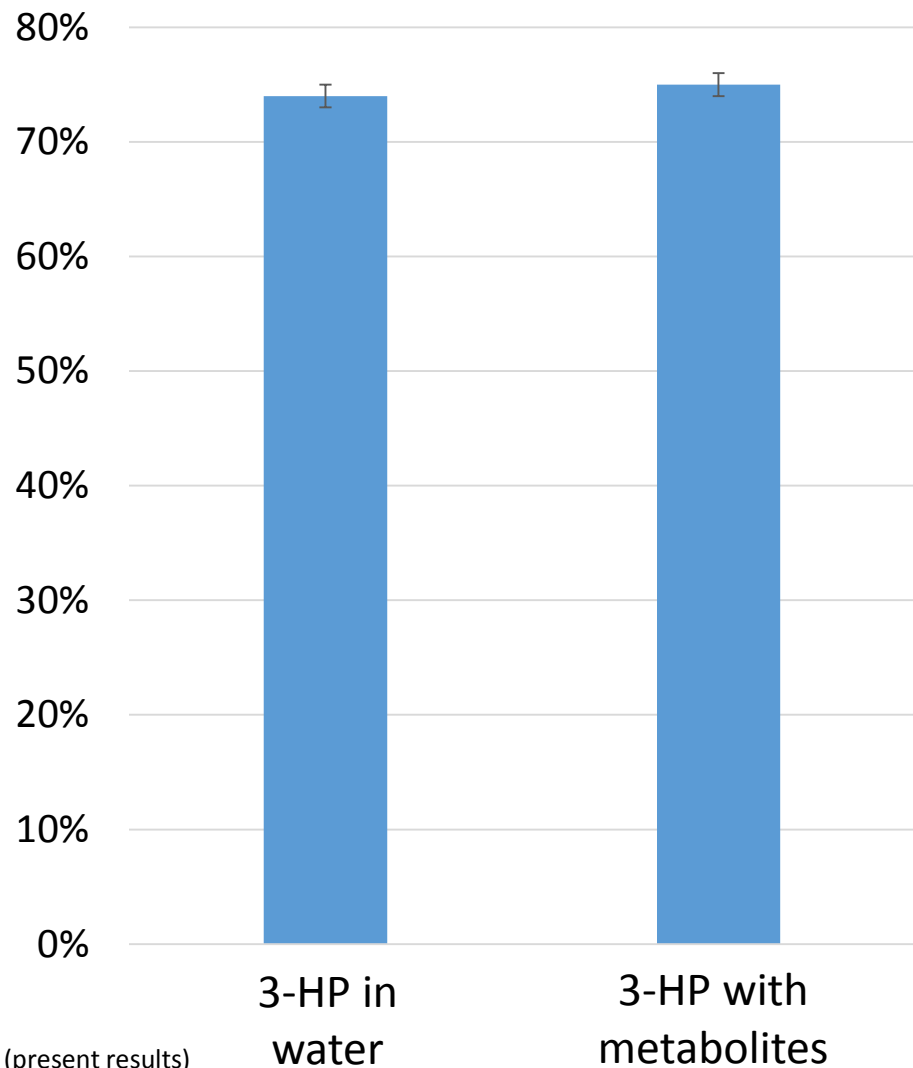


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# EXAMPLE OF A SALT-FREE BIOCONVERSION

Extraction yield without and with metabolites



The case of glycerol bioconversion with *Lactobacillus reuteri*

Substrate and metabolites:

- Glycerol OCC(O)CO
- 3-hydroxypropionaldehyde OCC(O)C=O
- 1,3-propanediol OCC(O)CO

→ No influence on the yield and very high selectivity for 3-HP