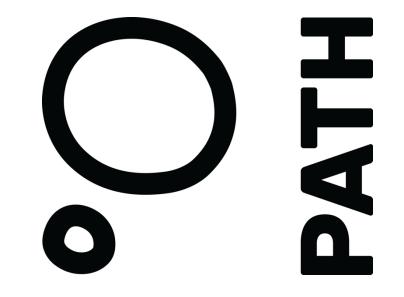
Smart solvent design: using COSMO-RS to unlock selective polymer dissolution



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What's our goal?

Plastics are extremely relevant in many applications. This relevance resulted in their massive production and a large amount of waste The recycling of mixed waste and multi-layered materials is still a challenge, due to the difficult separation steps

SELECTIVE DISSOLUTION-PRECIPITATION is a promising approach towards this problem, but hazard organic solvents are still the preferred choice

ΔIM

MORE **SUSTAINABLE** dissolution-precipitation process

Using **COSMO-RS** as a pre-selecting tool

Find eutectic solvents (ES)

for selective dissolution of...

Petroleum-based polymers: PET, PP, PE, PVC

Bio-based polymers: PLA

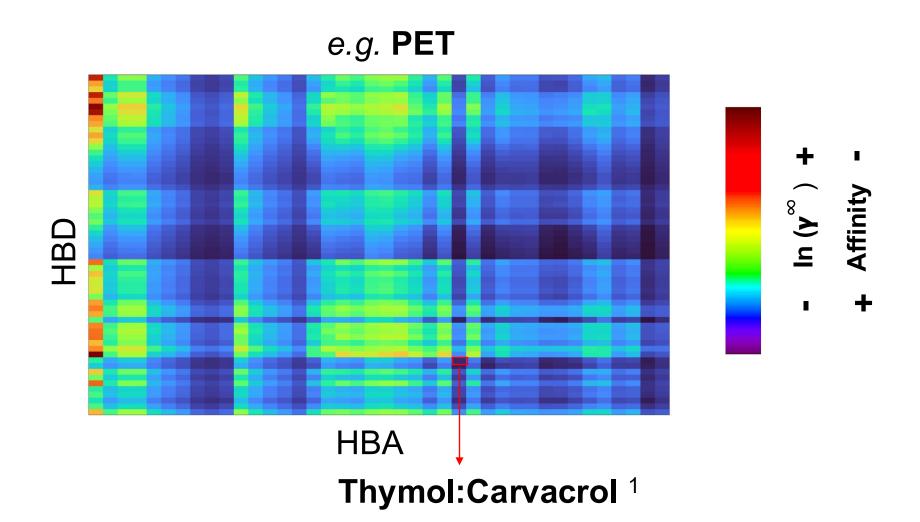
How can we achieve it?

1. COSMO-RS predictions

HBA:HBD molar ratio of 1:1
40 HBA + 59 HBD

2360 ES

∭00 °C



Monoterpenoid-based ES are suitable for PLA and PET

Menthol-based ES effectively dissolve

HDPE and PP

2. Dissolutionprecipitation (wet tests)

olution-precipitation

dis

Selective

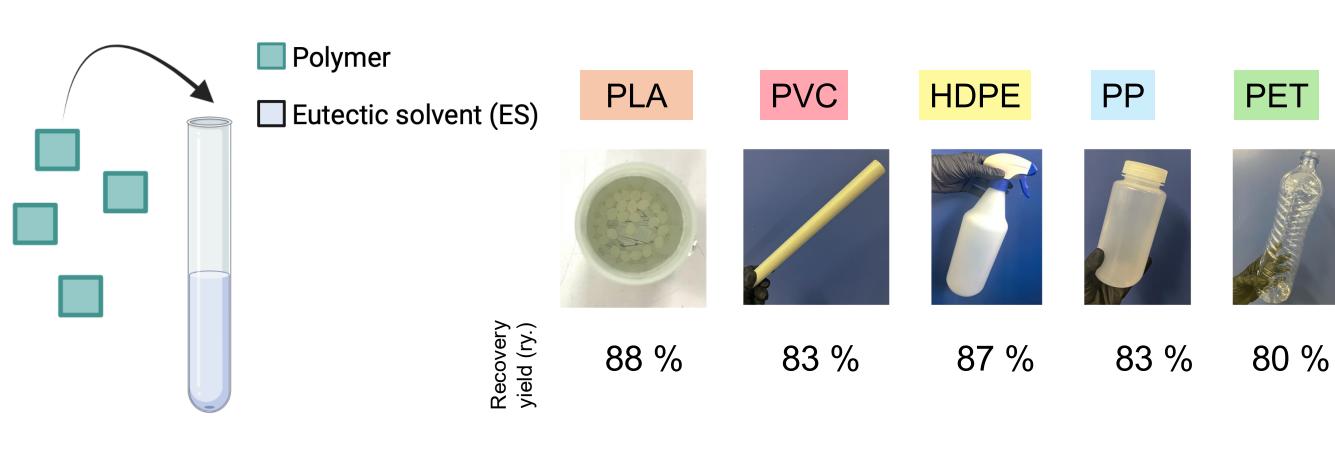
က<u>်</u>

polymer

of

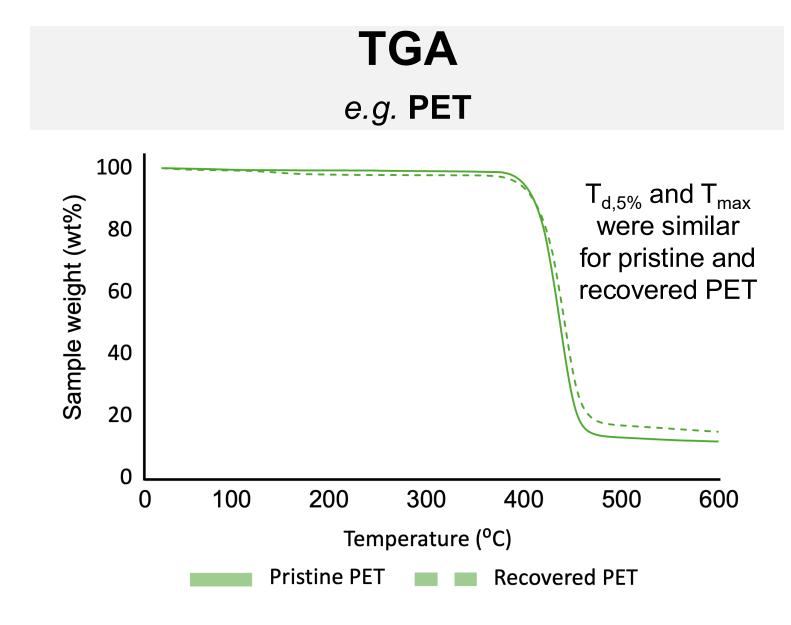
(wet

mixture



100 to 150 °C

Recovered polymers didn't present differences on FTIR, TGA and DSC



HDPE T_m 127.84 °C T_m 144.53 °C T_m 169.16 °C 141.24 °C Solid Dissolved ry. 56 % ry. 83 % ry. 92 % ry. 89 % PLA PVC PET HDPE 🛑 ry. 100 % PET Polymer dissolution Precipitation by adding an **Filtration** in solvent antisolvent and Filtration

Recovered HDPE seemed to have traces of PP Recovered PLA, PVC, PP and PET did not present differences

FTIR Recovered (mixture - step 3) Recovered (alone - step 2) **Pristine** Recovered (mixture - step 3) Recovered (alone - step 2) **Pristine** Recovered (mixture - step 3) HDPE Recovered (alone - step 2) **Pristine** Recovered (mixture - step 3) Recovered (alone - step 2) Pristine Recovered (mixture - step 3) Recovered (alone - step 2) **Pristine** Wavelength (cm)

Take home message

- > COSMO-RS enables rapid in silico evaluation of polymers' solubility in a wide range unconventional solvents ES.
- > ES proved to be suitable for selective dissolution of polymers by using different ES.
- > Selecting suitable ES for dissolving complex polymer mixtures in municipal waste and multilayer films can advance polymer recycling and circularity.







