Enzymatic conversion of mannosylerythritol lipids in natural deep eutectic solvents

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BioGEM
Bio-Chemical Green Engineering & Materials
University of Antwerp

EUBCE 2019
27th European Biomass Conference & Exhibition
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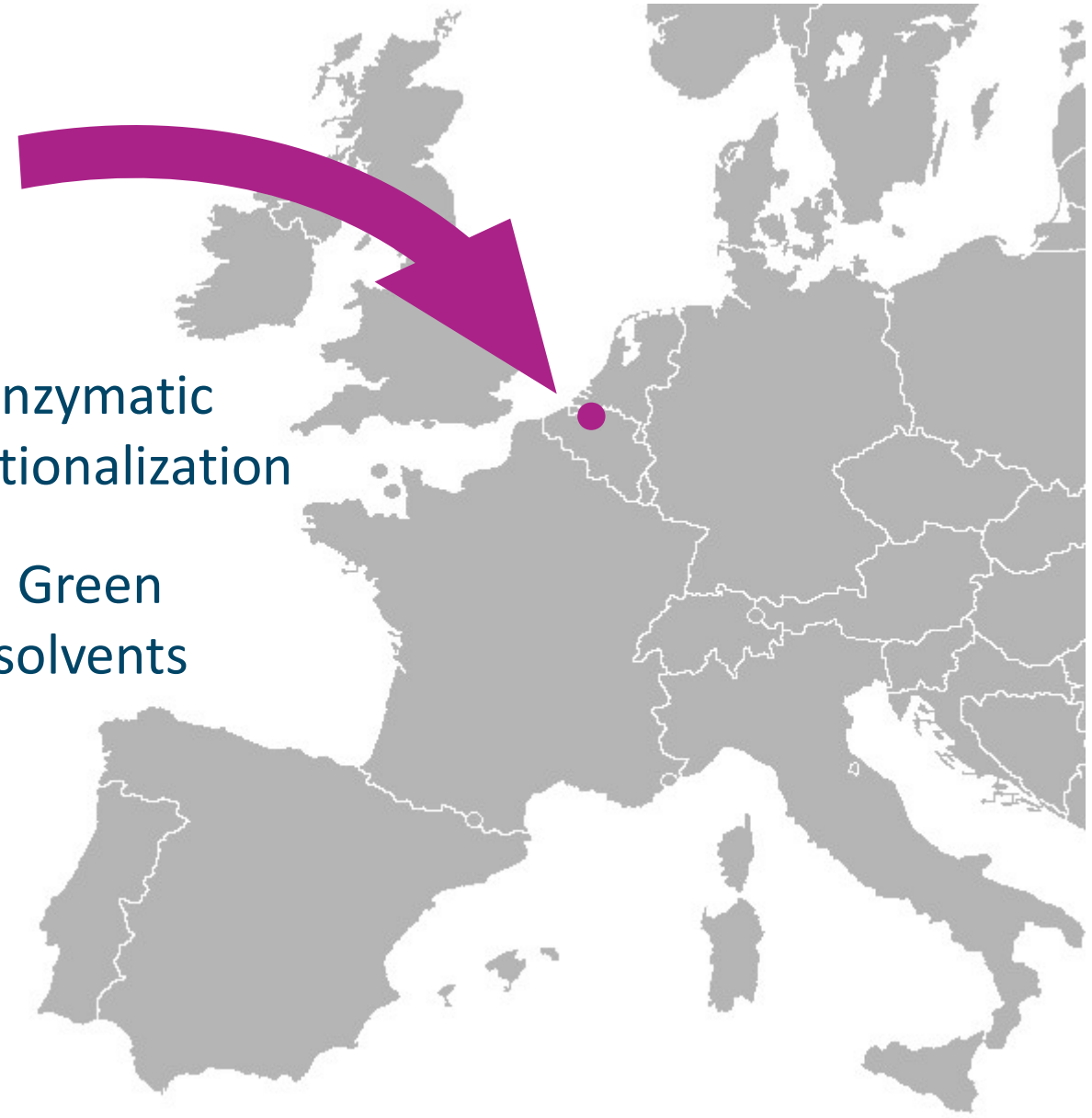
BioGEM group

Industrial biotechnology → Enzymatic functionalization

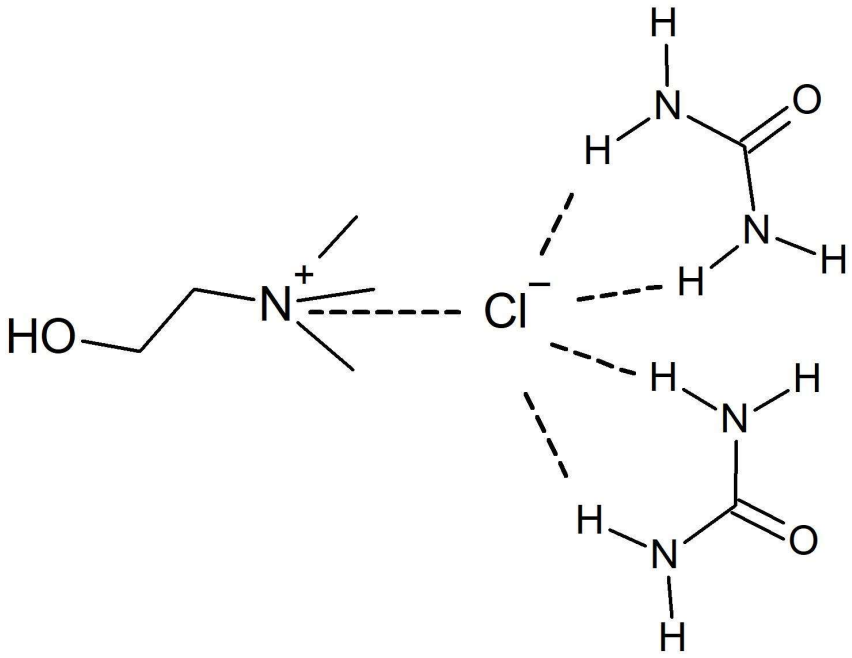
Green materials → Green solvents

Industrial wastewater treatment



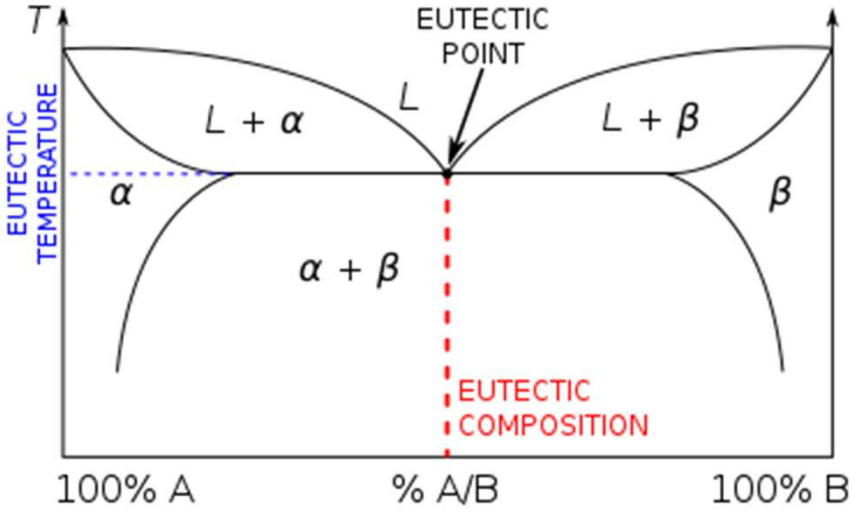
Natural deep eutectic solvents

Interactions in NADES



1 Choline chloride 2 Urea

Decreased melting point



Natural deep eutectic solvents

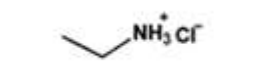
Composition of NADES

- Quaternary ammonium salts
- Organic acids
- Amino acids
- Sugars

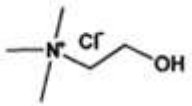
Advantages

- Low volatility
- Non-flammable
- Low toxicity
- Biodegradable
- Low price

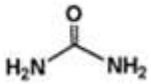
Common components in NADES:



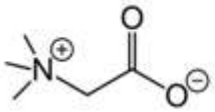
Ethylammonium chloride



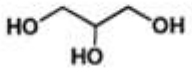
Choline chloride



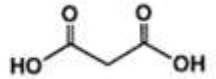
Urea



Betaine



Glycerol



Malonic acid

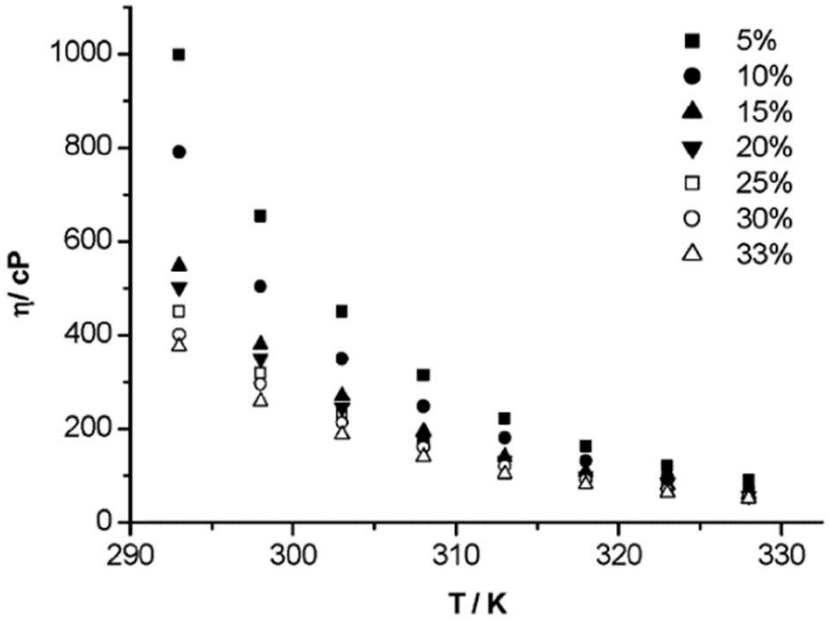
NADES as designer solvent

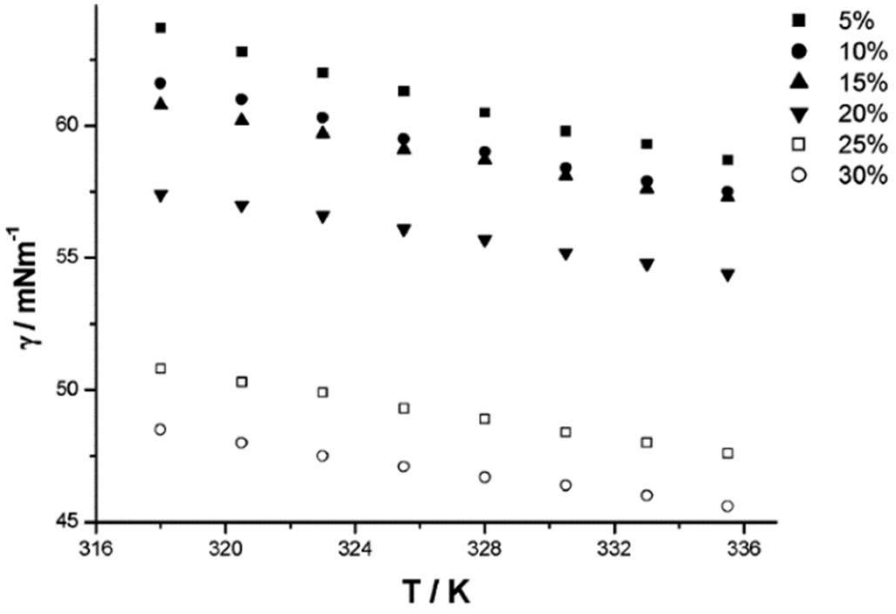
Properties are tailorable

Composition

Constituents

Changes in viscosity and surface tension of choline chloride-glycerol NADES by altering composition



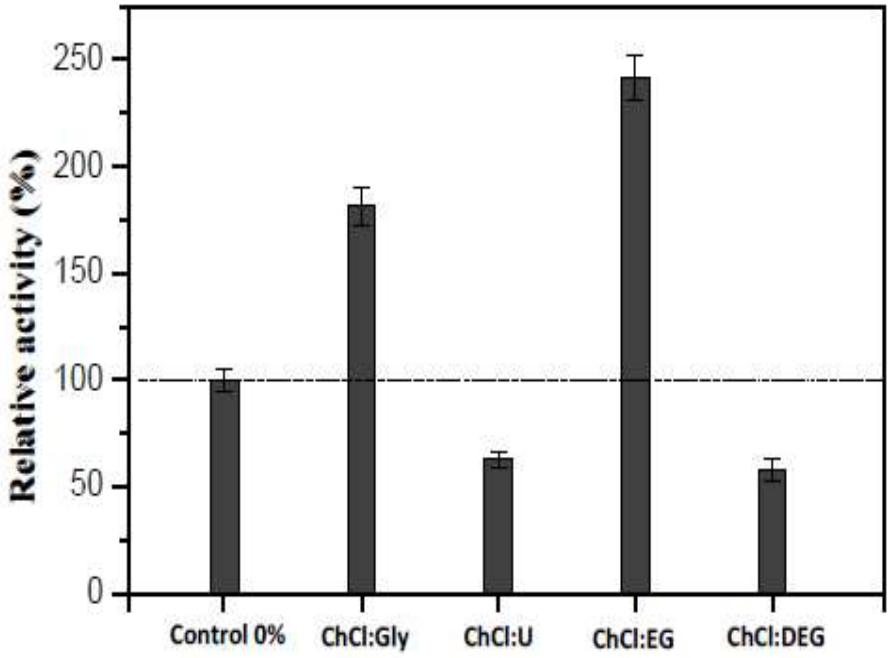


Abbott *et al.*, 2011.

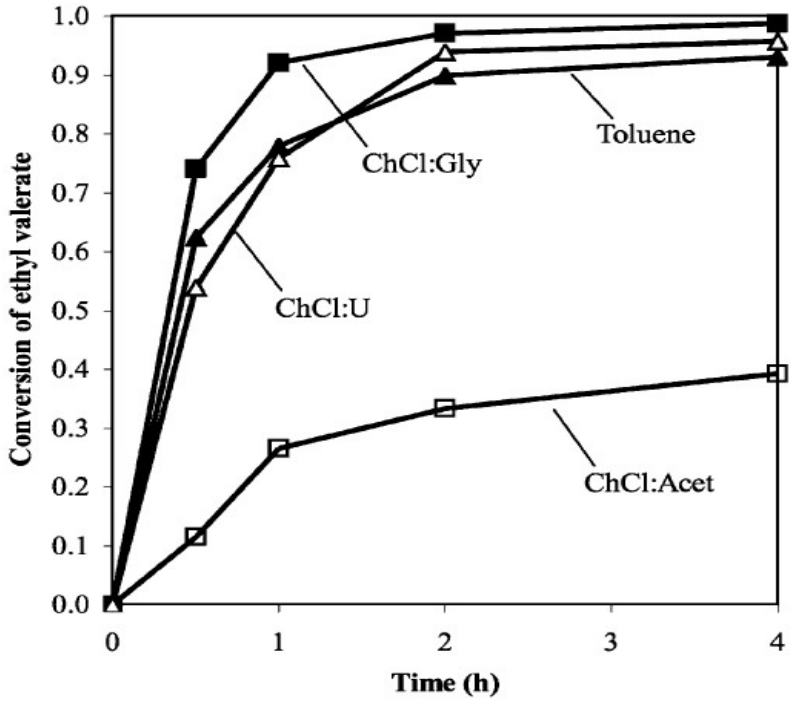
NADES in biocatalytic reactions

The applied NADES determines the reaction parameters

Changes in initial activity and conversion rate in lipase catalyzed reactions in different NADES

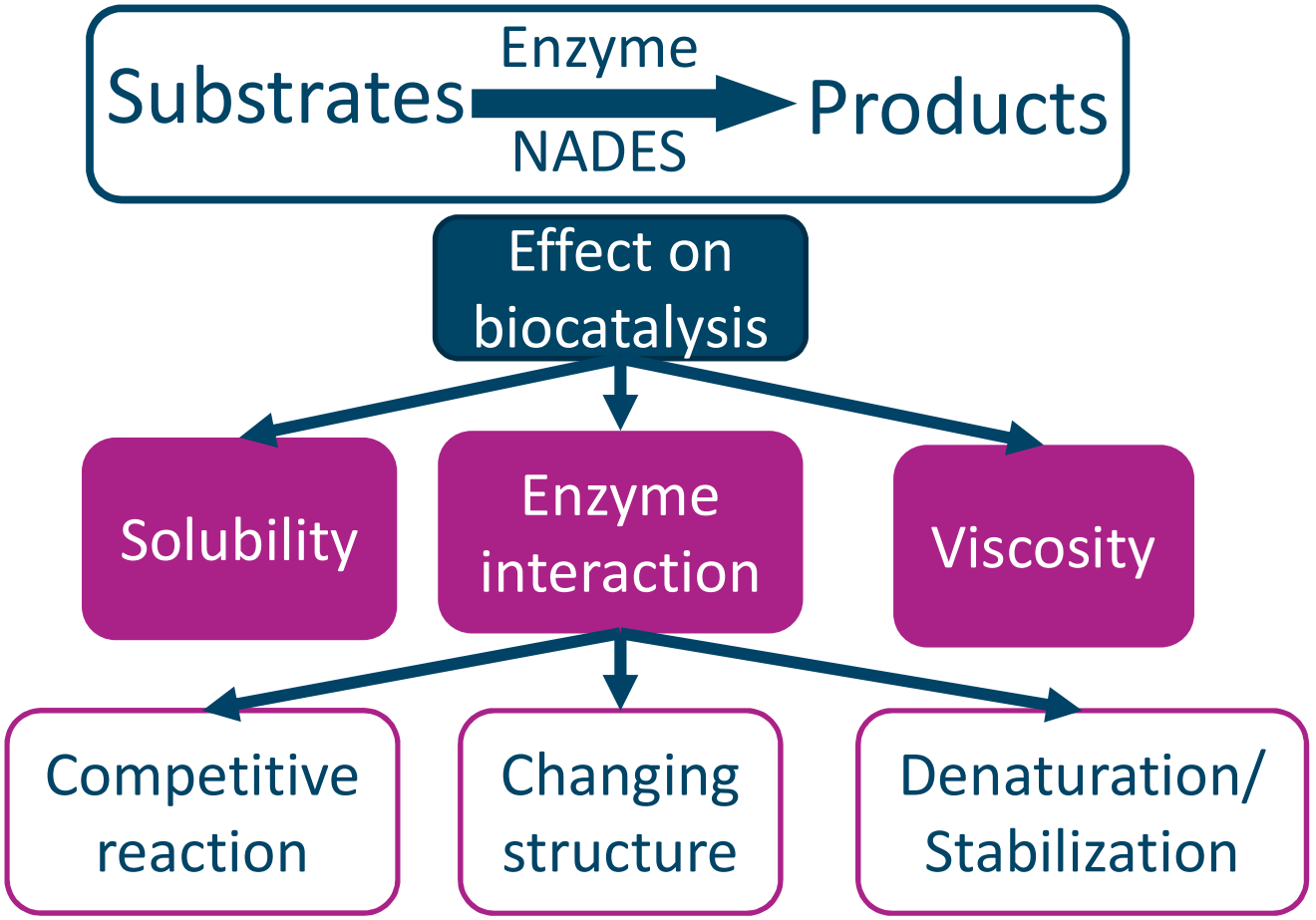


Juneidi *et al.*, 2017.



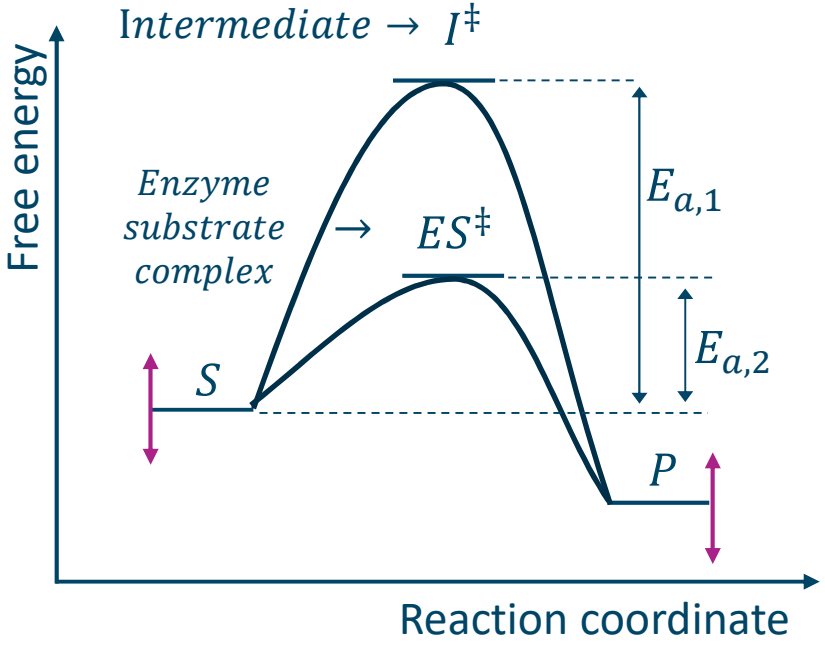
Gorke *et al.*, 2008.

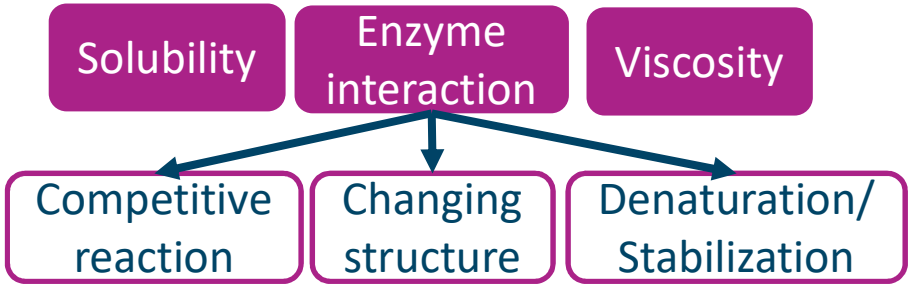
NADES in biocatalytic reactions



NADES in biocatalytic reactions

Effect of solvation energy





Michaelis-Menten kinetics

$$v_0 = k_{cat}[E_0]\frac{[S]}{K_M + [S]}$$

$$k_{cat} = Ae^{-E_a/RT}$$

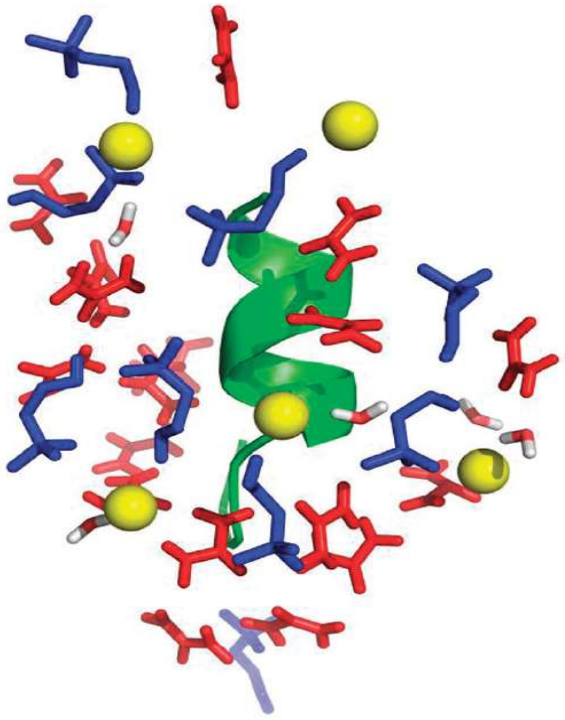
Assumed effect of NADES

Kinetic parameter:	Affected by:
K_M	Solvation
$[E_0]$	Enzyme inactivation
k_{cat}	Mass transfer limitation
E_a	Solvation/Conformation change of the enzyme

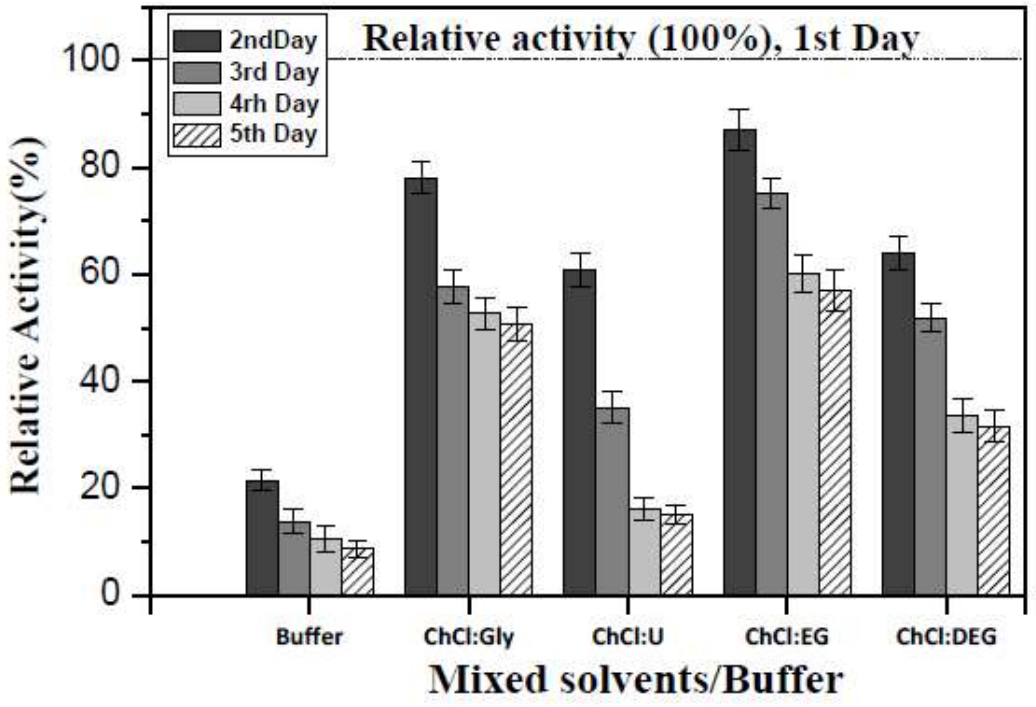
NADES in biocatalytic reactions

NADES could stabilize the enzyme structure

Hydrogen bonding network: prevents denaturation and promotes stabilization



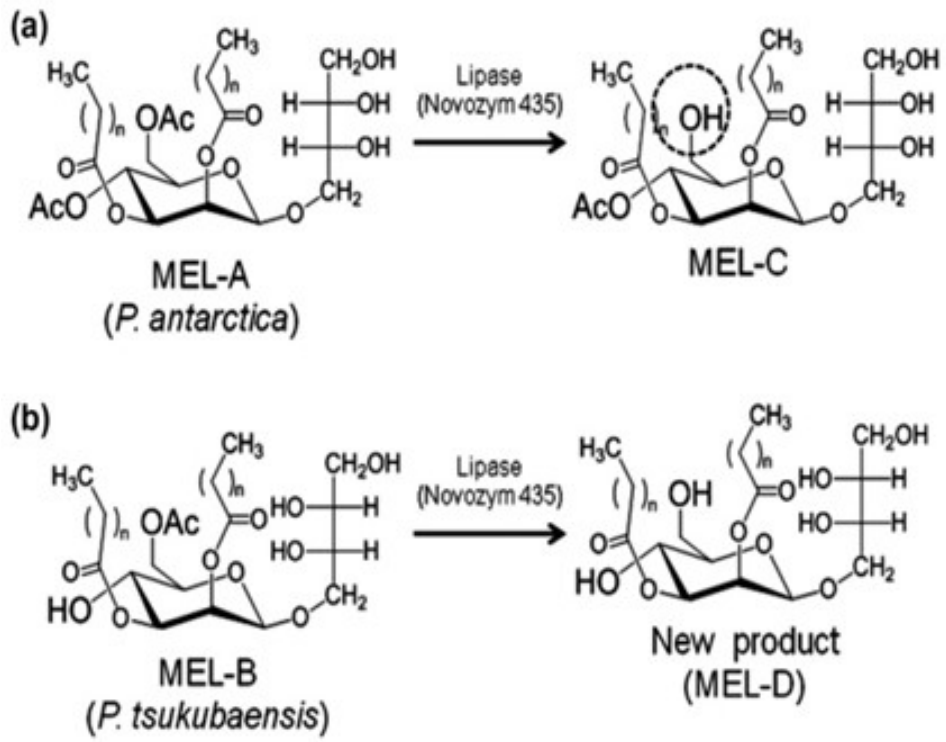
Monhemi *et al.*, 2014.



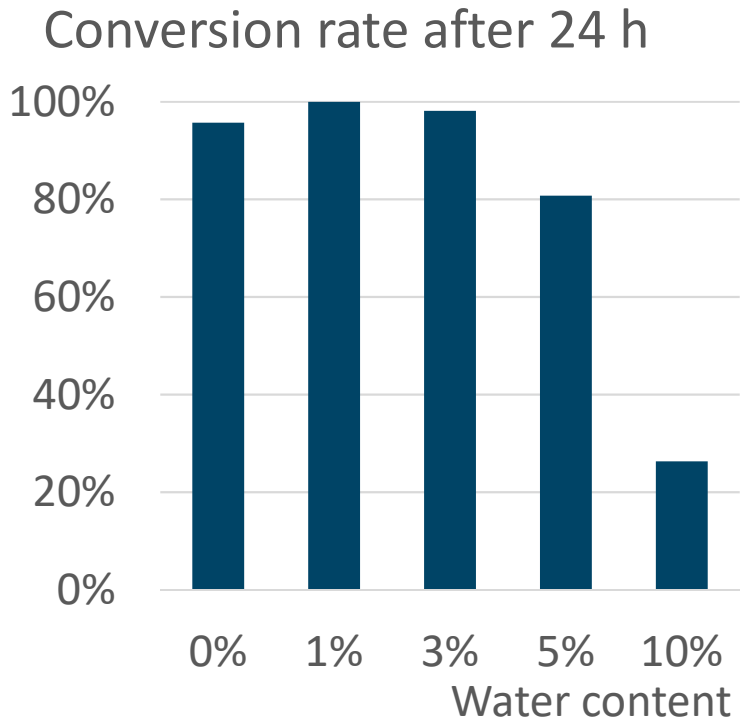
Juneidi *et al.*, 2017.

Mannosylerythritol lipids

Enzymatic deacetylation of MELs



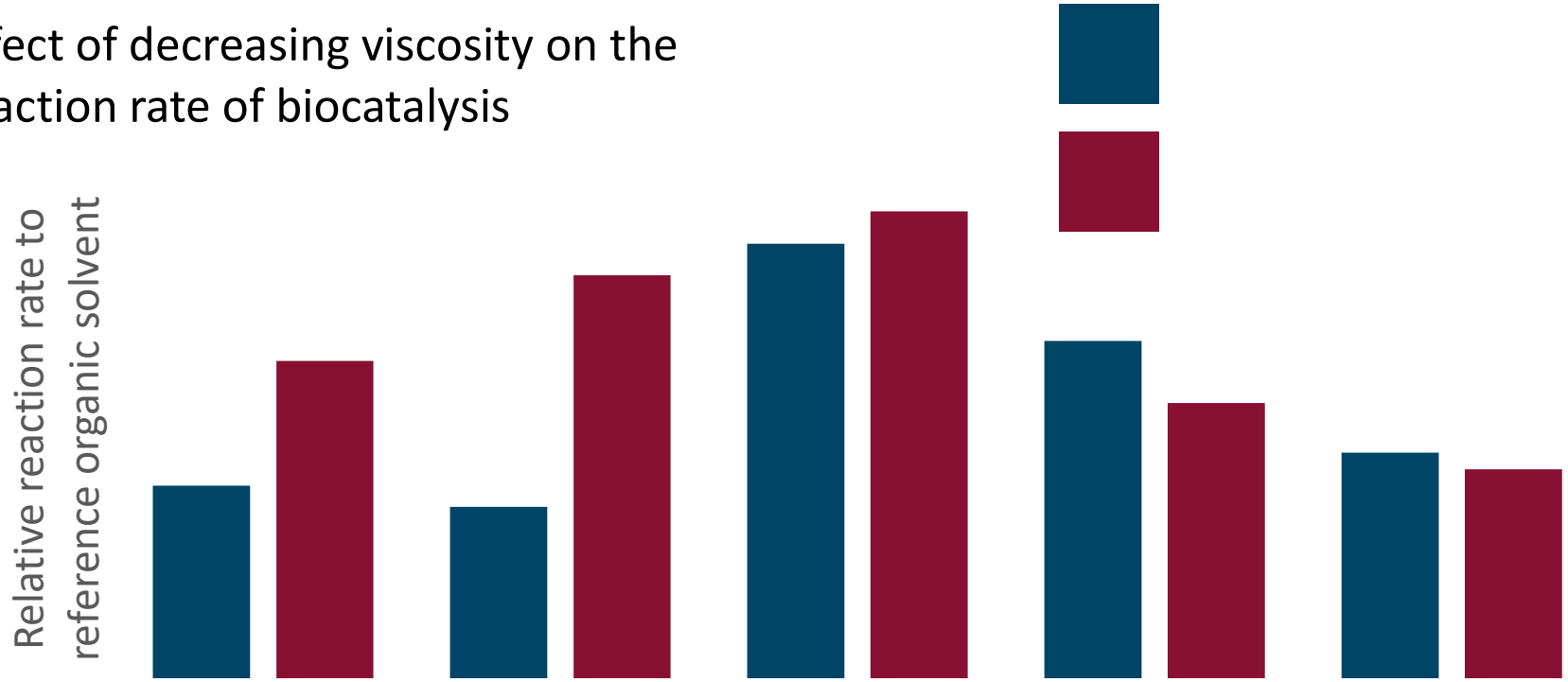
Water: negative effect on reaction



Goosens and Levi, 2016

Effect of viscosity

Effect of decreasing viscosity on the reaction rate of biocatalysis



Source of data: Gorke *et al.*, 2008.
Durand *et al.*, 2013.
Kleiner and Schörken, 2015.
Zhao *et al.*, 2011.

Effect of solubility

Modelling solubility: no proper model

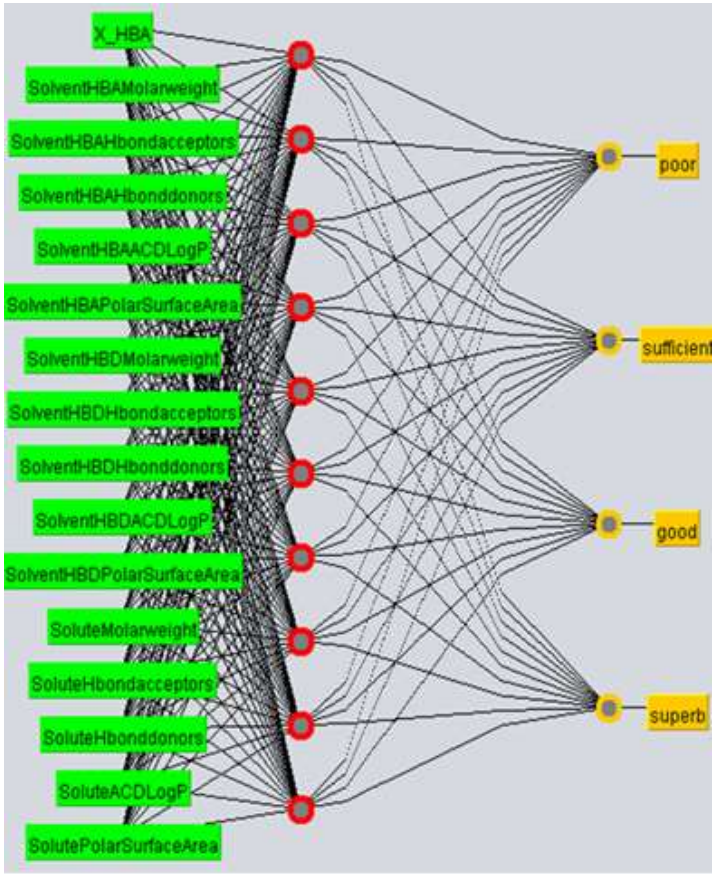
Hansen solubility parameters?
COSMO-RS?

Own model: Artifical neural network

Classification model
Input: molecular properties of NADES constituents
Output: solubility classes

Solubility [g/g]	Classes
<0.002	Poor
0.002-0.1	Sufficient
0.1-0.5	Good
0.5<	Superb

	Baseline of prediction	Artificial neural network
Total Number of Instances	62	
Correctly Classified Instances	27	53
Percentage of Correct Classification	44%	85%

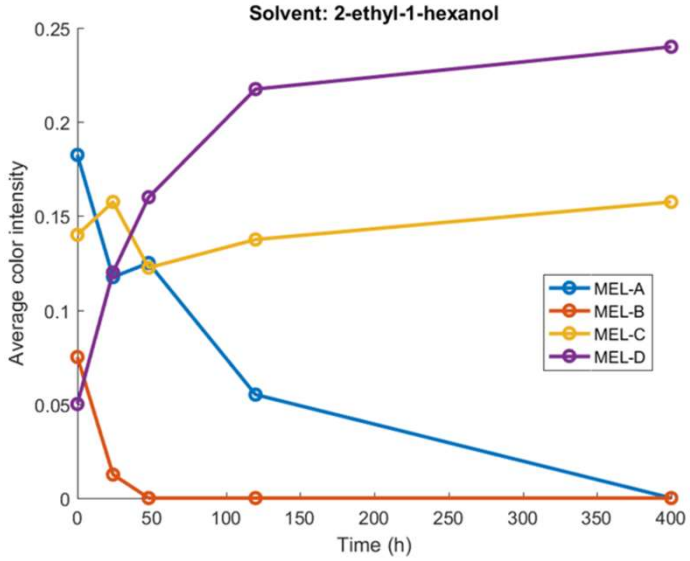


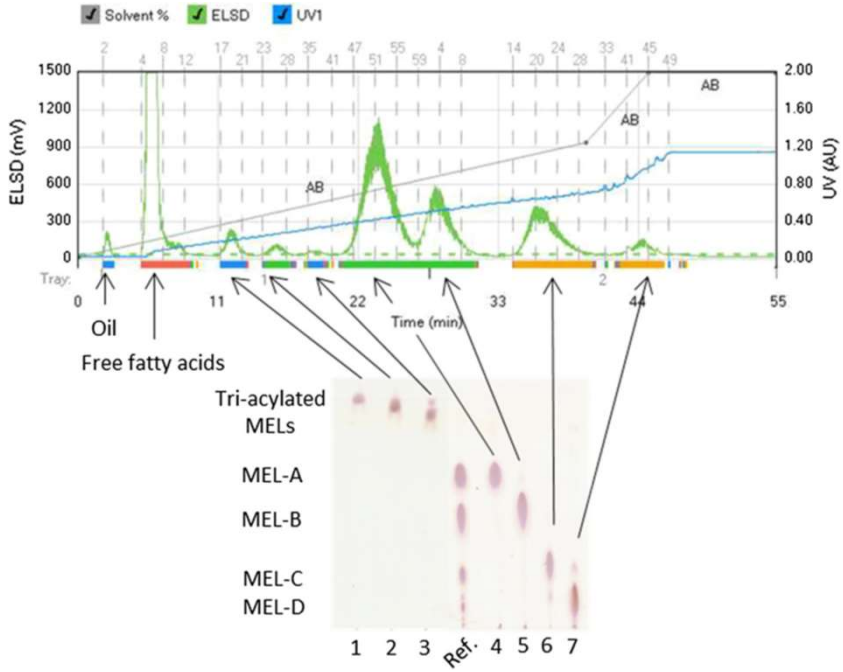
NADES effect on biocatalysis

Case study: deacetylation of MELs

Reaction in organic solvents ✓ ⇨ Reaction in NADES ✓ ⇨ Determination of reaction kinetics !!!

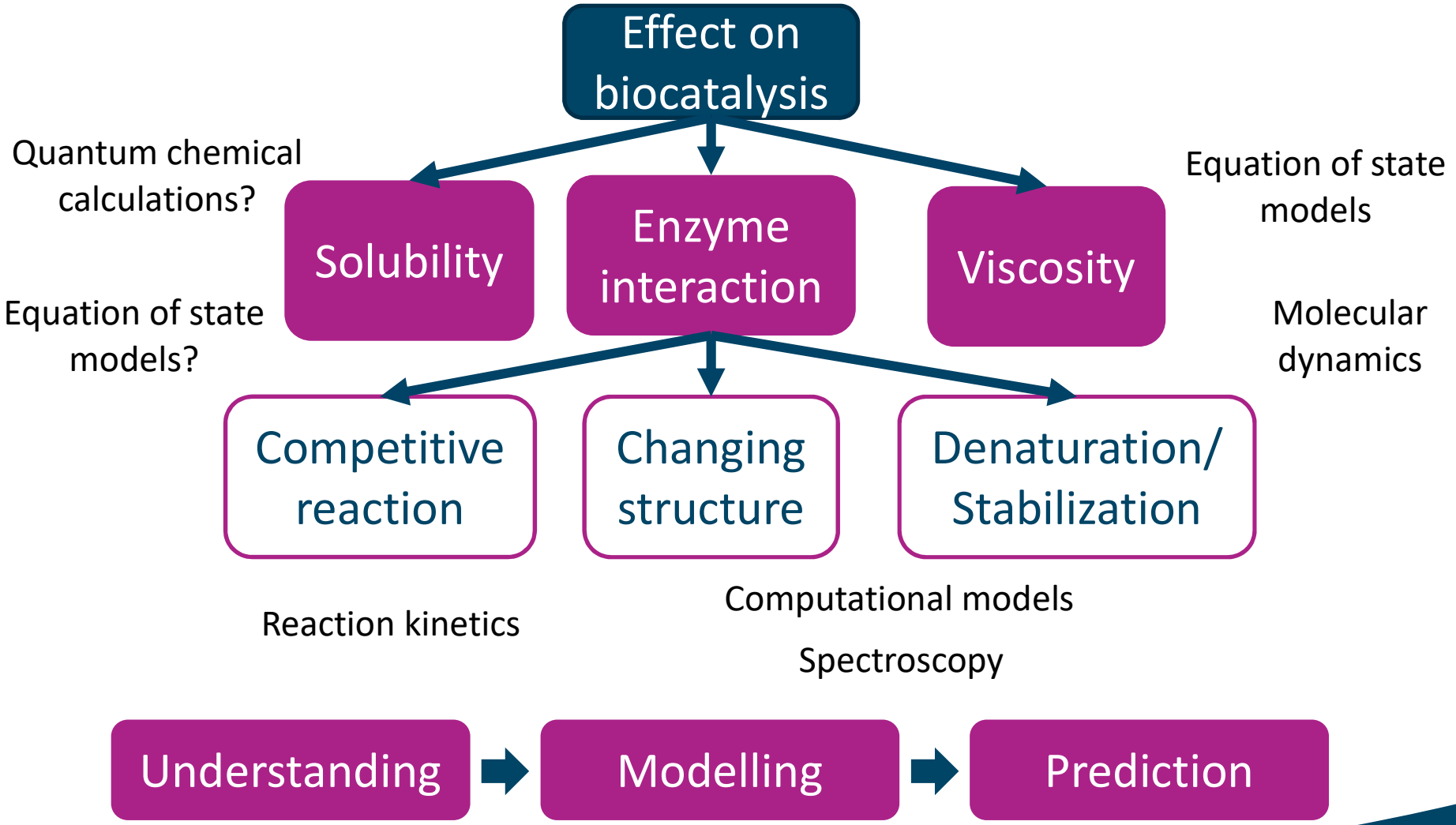
Deacetylation of MELs in common organic solvent





Goossens *et al.*, 2016.

Modelling NADES effect: How to?



Further investigation

Identify and quantify these effects

$$v_0 = k_{cat}[E_0]\frac{[S]}{K_M + [S]} \qquad k_{cat}=Ae^{-E_a/RT}$$

	Affected by:
K_M	Solvation
$[E_0]$	Enzyme inactivation
k_{cat}	Mass transfer limitation
E_a	Solvation/Conformation change of the enzyme

Determination of kinetic parameters

Calculation of activation energy

Computational chemistry

Articles in preparation – Fall 2019:

Review article on NADES modelling

Kinetic parameters of MELs deacetylation

Take home message

- NADES as reaction media for MELs deacetylation is proven
- Determination of kinetic parameters is essential to determine NADES effect on reaction
- Modelling solubility is feasible, but quantiative model is not yet available
- Preliminary results are promising, but large amount of additional data is needed

Thank you for your attention!

Further information:

Attila Kovács
Research Gate

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Vlaanderen
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