ReSolve
SAFE AND EFFECTIVE BIO-BASED SOLVENTS

Introducing the ReSolve Project

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BBI JU

Bio-based Industries Consortium

Horizon 2020
European Union Funding
for Research & Innovation

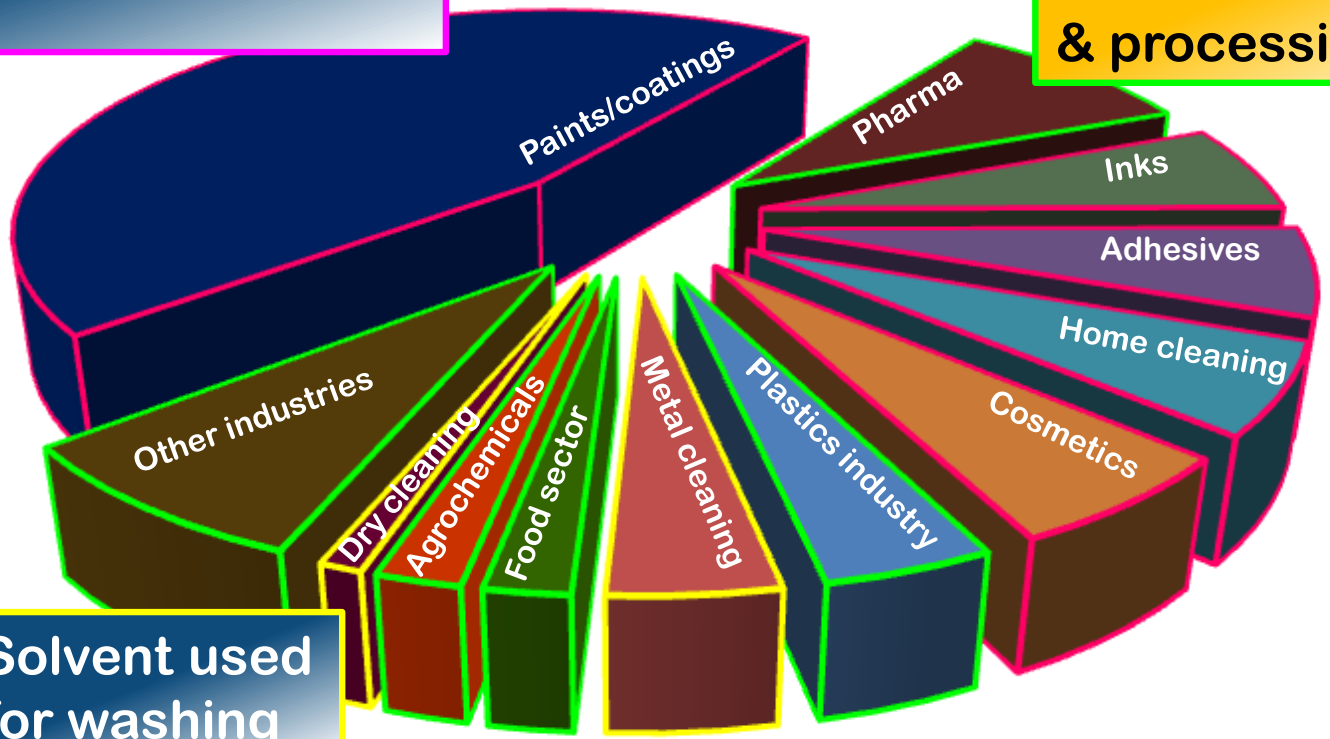
This project has received funding from the Bio Based Industries Joint Undertaking under the European Union‘s Horizon2020 research and innovation programme under agreement No 745450.

Solvent market

Market: 20 Million Tonnes /year

Solvent is the major ingredient (the 'wet' bit)

Solvent is needed in manufacturing & processing



Solvent used for washing

ESIG data, 1997

Basis for ReSolve project

- REACH regulation introduced to protect human health and the environment from risks posed by chemicals
  - Restriction of use of certain solvents
- ReSolve project targeting the replacement of two solvents restricted under REACH regulation:
  - NMP – categorised as a Substance of Very High Concern (SVHC) and restriction for certain uses in place from 2020
  - Toluene – restricted for products supplied to the public
- Conventional solvents generally fossil-based
  - Substitution with sustainable bio-based alternatives

NMP info card

RSS

1-methyl-2-pyrrolidone

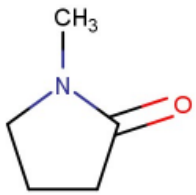
Regulatory process names 3 Translated names 34 CAS names 1 IUPAC names 19 Trade names 16 Other identifiers 5

Substance identity

EC / List no.: 212-828-1

CAS no.: 872-50-4

Mol. formula: C5H9NO



Hazard classification & labelling

Danger! According to the **harmonised classification and labelling** (ATP09) approved by the European Union, this substance may damage the unborn child, causes serious eye irritation, causes skin irritation and may cause respiratory irritation.

Additionally, the classification provided by companies to ECHA in **REACH registrations** identifies that this substance may damage fertility or the unborn child.

Properties of concern

R Toxic to Reproduction

Important to know

- Substance of very high concern (SVHC) and included in the candidate list for authorisation.
- Some uses of this substance are restricted under Annex XVII of REACH.

How to use it safely

- ECHA has no data from registration dossiers on the precautionary measures for using this substance.
- Guidance on the safe use of the substance provided by manufacturers and importers of this substance.

About this substance

This substance is manufactured and/or imported in the European Economic Area in 10 000 - 100 000 tonnes per year.

This substance is used in articles, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

https://echa.europa.eu/substance-information/-/substanceinfo/100.011.662

Toluene info card

RSS

Toluene

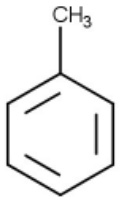
Translated names 13 CAS names 1 IUPAC names 16 Trade names 23 Other identifiers 4

Substance identity

EC / List no.: 203-625-9

CAS no.: 108-88-3

Mol. formula: C7H8



Hazard classification & labelling

Danger! According to the **harmonised classification and labelling** (CLP00) approved by the European Union, this substance may be fatal if swallowed and enters airways, is a highly flammable liquid and vapour, is suspected of damaging the unborn child, may cause damage to organs through prolonged or repeated exposure, causes skin irritation and may cause drowsiness or dizziness.

Additionally, the classification provided by companies to ECHA in **REACH registrations** identifies that this substance is suspected of damaging fertility or the unborn child, is harmful to aquatic life with long lasting effects and causes serious eye irritation.

About this substance

This substance is manufactured and/or imported in the European Economic Area in 1 000 000 - 10 000 000 tonnes per year.

This substance is used by consumers, in articles, by professional workers (widespread uses), in formulation or re-packing, at industrial sites and in manufacturing.

Properties of concern

R Possibly Toxic to Reproduction

Important to know

- Substance included in the Community Rolling Action Plan (CoRAP).
- Some uses of this substance are restricted under Annex XVII of REACH.

How to use it safely

- Precautionary measures suggested by manufacturers and importers of this substance.
- Guidance on the safe use of the substance provided by manufacturers and importers of this substance.

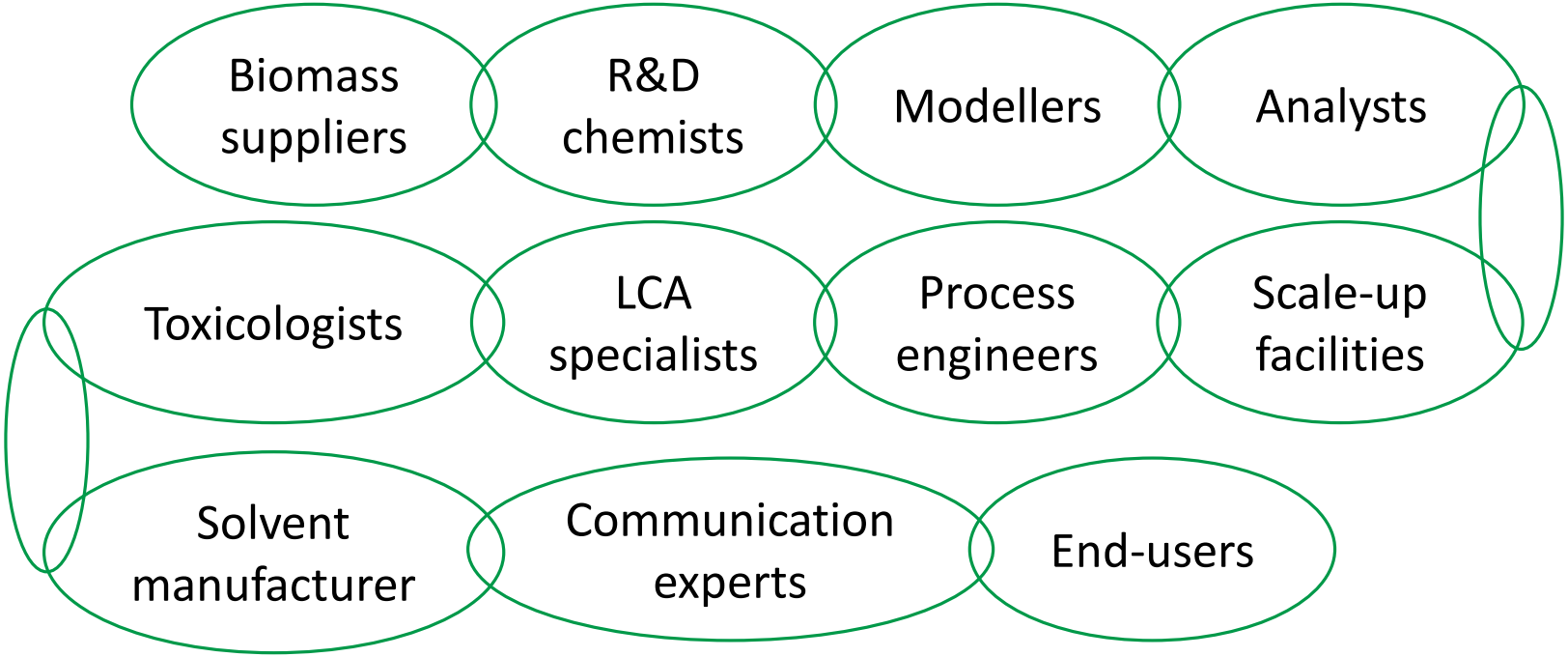
https://echa.europa.eu/substance-information/-/substanceinfo/100.003.297

Current solutions

- Replacement of NMP by similar solvents
  - DMF and DMAc already categorised as SVHC
  - Other N-containing solvents are likely to pose a similar risk to both health and the environment
- Toluene used as the easy solution to replace benzene
  - However causes organ damage and suspected of damaging the unborn child
  - Xylenes used to replace toluene but have their own issues
- Need a new approach
  - Multi-disciplinary collaboration
  - Avoid similar structures (and risks) to the target solvents

The ReSolve approach

- Bring together partners based throughout the value chain
- Developing a methodology that can be applied elsewhere

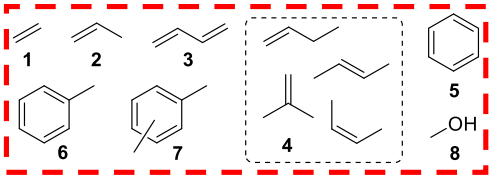


The bio-based advantage

- Improved sustainability over fossil-based solvents
  - Use of renewable non-food carbohydrates - no competition with the food chain
  - Use of existing side streams e.g. sawdust, co-products from other processes

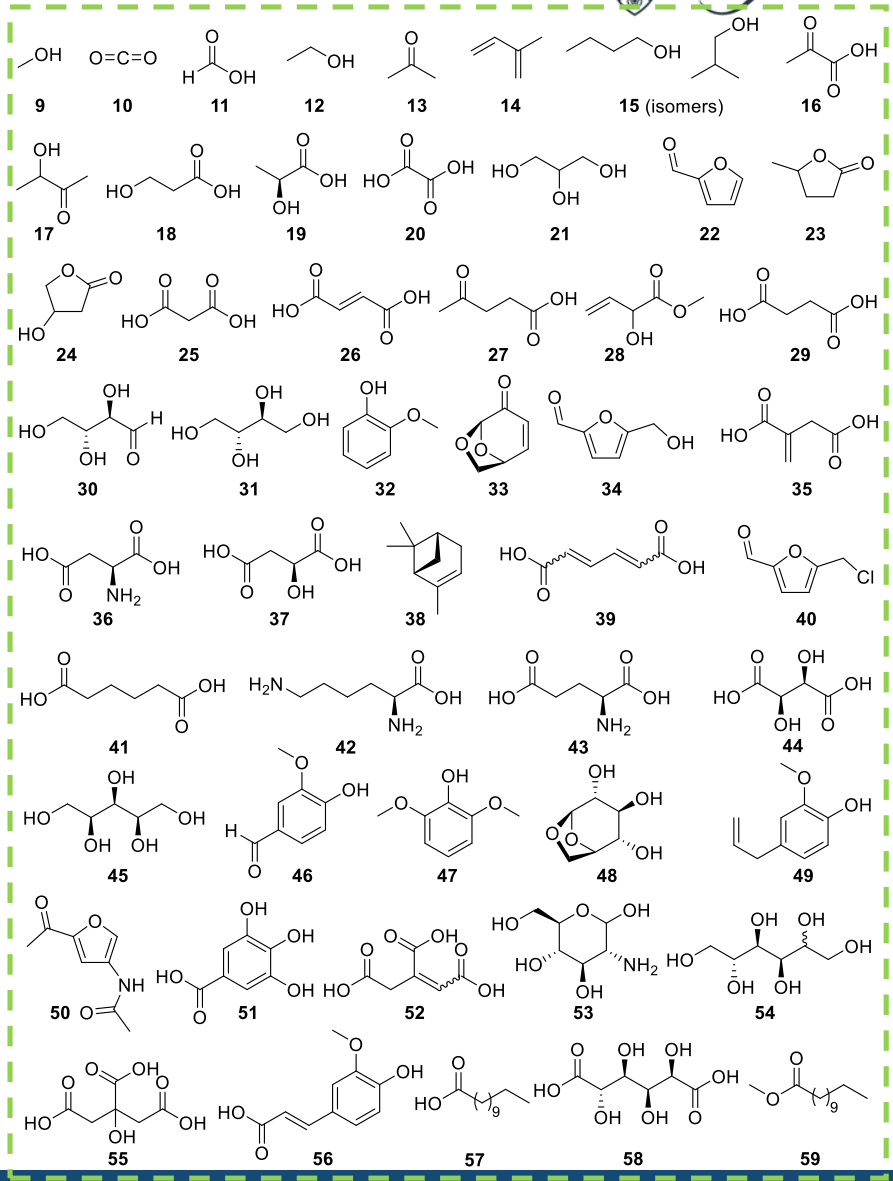
- Interesting structures providing in-built functionality

Bio-based: built-in functionality



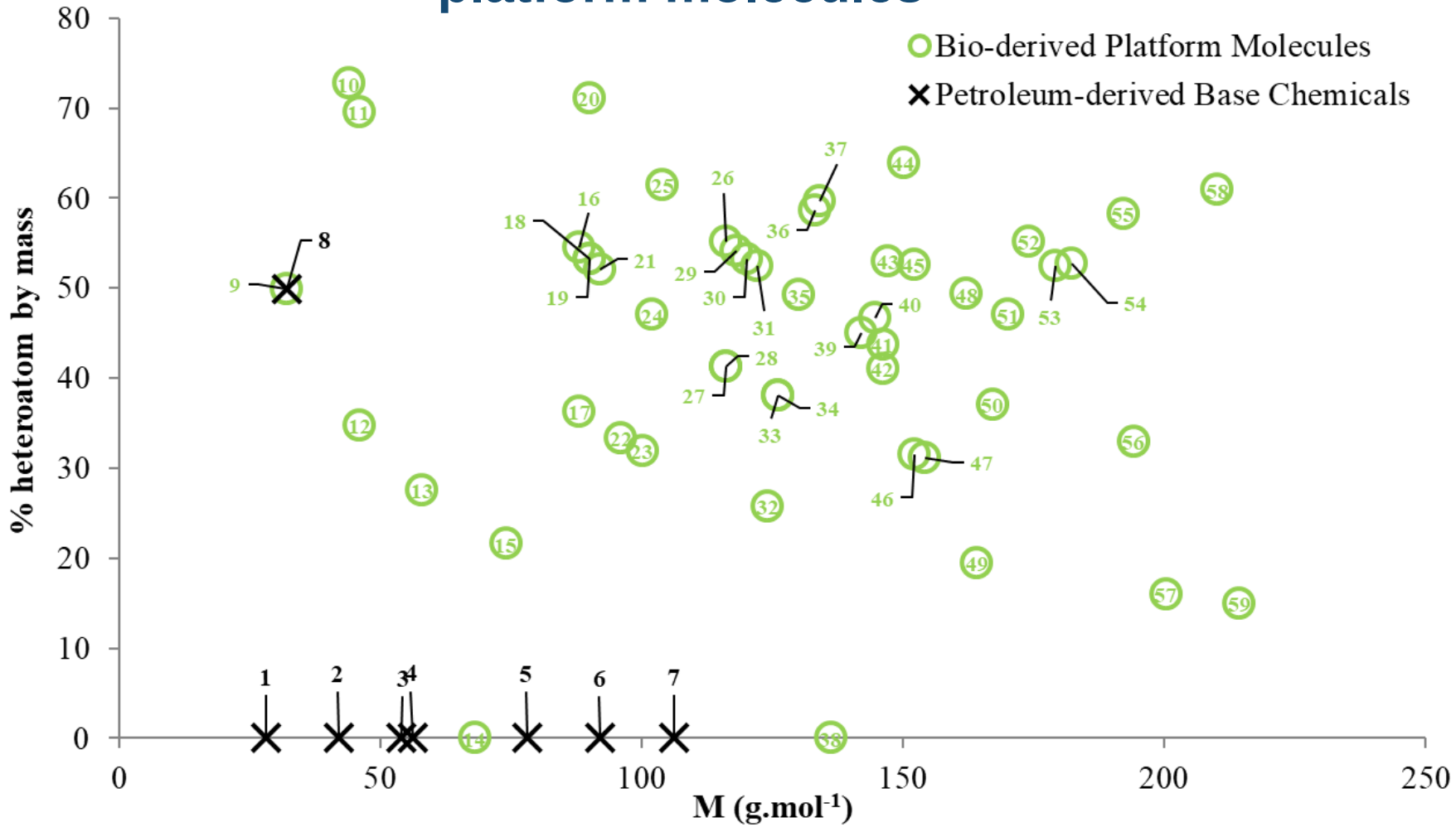
Base chemicals

Bio-based platform molecules



[1] *BioLogicTool:* A Simple Visual Tool for Assisting in the Logical Selection of Pathways from Biomass to Products
Y. Lie, P. Ortiz, R. Vendamme, K. Vanbroekhoven & T. J. Farmer, *Ind. Eng. Chem. Res.*, 2019, 58, 15945-15957

Higher heteroatom content of platform molecules



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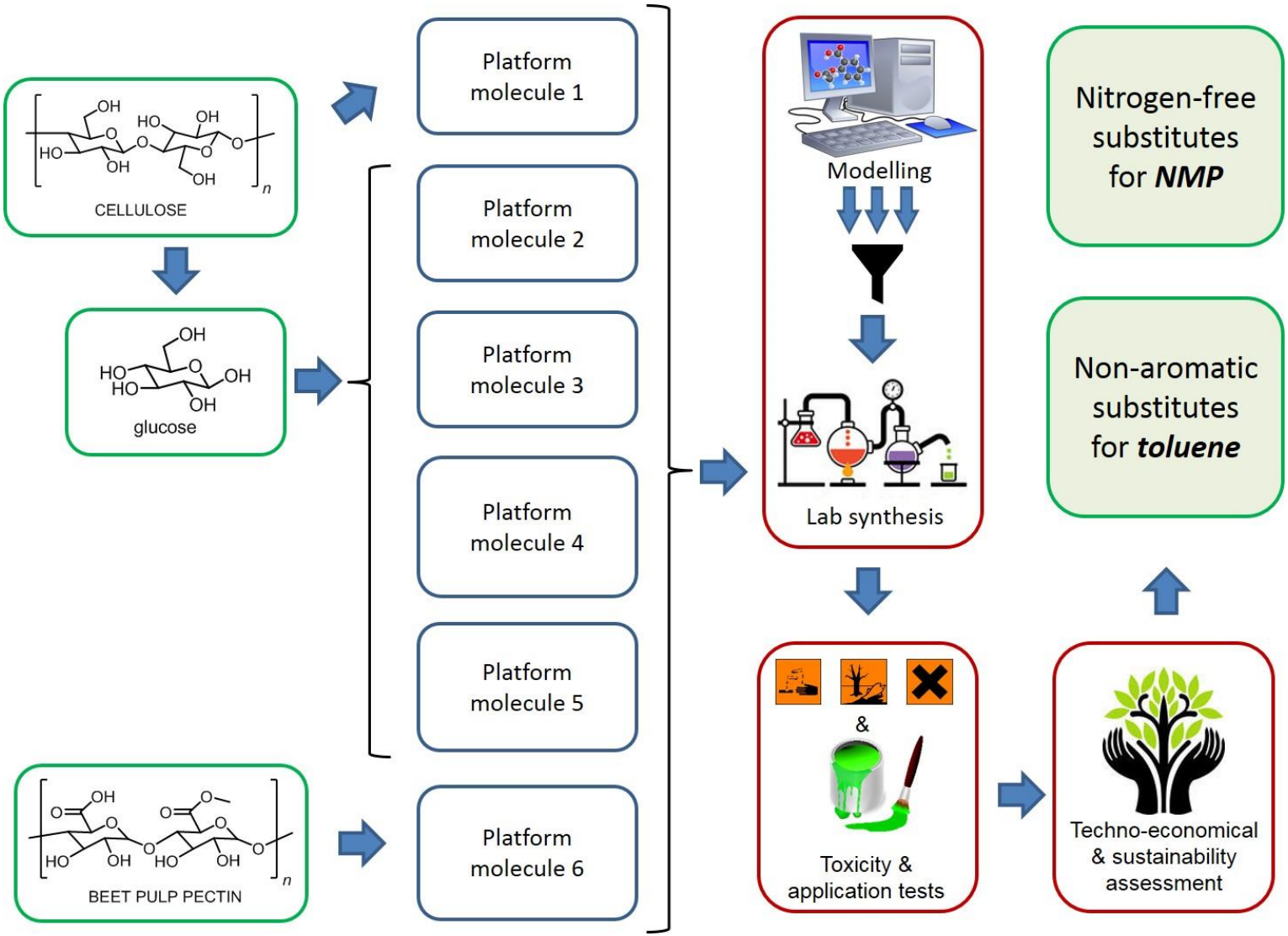
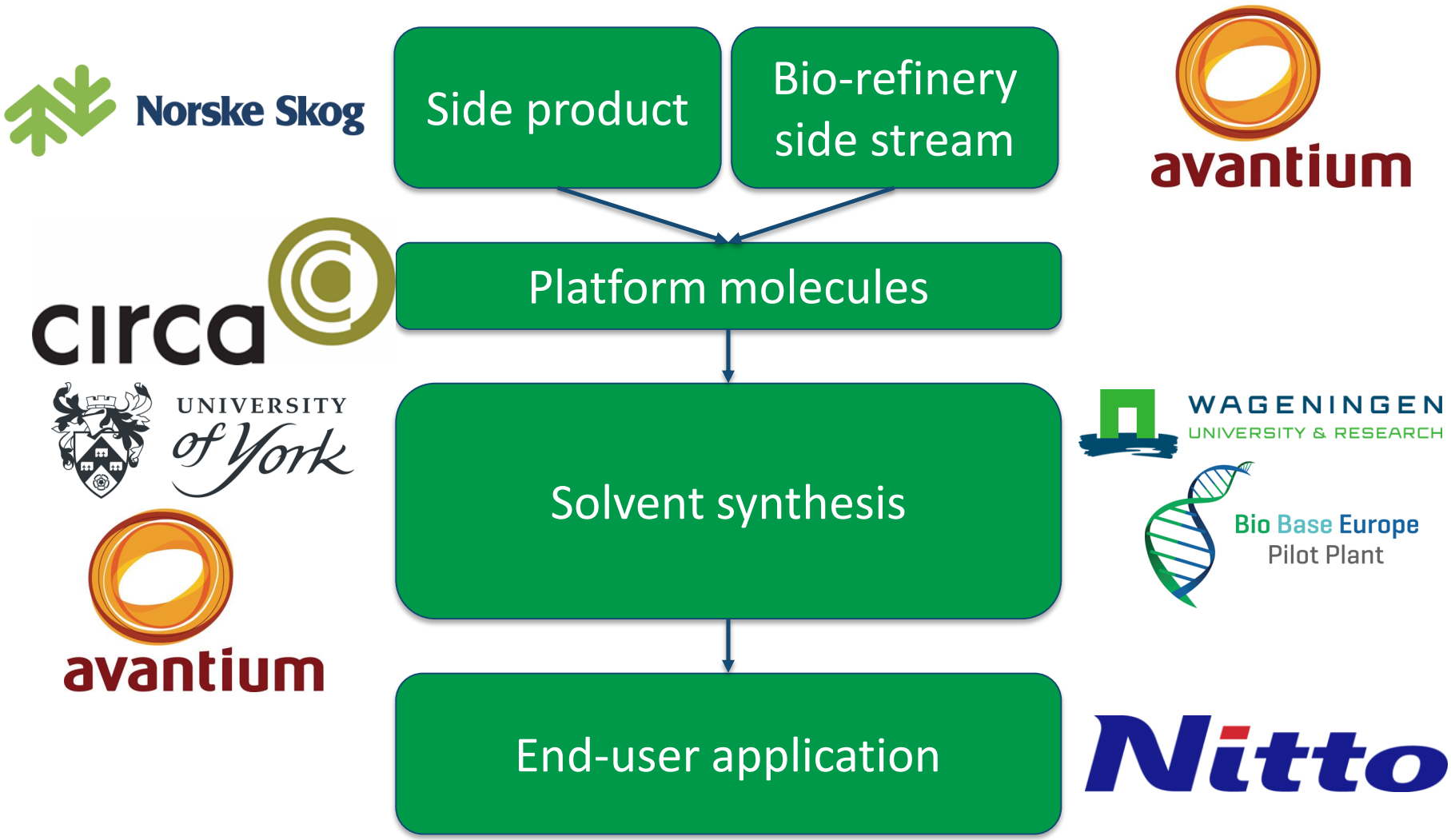
Aims for project

- Two solvents to replace toluene and NMP that will:
  - Be derivable from non-food carbohydrates (bio-based)
  - Have a lower impact on health and the environment
  - Have high performance in target applications
  - Offer economically viable and industry-relevant routes to manufacture

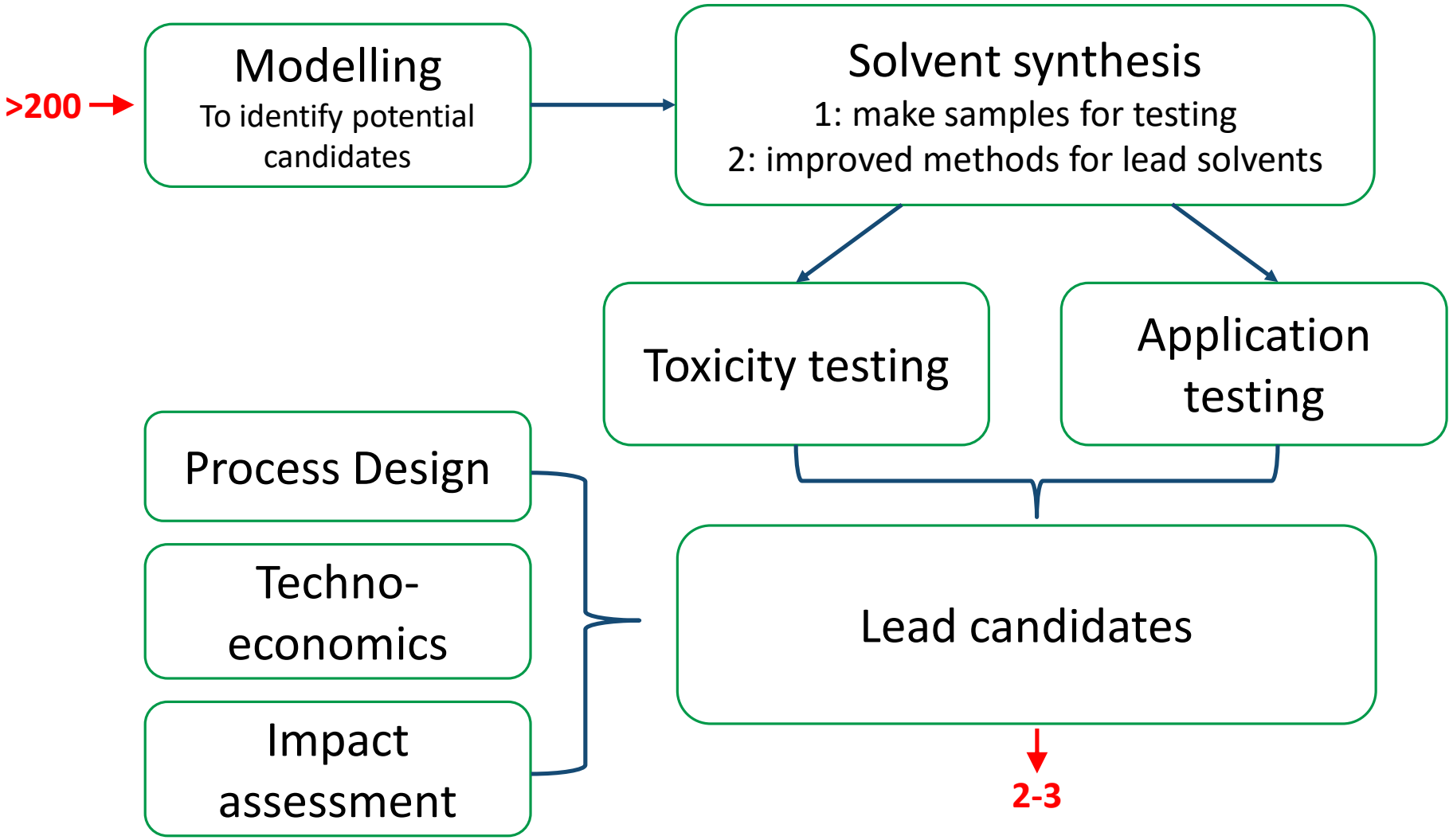
The concept


CELLULOSE
glucose
BEET PULP PECTIN
Platform molecule 1
Platform molecule 2
Platform molecule 3
Platform molecule 4
Platform molecule 5
Platform molecule 6
Modelling
Lab synthesis
&
Toxicity & application tests
Techno-economical & sustainability assessment
Nitrogen-free substitutes for NMP
Non-aromatic substitutes for toluene

Value chain


Side product
Bio-refinery side stream
Platform molecules
Solvent synthesis
End-user application
Norske Skog
avantium
circa
UNIVERSITY of York
WAGENINGEN UNIVERSITY & RESEARCH
Bio Base Europe Pilot Plant
avantium
Nitto

Project structure



Project progress

Modelling

Solvent synthesis

Physical properties for >200 compounds calculated and compared with experimental data

New method for calculating KAT parameters developed

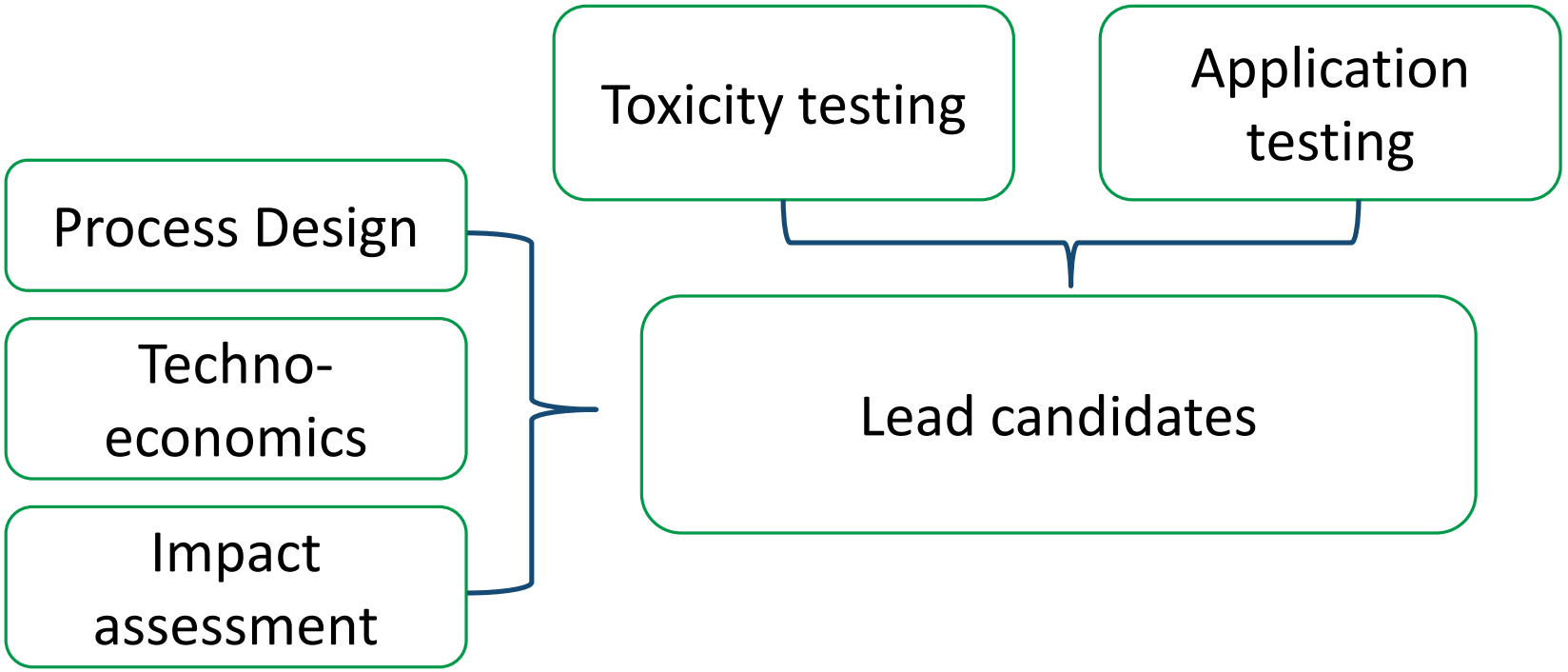
doi: 10.3390/molecules24122209

Samples sent for toxicity and application testing

Solvents chosen for lab-scale up/improved methods

Project progress

In the next talks you will hear more about:

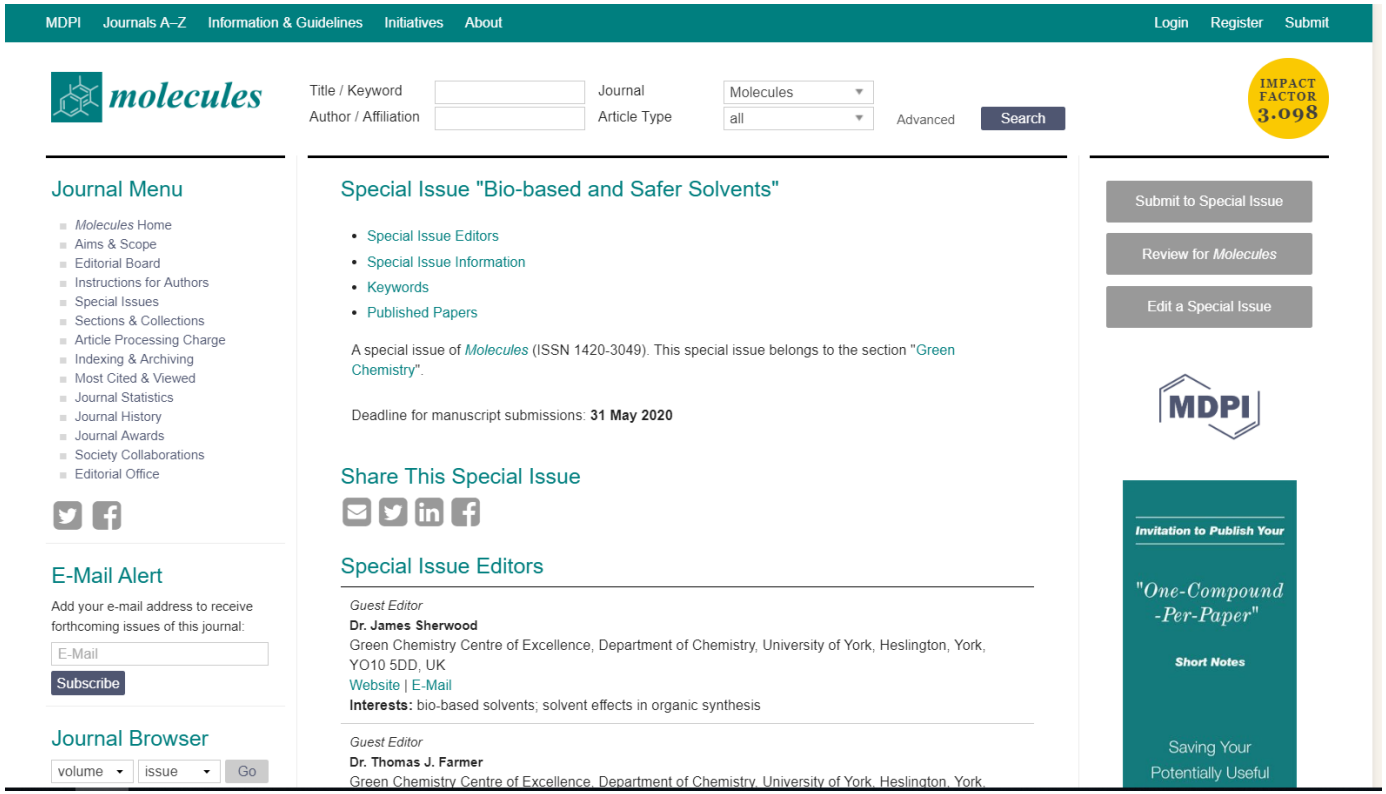


Plans for rest of the project

- Pilot-scale testing of lead toluene replacement in an industrial setting
- Lab-scale up for the most promising additional solvents
- Life-Cycle Analysis and Techno-Economic Evaluation completed for key solvents
- Application case studies published

Advertisement

- ReSolve is running a Special Issue on "Bio-based and Safer Solvents" hosted by *Molecules* (MDPI, Open Access), **submission deadline May 2020**



Project partners