XXIX ENCONTRO LUSO-GALEGO DE QUÍMICA
10-12 NOV '25 FÓRUM BRAGA PORTUGAL

ILIMITED

IONIC LIQUID SORBENT-ENHANCED CO_2 CONVERSION

COSMO + AI for screening of solvents. Case study of Methanol synthesis

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Funded by the European Union

Funded by the European Union's Horizon Europe Research and Innovation Actions programme under grant agreement No. 101192964

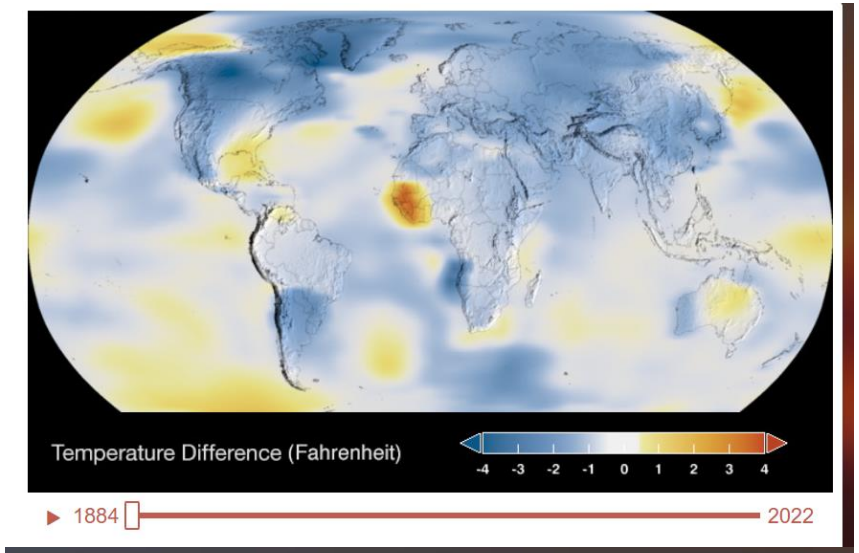
Project funded by

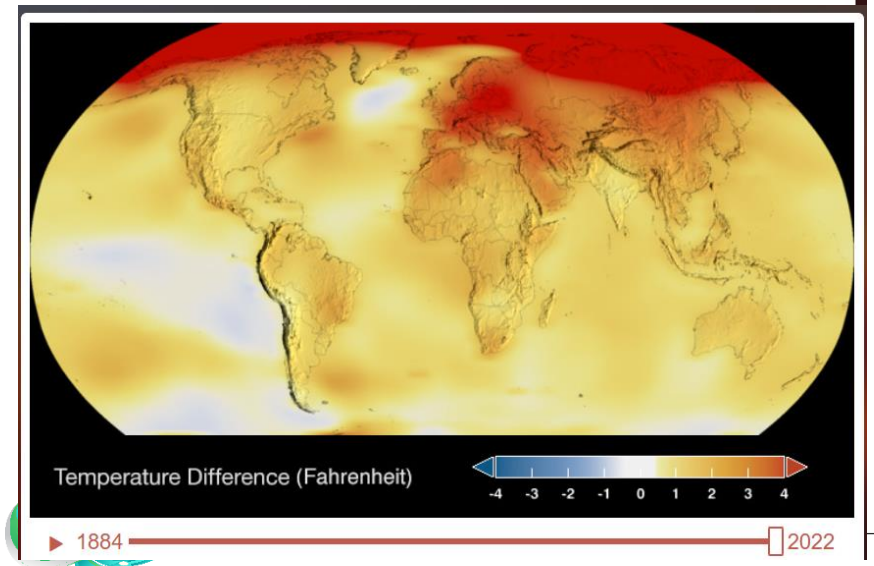
Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

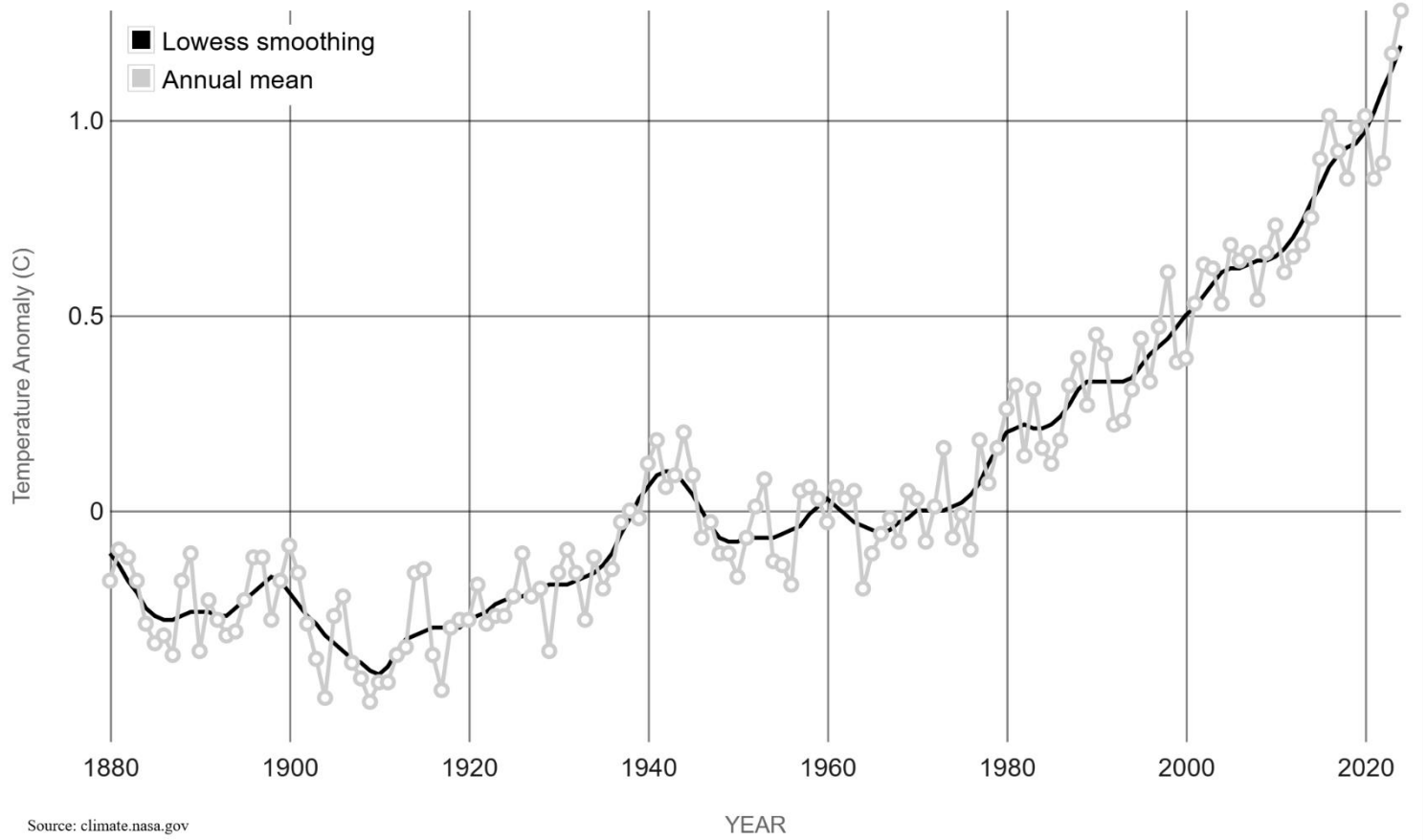
Swiss Confederation

Federal Department of Economic Affairs, Education and Research EAER
State Secretariat for Education, Research and Innovation SERI

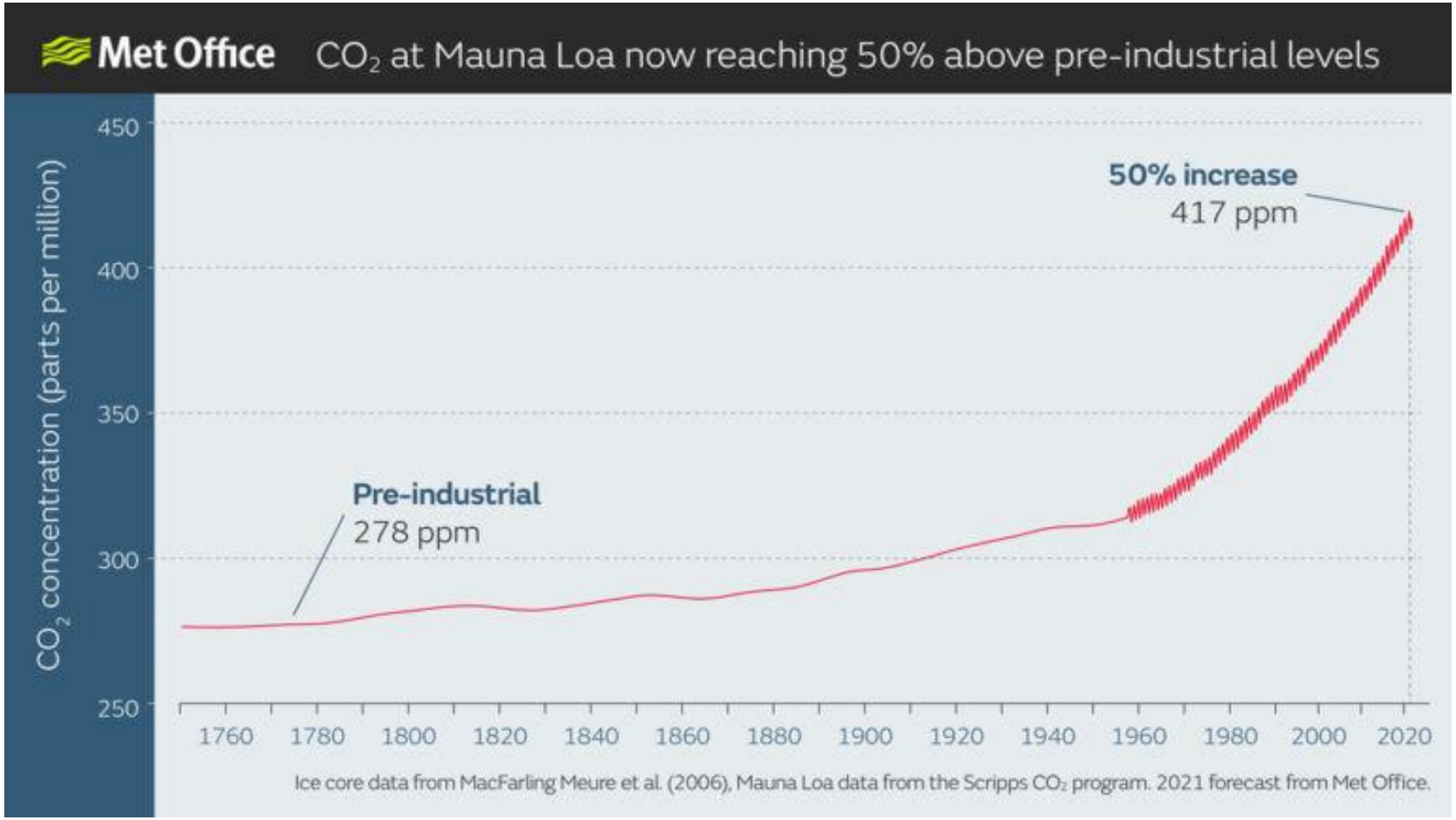
Global warming over 50y



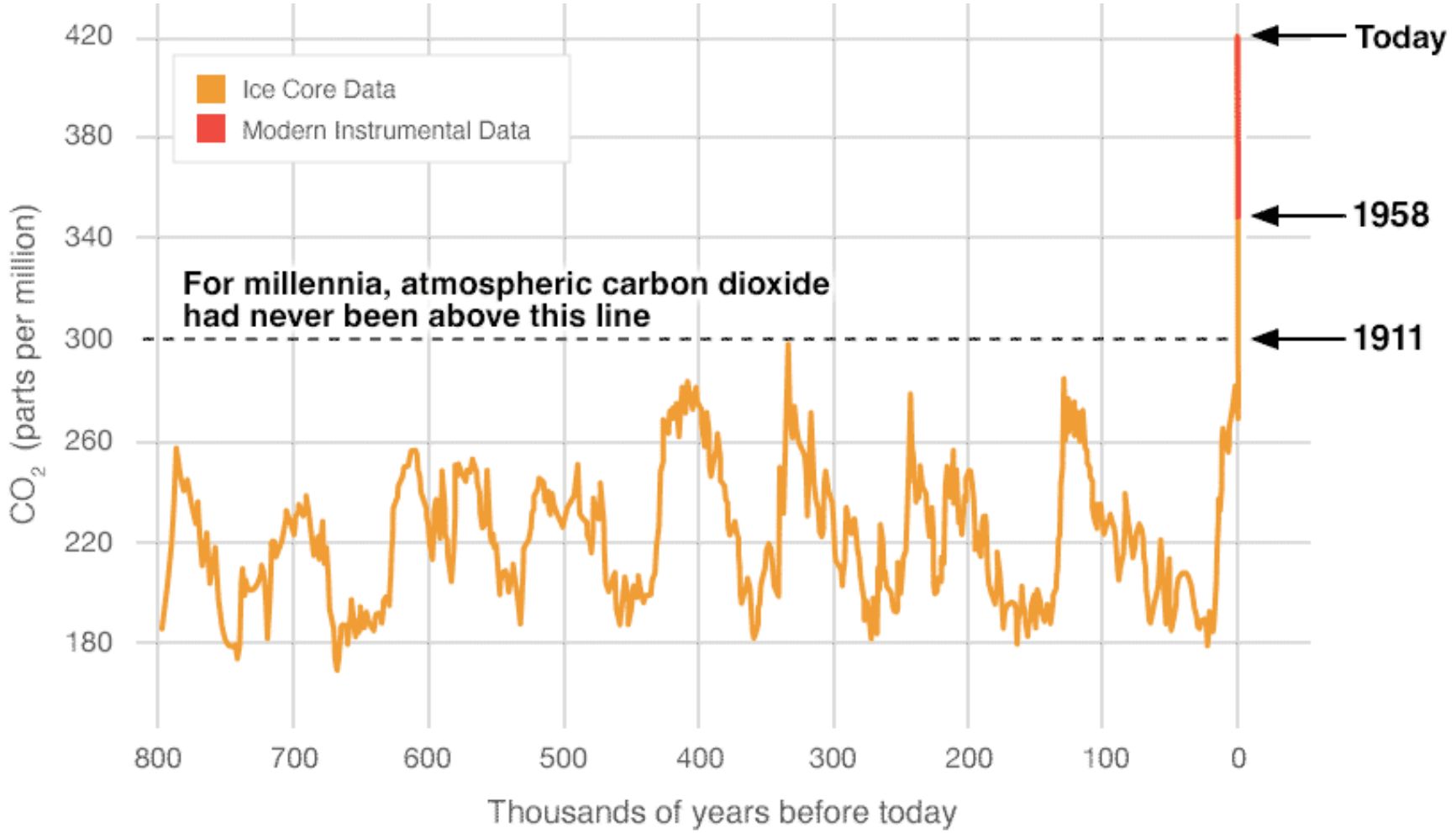




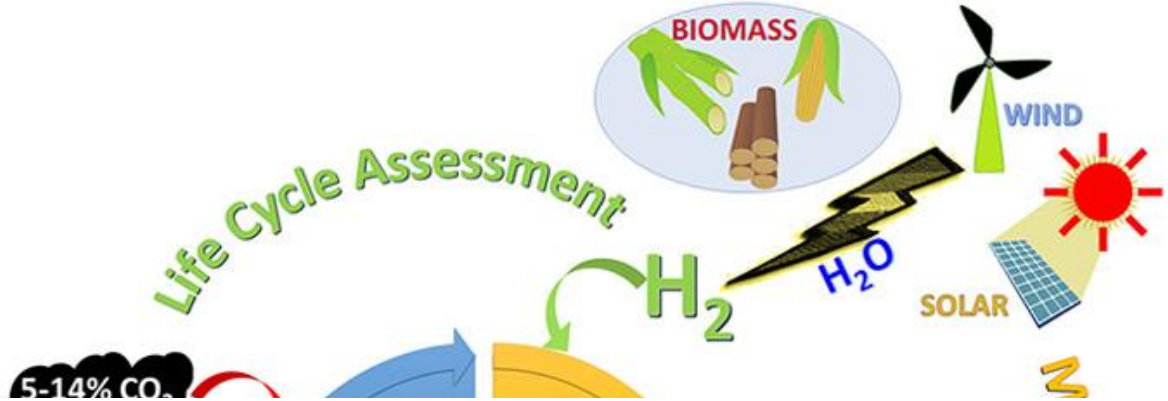
CO2 concentration in the atmosphere



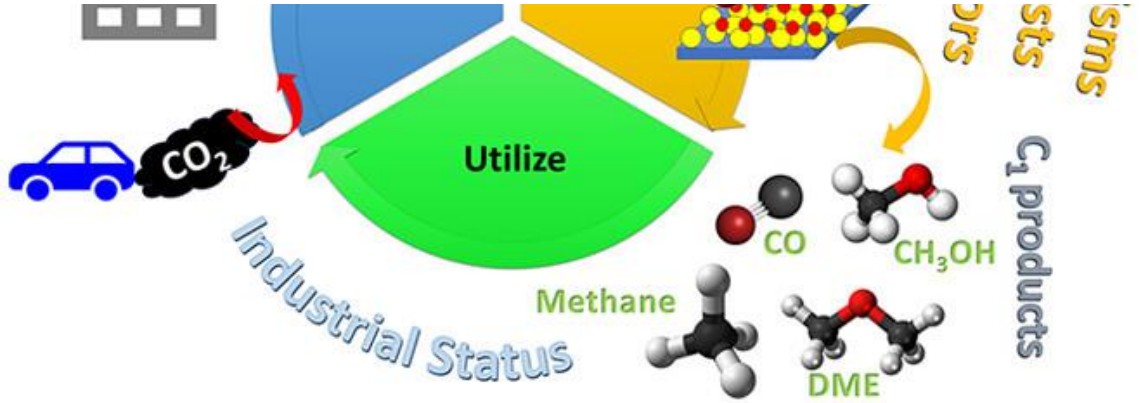
CO2 concentration in the atmosphere



CO_2 conversion life cycle



How can we do it sustainable and affordable?



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ACS Energy LETTERS

Cite This: *ACS Energy Lett.* 2018, 3, 1938−1966

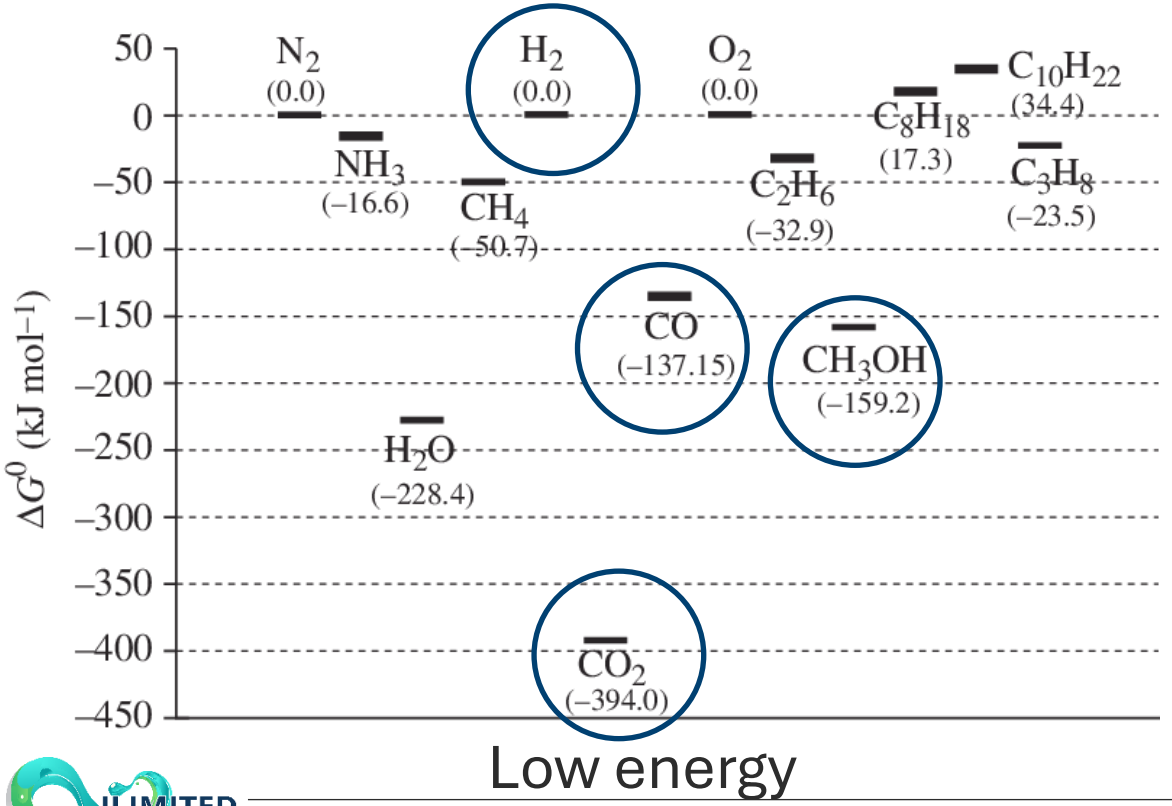
Thermochemical CO_2 Hydrogenation to Single Carbon Products: Scientific and Technological Challenges

Soumyabrata Roy[#] Arjun Cherevotan[#] and Sebastian C. Peter[*]

CO_2 conversion

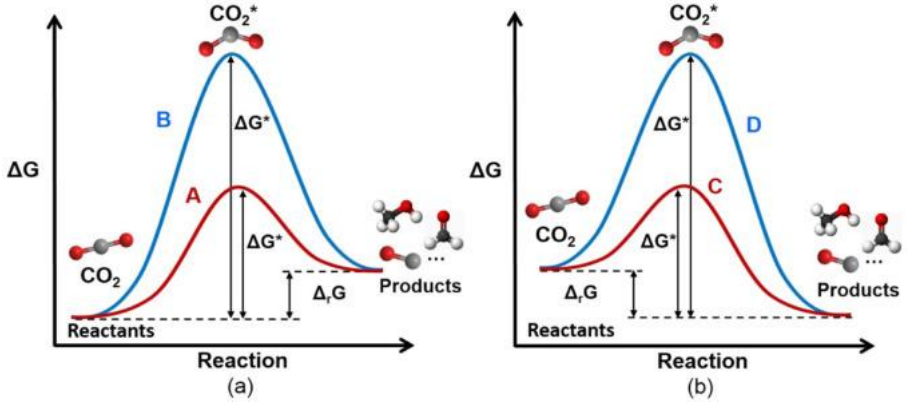
Thermodynamic problem

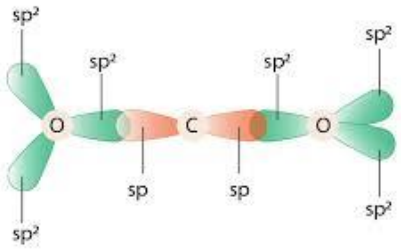
High energy

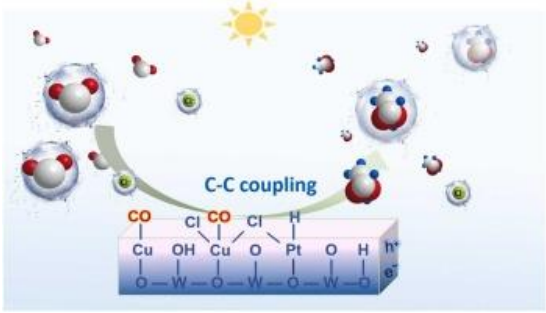


Low energy

Kinetic problem





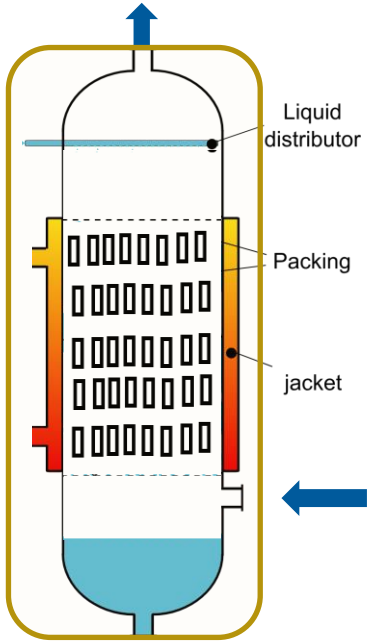


Illimited Project – EIC

$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$

~18.2 %/pass

$CH_3OH + H_2O$ + unreacted gas



Operational temperature
200°C

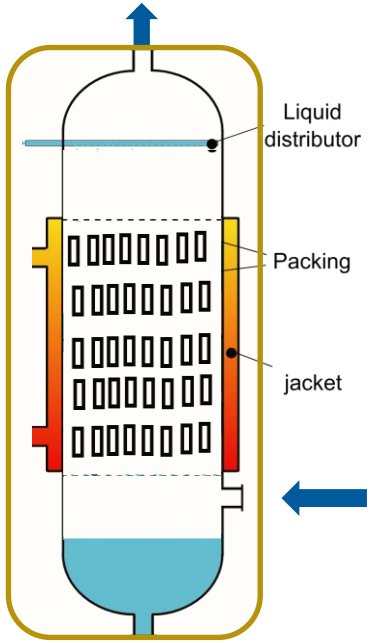
$CO_2 + 3H_2$

Liquid+ **CH_3OH & H_2O**

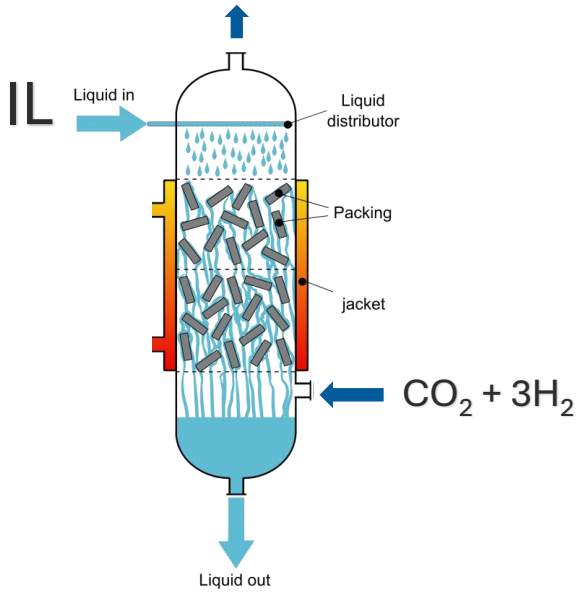
Illimited Project – EIC

Thermodynamic shift

$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$

~~~18.2 %/pass~~~

~80%/pass

$CH_3OH + H_2O$ + unreacted gas



Operational temperature
200°C

$CO_2 + 3H_2$

Liquid+ **CH_3OH & H_2O**
~~~

Objective



Goal: To screen for a stable liquid solvent able to capture methanol and water at 200°C

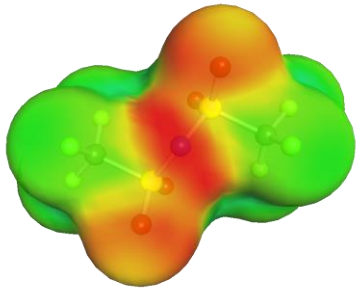
Metrics:

- Thermal stability (**Td**) above **500K**
- Melting temperature (Tm) above **298 K**
- Viscosity (**μ**) below **1000 mPa.s**
- MeOH & H_2O **solubility/selectivity** (γ^{∞}_{MeOH} **&** $\gamma^{\infty}_{H_2O}$)

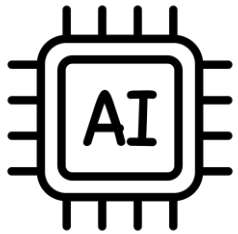
Goal

Ionic Liquids

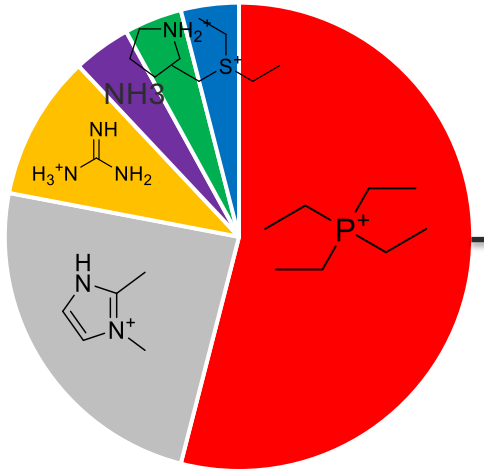
- Td > 513 K
- Tm > 298 K
- η_{298k}<1000 mPa.s
- MeOH & H_2O sol.



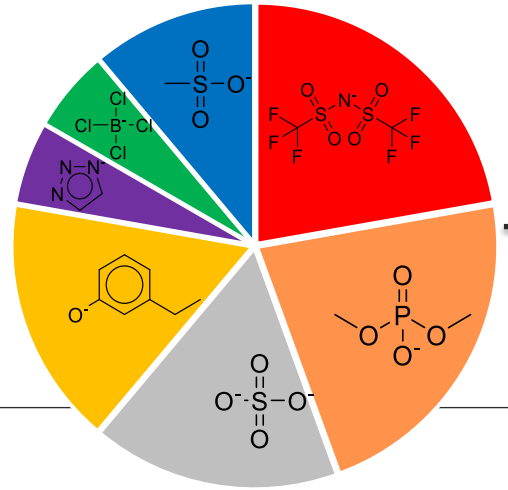
COSMO-RS



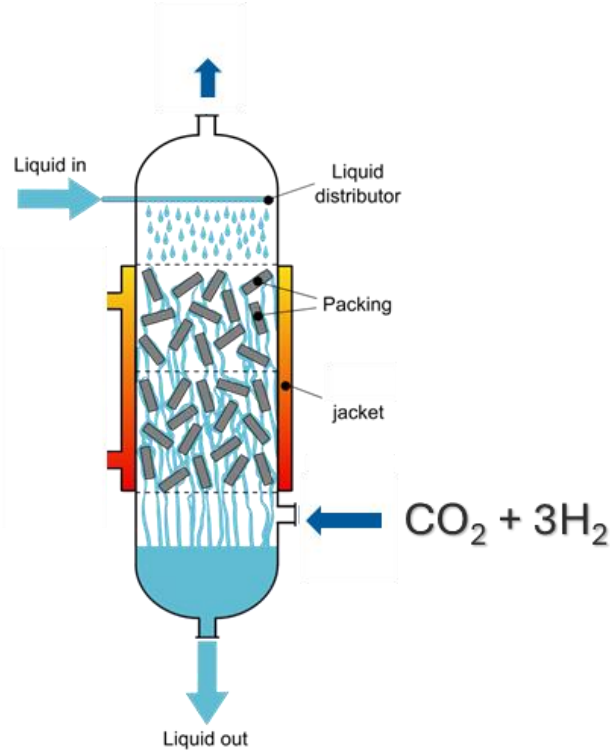
CATIONS



ANIONS



IL



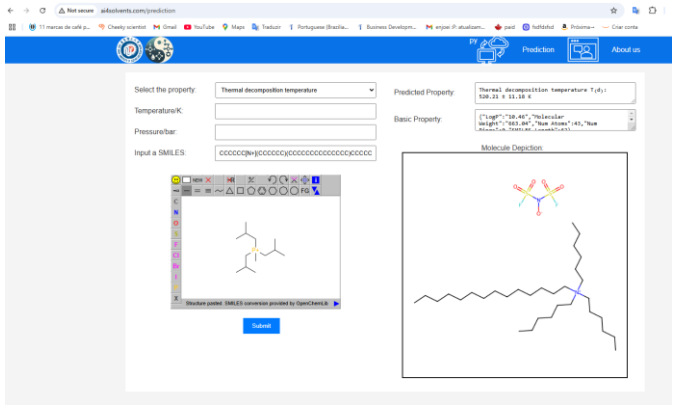
$MeOH + H_2O$

Methods

AI – ILBERT

http://ai4solvents.com/

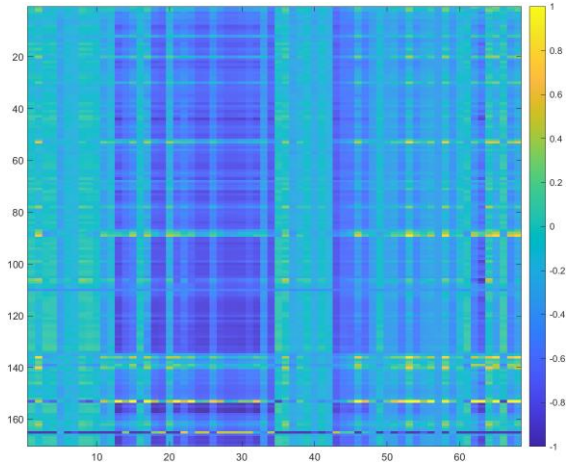
Td, Tm & μ



19.5 mi ILs

COSMO-RS

activity coefficient (γ)
Methanol & Water



Top 0.1% => 20k ILs

Ranking
Metrics & Limitations

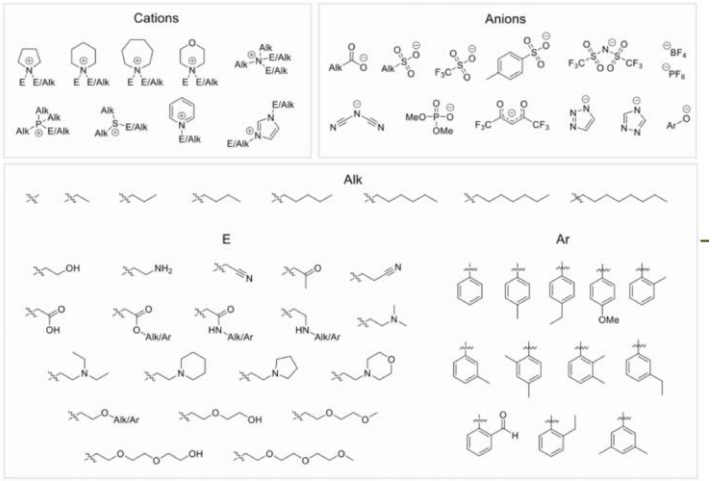
Ranked shortlist
(not shown)

Top 0.0002% => 40 ILs

Chemical Space

19.5 millinon ILs

- **8.5 mi synthesizable**

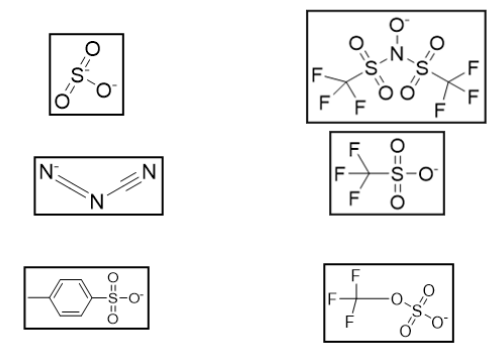


The Ionic Liquid Property Explorer: An Extensive Library of Task-Specific Solvents

by Vishwesh Venkatraman *, Sigvart Evjen and Kallidanthiyil Chellappan Lethesh

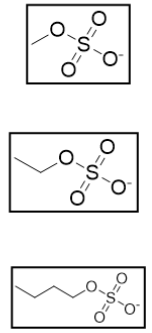
https://doi.org/10.3390/data4020088

- **11 mi Literature review**

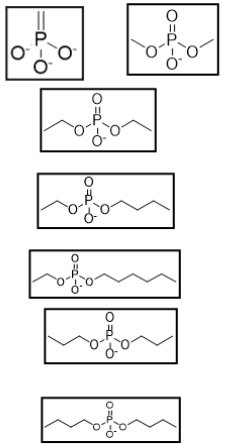


industry

Fluorate



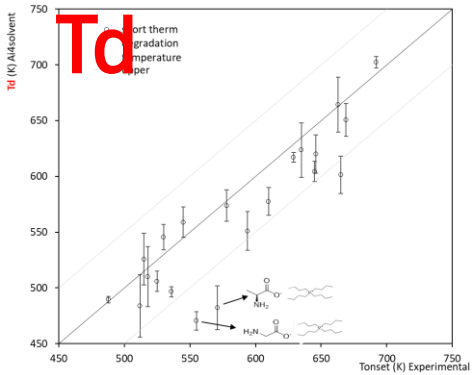
Sulfate

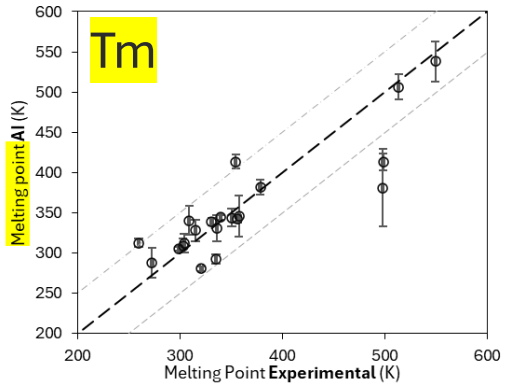


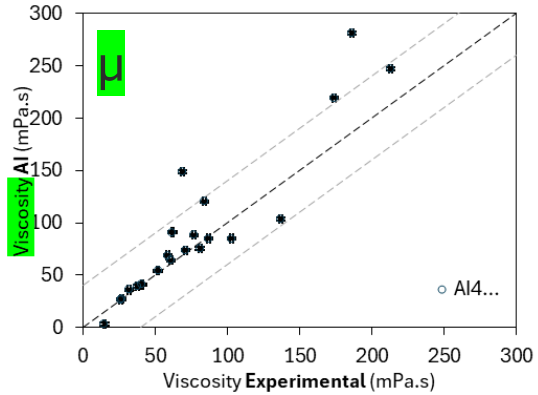
Phosphate

Validation AI / COSMO

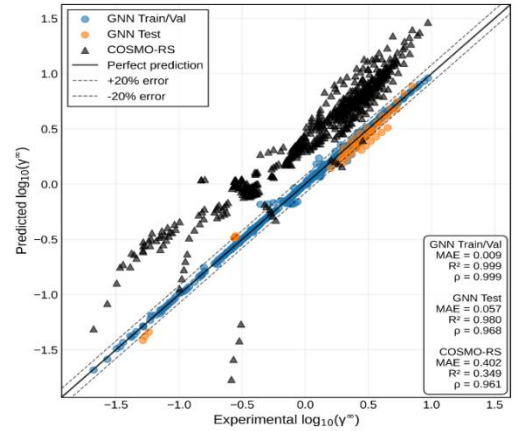
AI - ILBERT

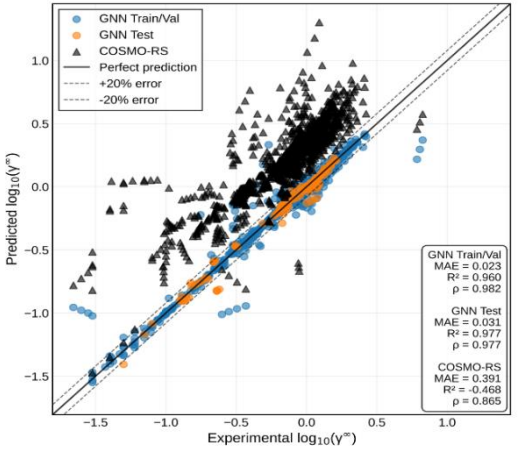




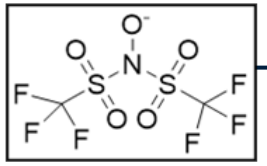


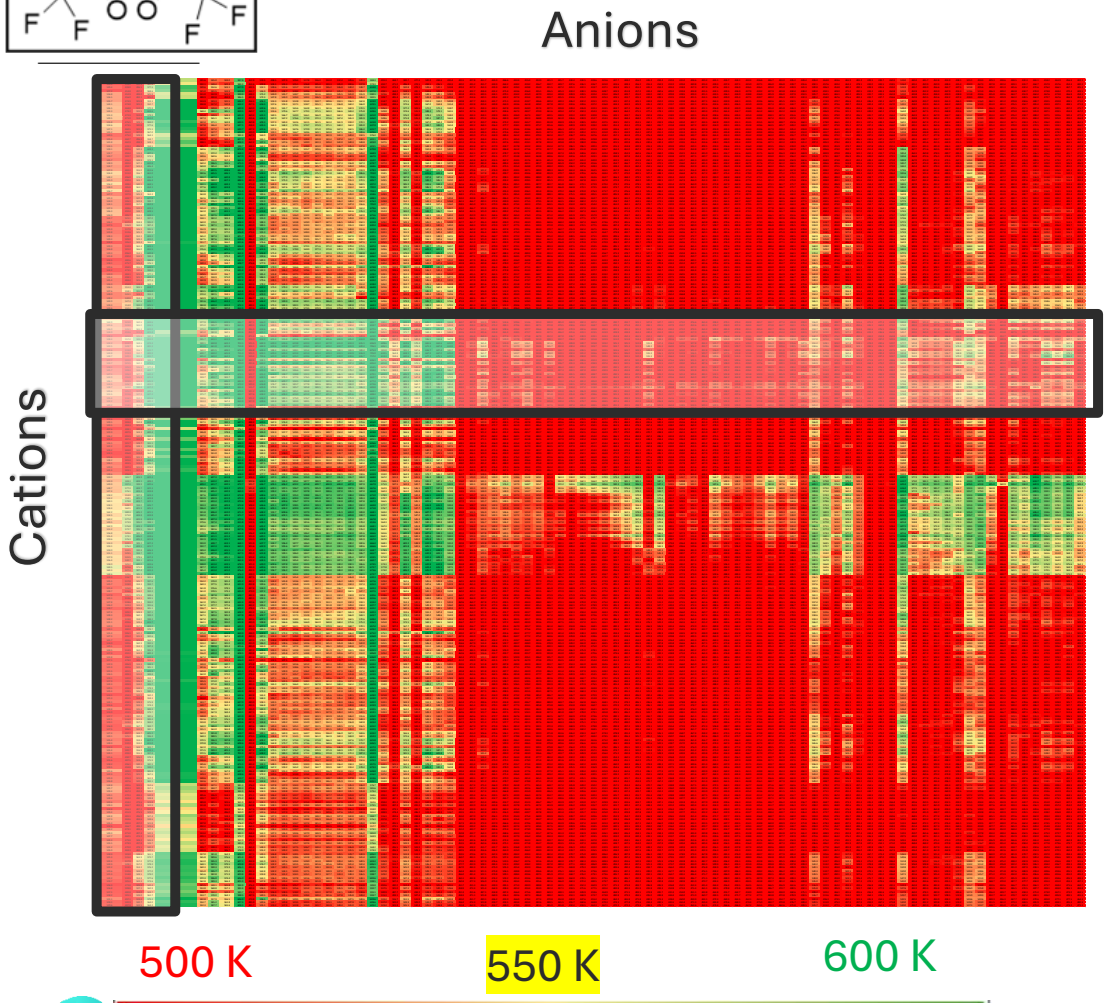
COSMO-RS - GNN

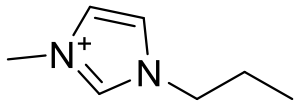




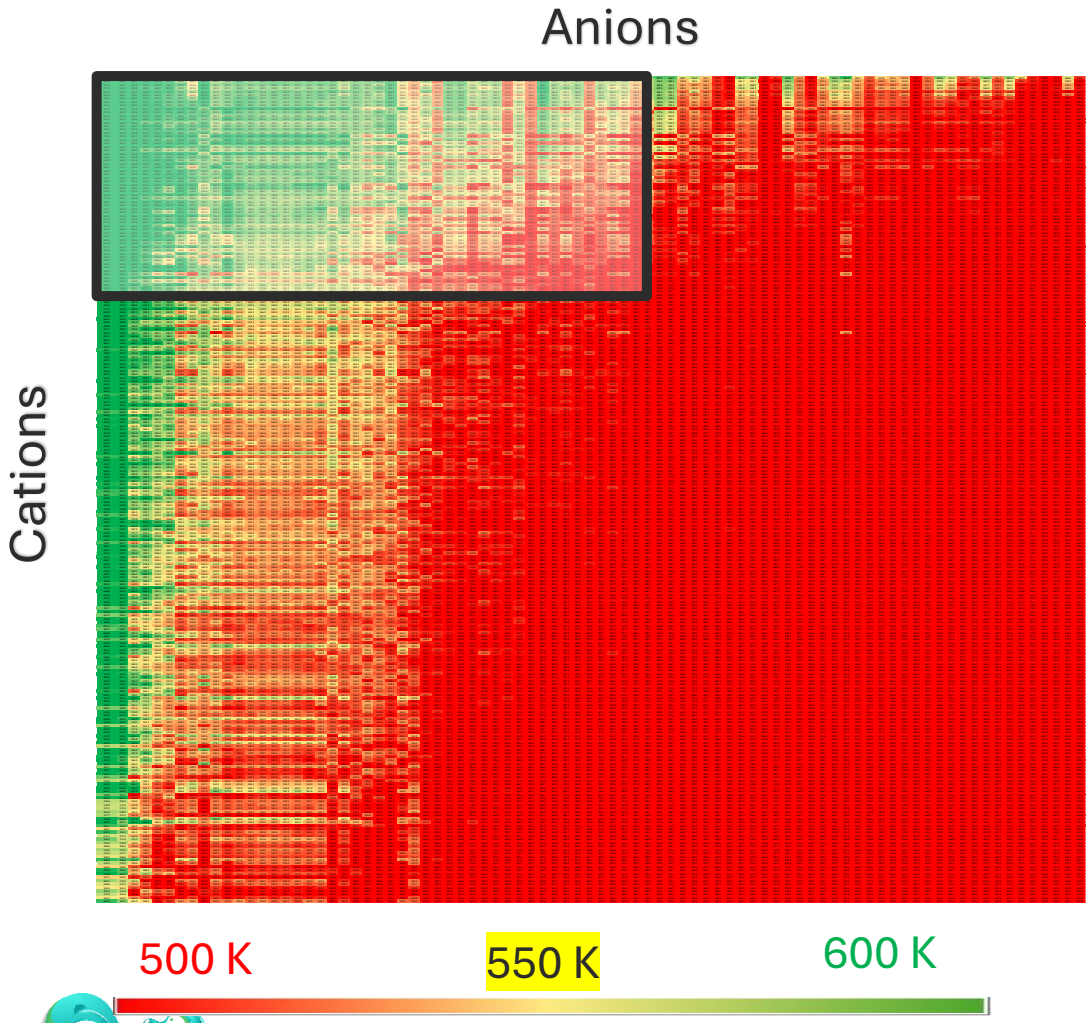
Degradation temeprature (Td) of 20,000 ILs

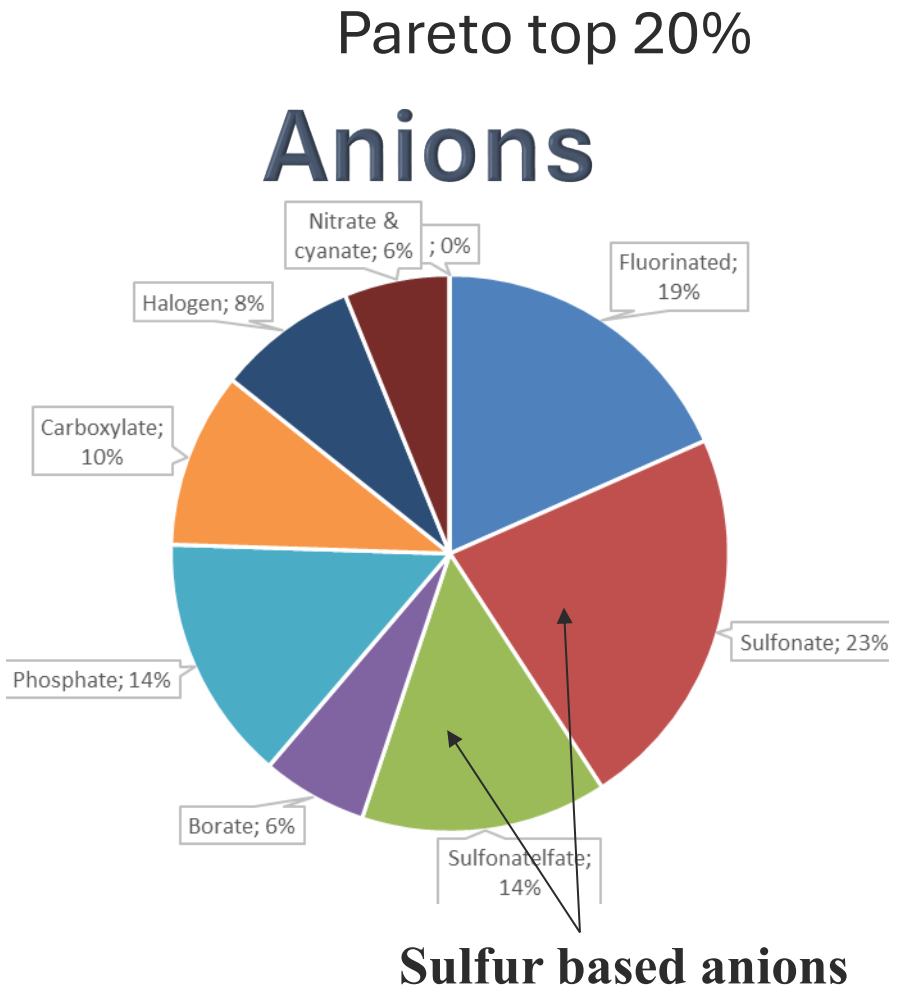




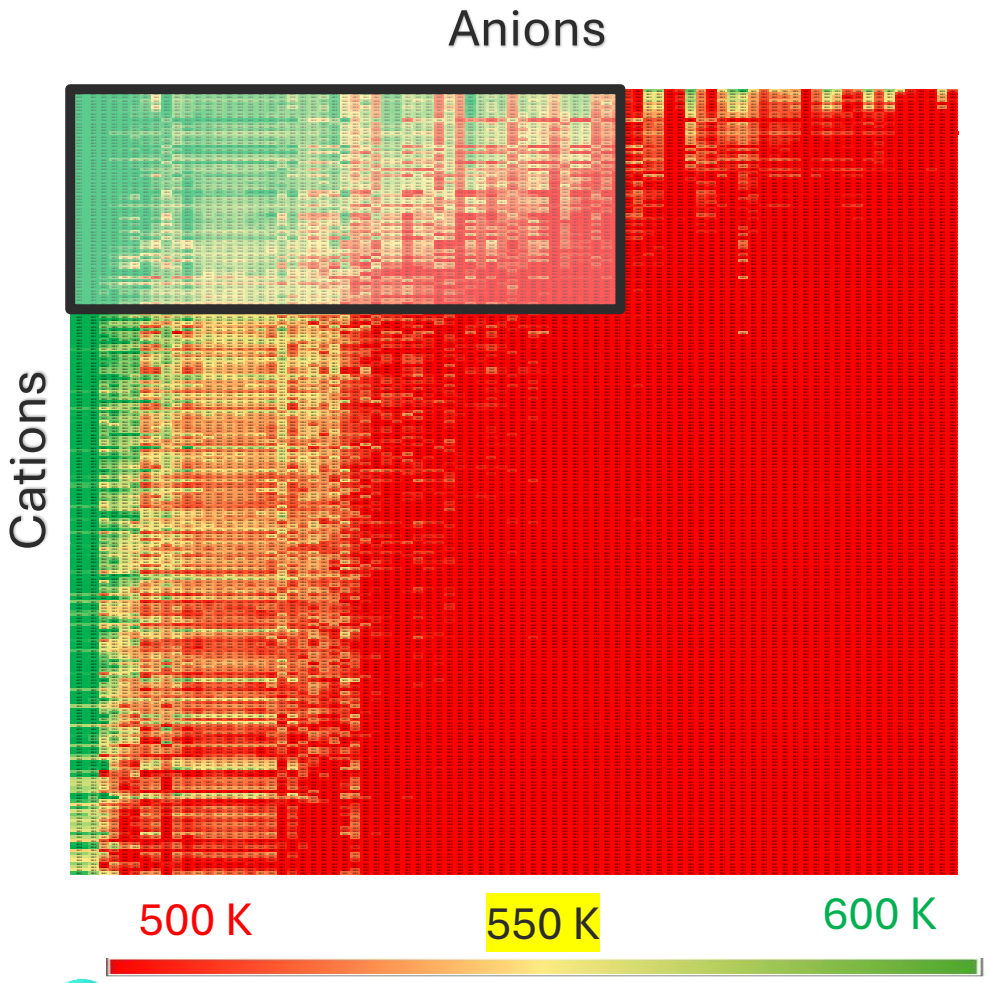


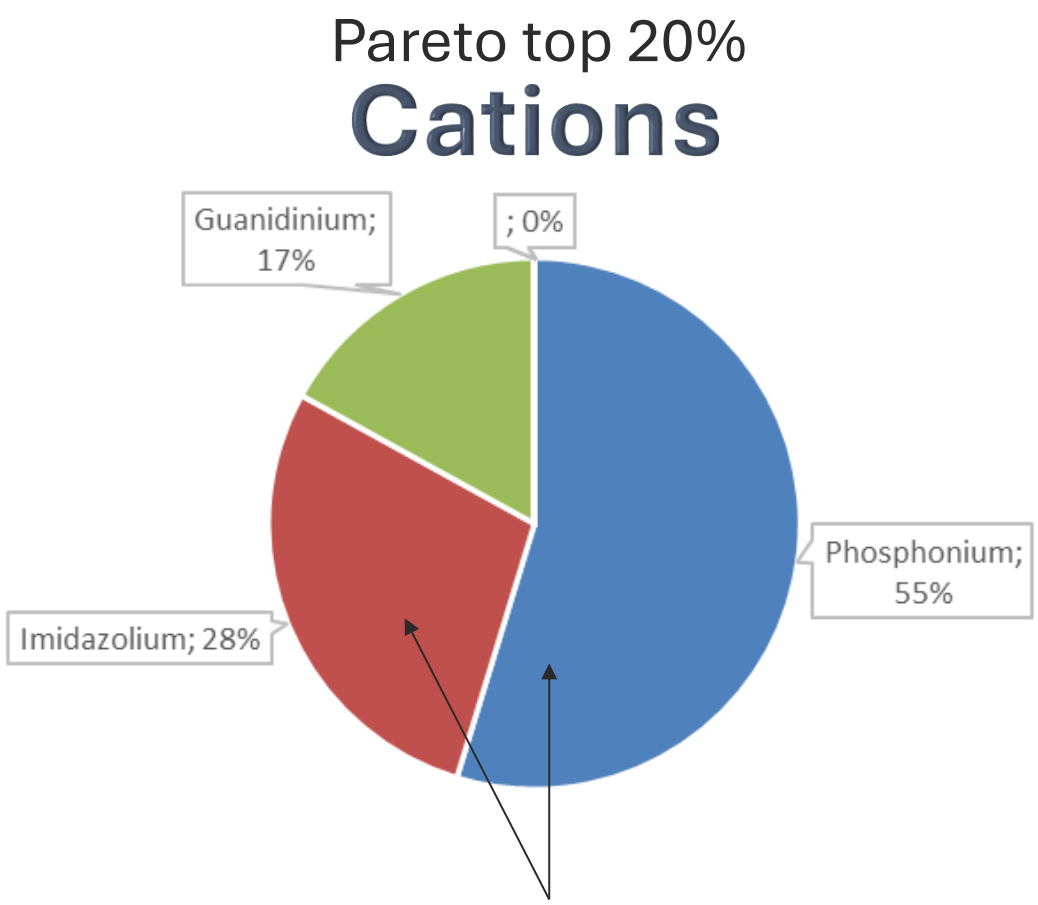
Degradation temeprature (Td) of 20,000 ILs





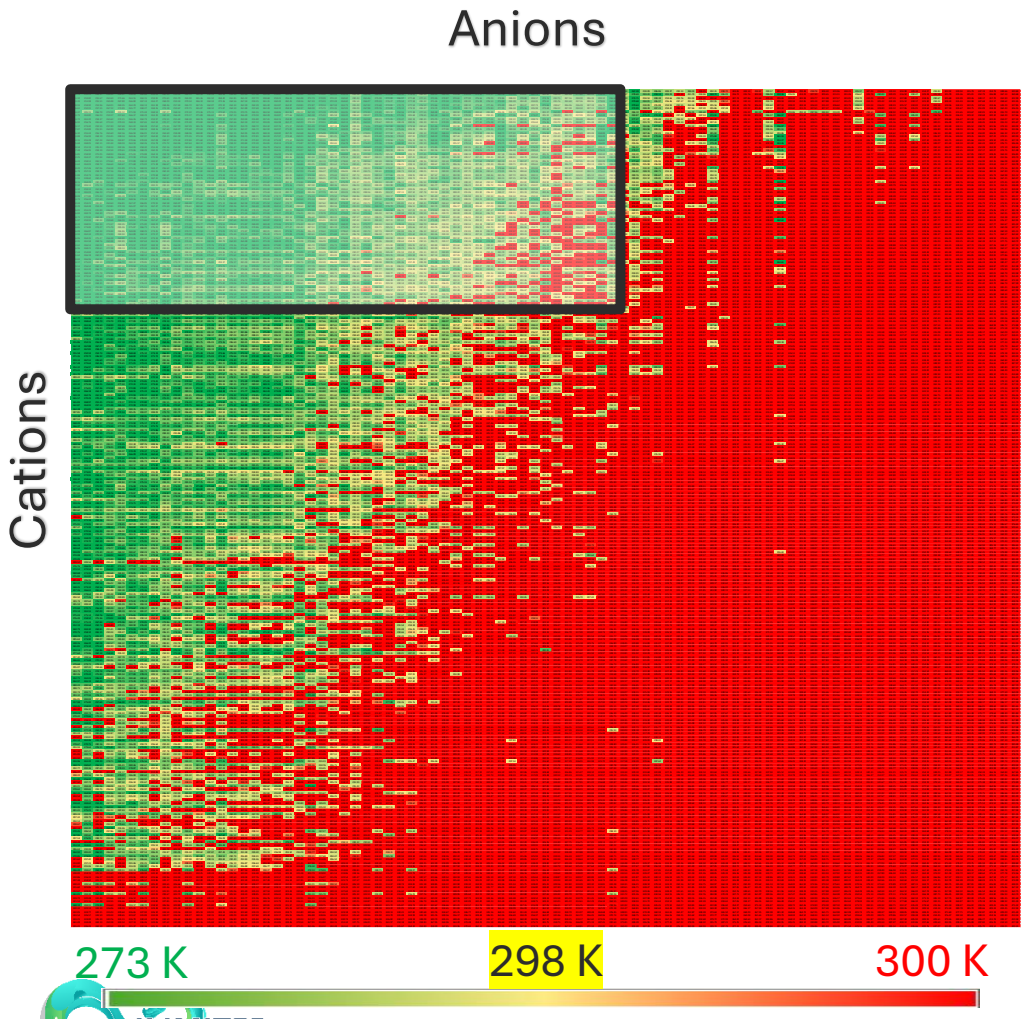
Degradation temeprature (Td) analysis

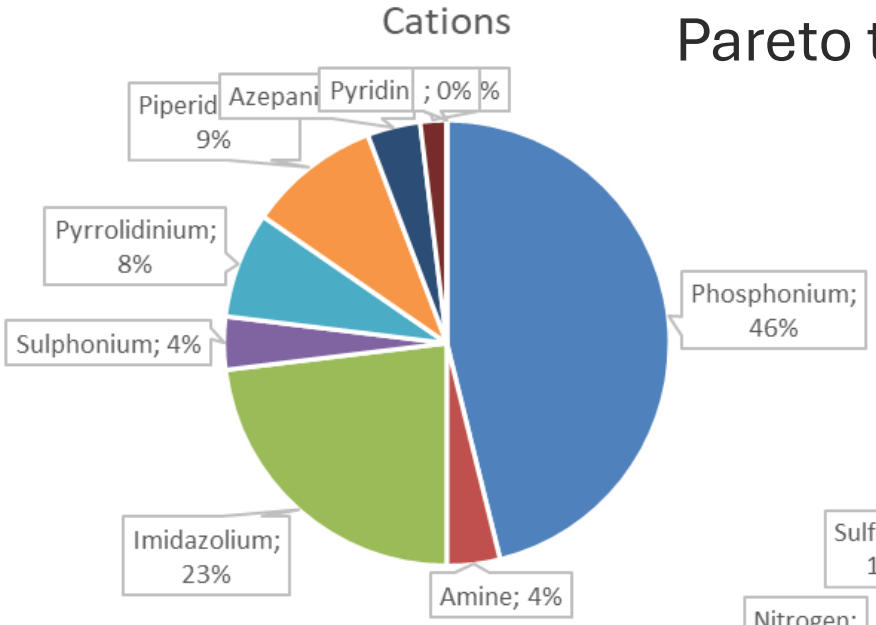




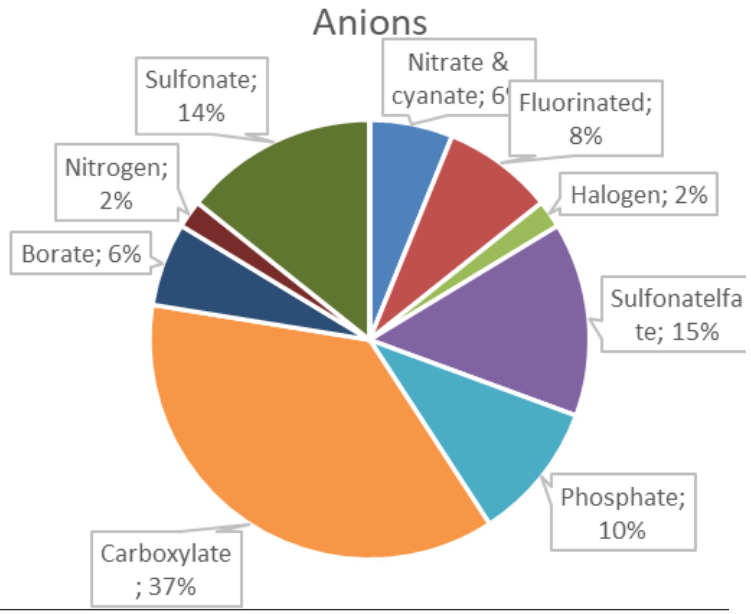
Phosphonium and Imidazolium cations

Temperature of melting (Tm)

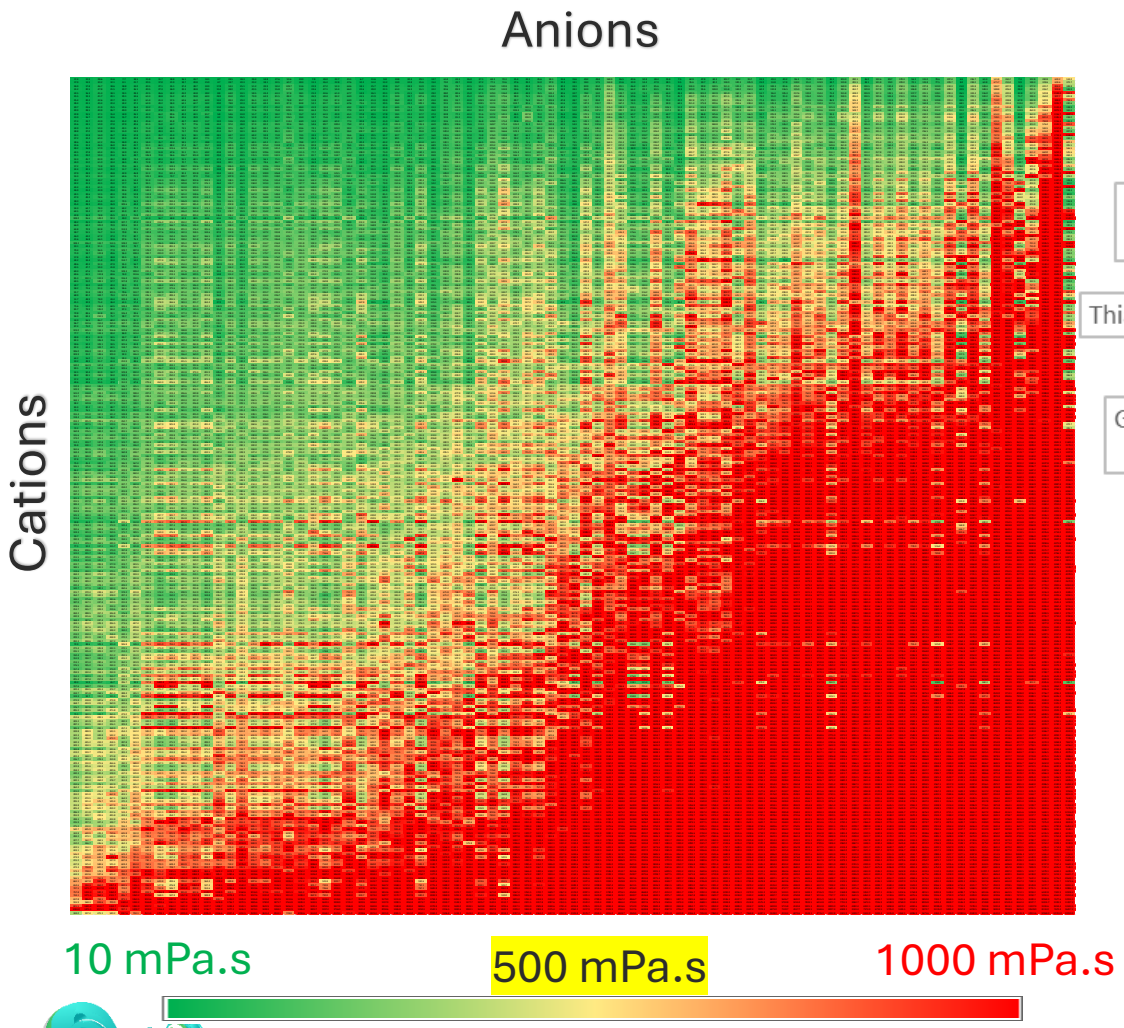


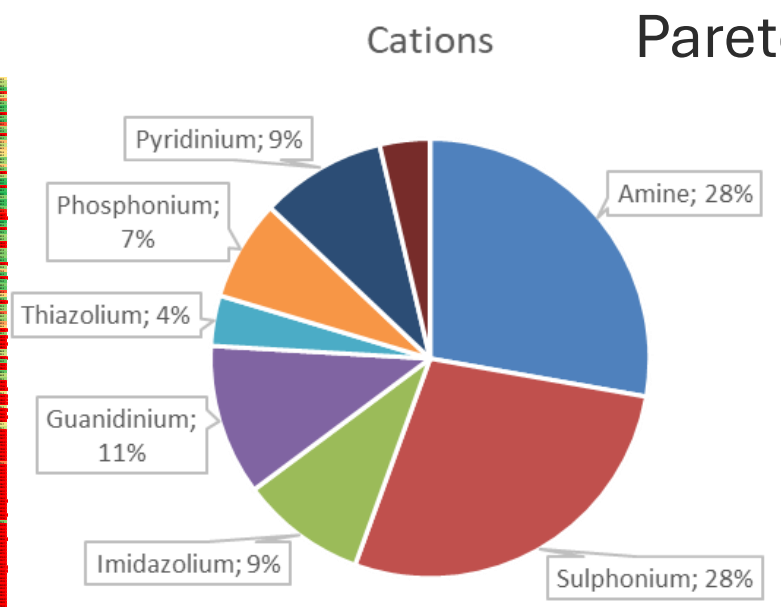


Pareto top 20%

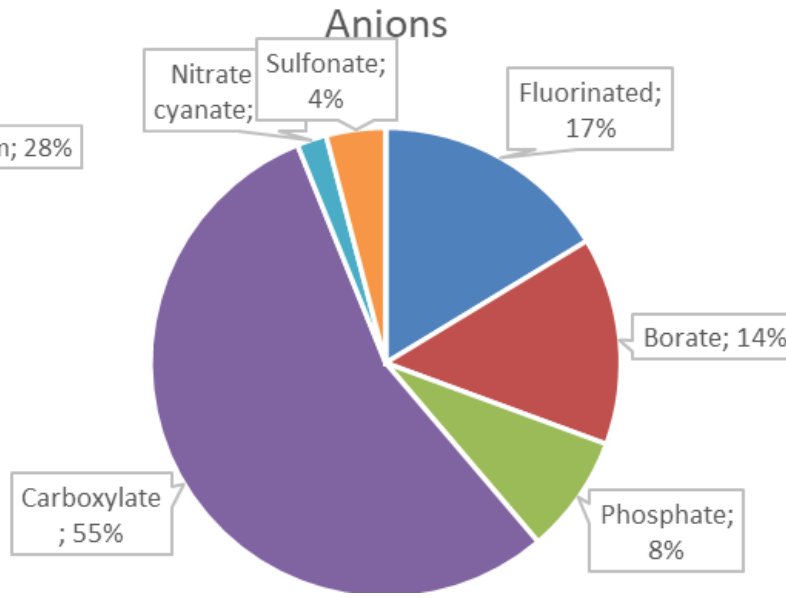


Viscosity (μ)

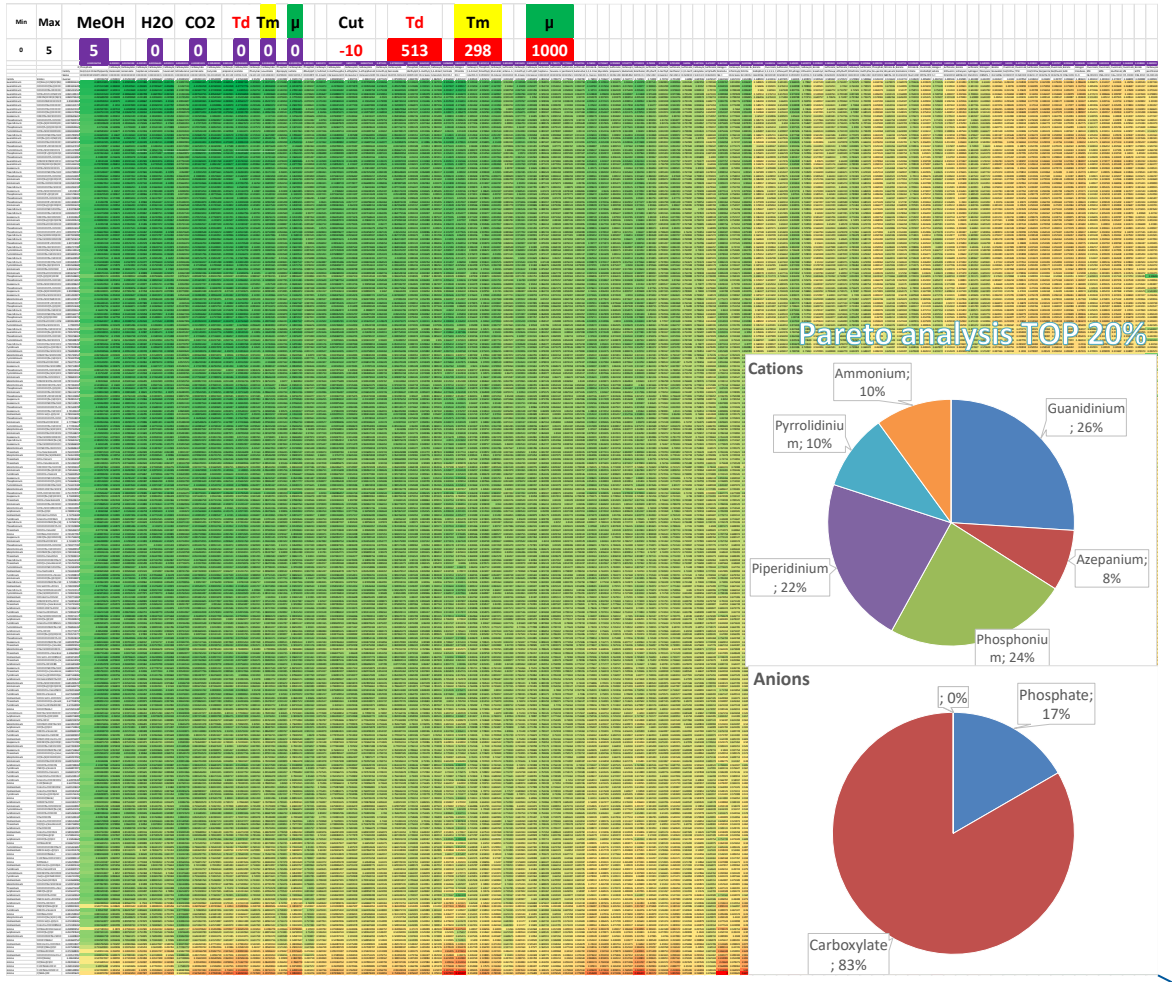


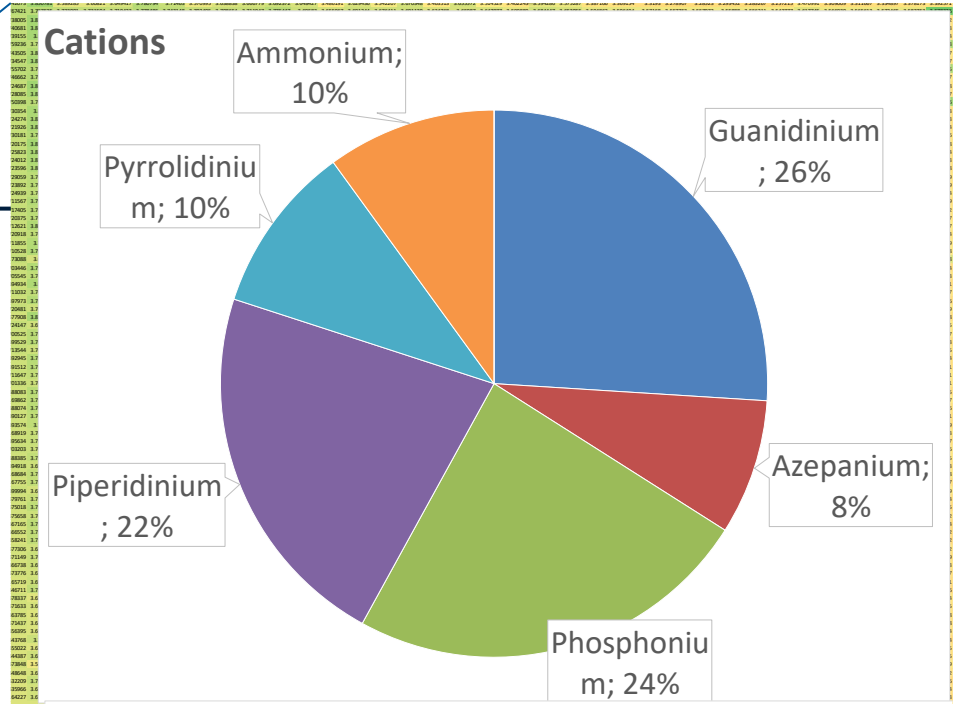


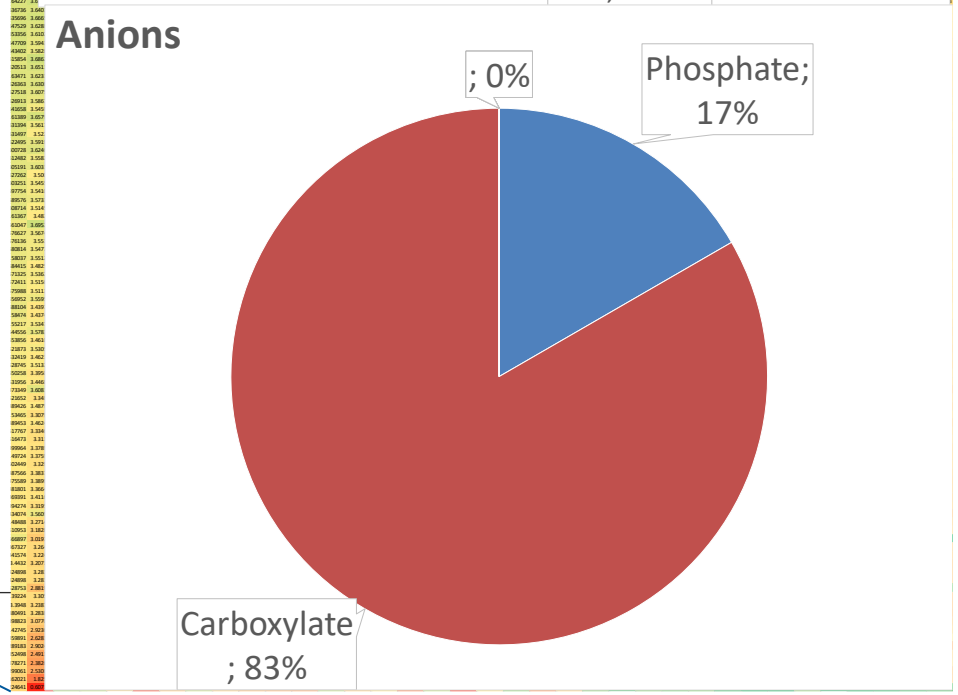
Pareto top 20%



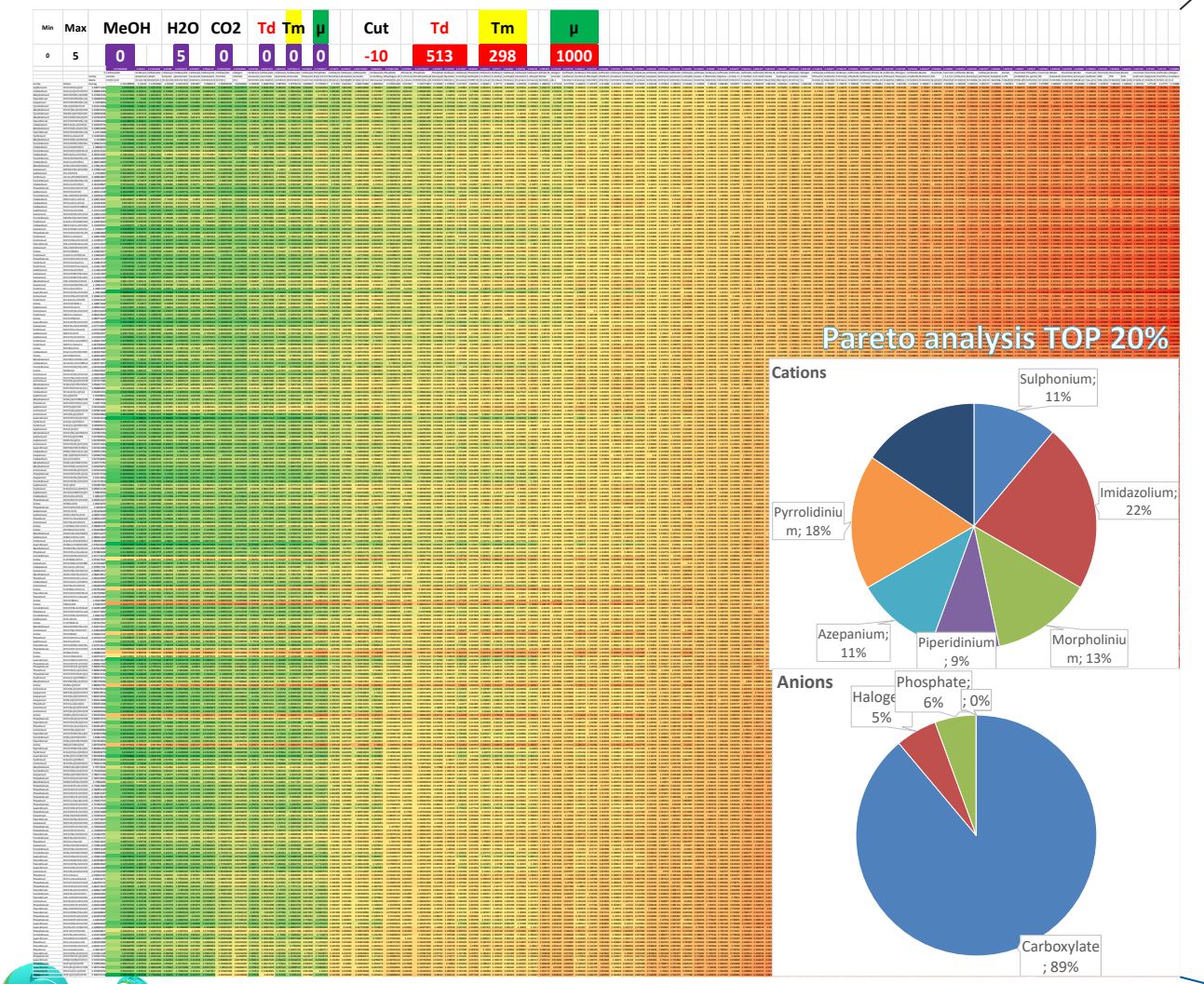
Activity coefficient (γ^{∞}_{MeOH})

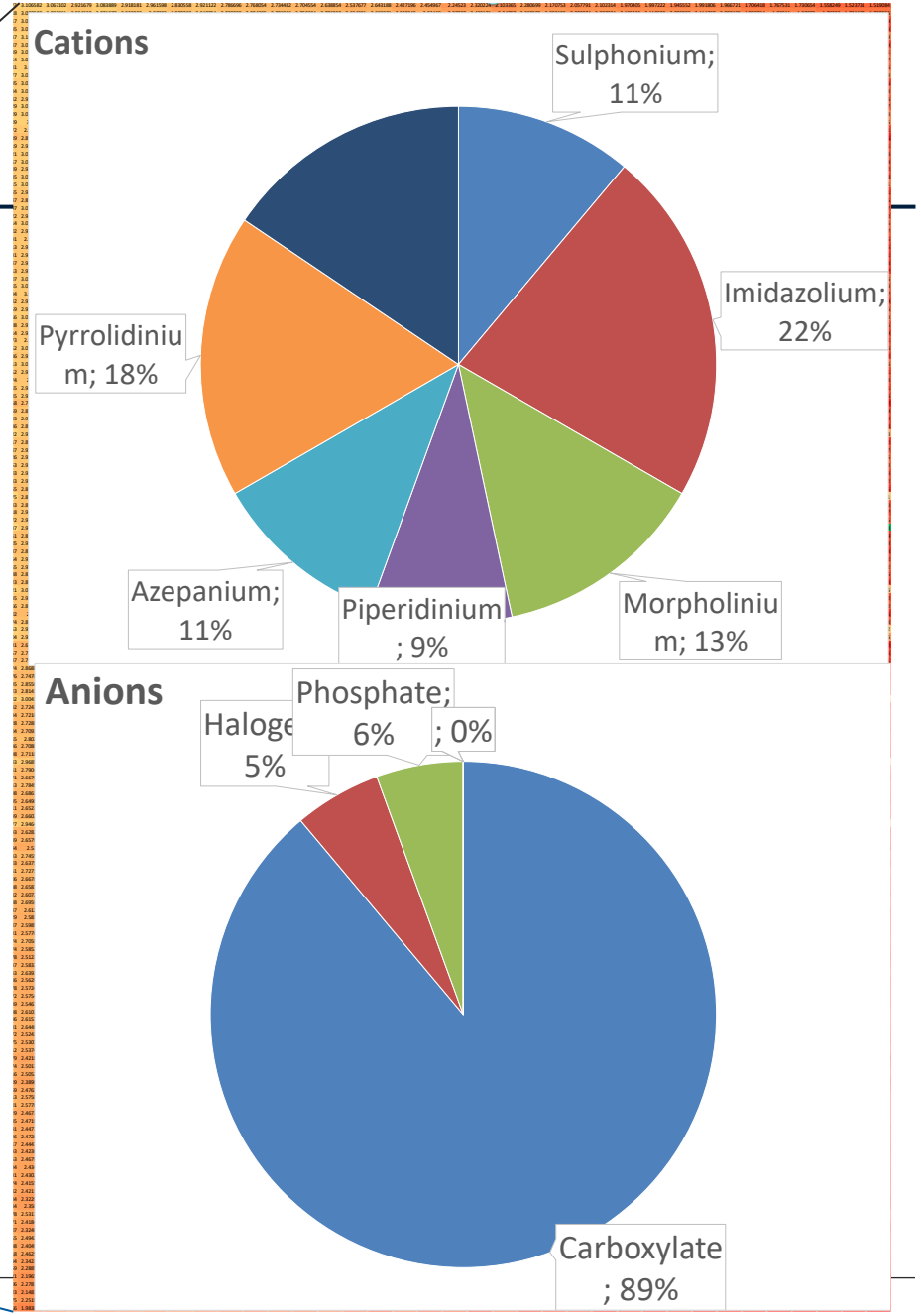






Activity coefficient ($\gamma_{H_2O}^{\infty}$)





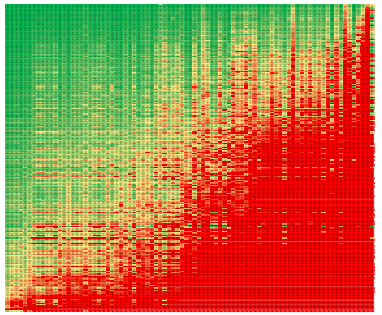
Ranking

3 Limitations

- Thermal stability (**Td**) above **500 K**
- Melting temperature (Tm) above **298 K**
- Viscosity (**μ**) below **1000 mPa.s**

5 metrics

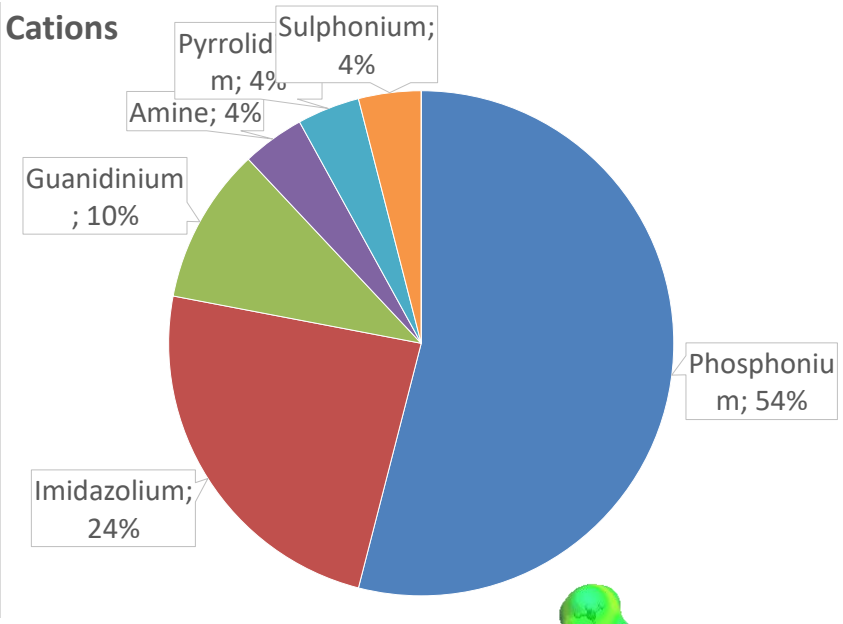
γ_{MeOH}, γ_{H_2O}, **Td** , Tm , **μ**

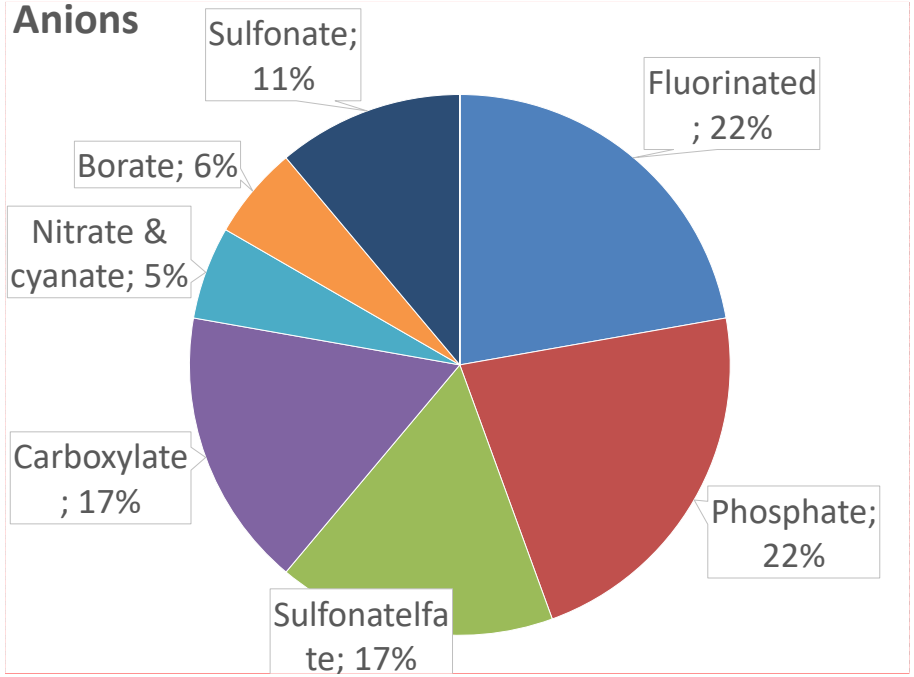


Weighted ranking (standardized)

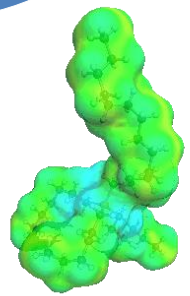
Fobj= 4.γ_{MeOH} + 3.γ_{H_2O}+2.**Td**+ Tm + **μ**

Ranking

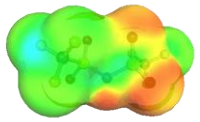


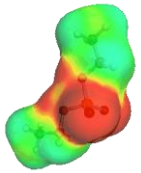


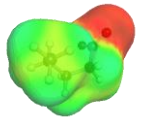




Imidazolium Phosphonium







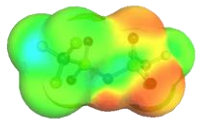
Fluor Sulfate Phosphate Carboxylate

Conclusions

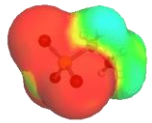
COSMO-RS + AI allowed screenning over 20 mi Ils
5 metrics & 3 limitations

19.5 mi ILs -> 20k ILs -> 40 ILs
Shortlist of candidate ILs not shown (results under evaluation)

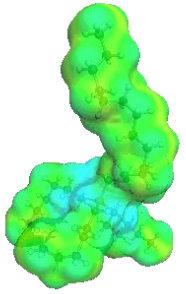
Identification of trends and best ILs



Fluor Sulfate



Sulphate



Phosphonium

TESTE TEXTO TESTE

Thank you

Questions?



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