inKemia
green chemicals

Company Overview

Driving Innovative Performance And Function Through The Transformational Power Of Green Chemistry

InKemia Green Chemicals, Inc.

Company Background

- InKemia Green Chemicals, Inc. is a subsidiary of InKemia IUCT Group.

- Company Mission: Development & commercialization of top performing and economical green chemical technologies.

InKemia IUCT Group in Figures

Team

- Knowledge division staff : 65 full time employees and 200 part time collaborators.
- All divisions and subsidiaries: more than 100 full time employees and 220 part time collaborators.

Patents

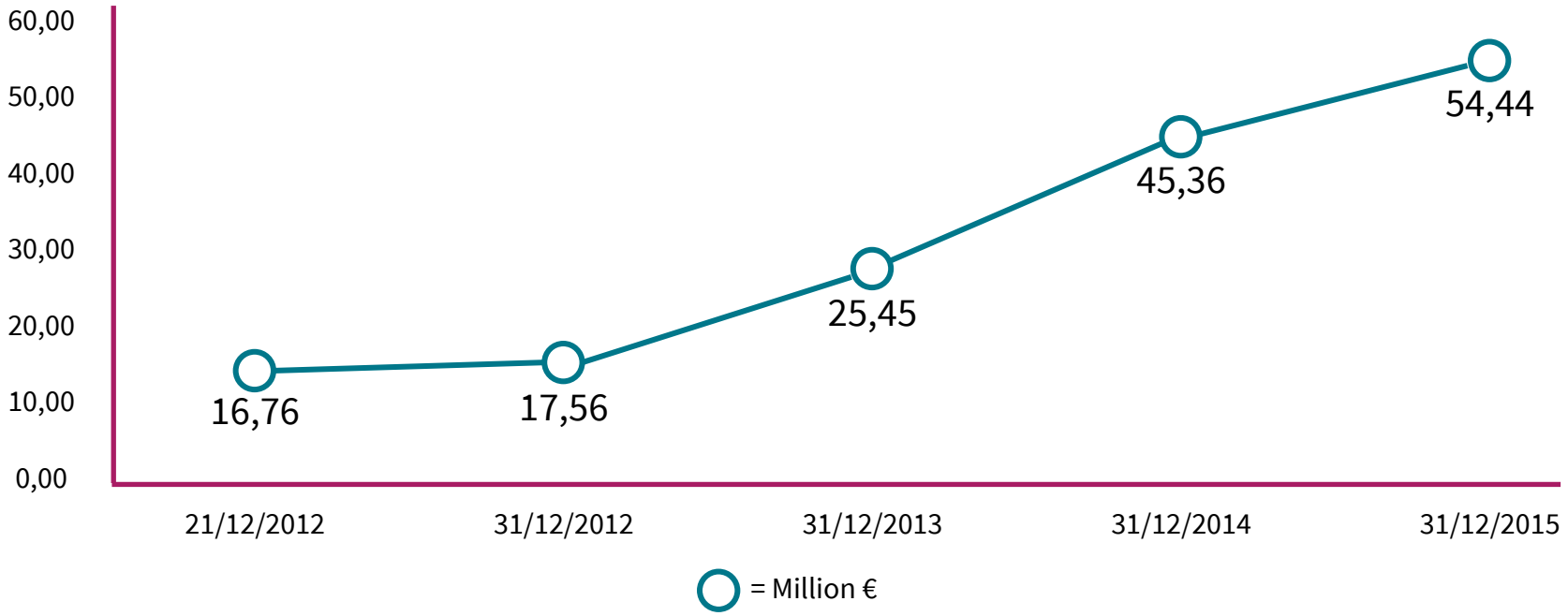
- International granted patents: 68 (26 patent families).
- Under examination: 150

Clients

- Industrial sector > 300

InKemia IUCT Group is listed in the Spanish Stock Market (MAB) since 2012: Ticker IKM

Value of IKM in Spanish Stock Market:



What Is Green Chemistry?

> “Green Chemistry is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances.”

Anastas, P. T. and Warner, J. C. Green Chemistry: Theory and Practice. Oxford University Press: New York, 1998, p. 30. By permission of Oxford University Press.

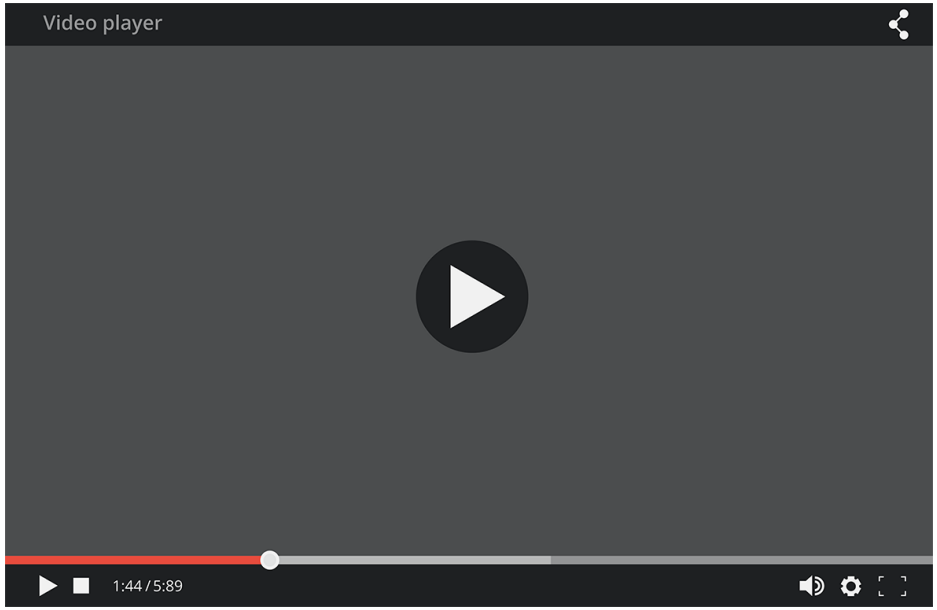
The 12 Principles of Green Chemistry

1. **Prevention**
2. **Atom Economy**
3. **Less Hazardous Chemical Syntheses**
4. **Designing Safer Chemicals**
5. **Safer Solvents and Auxiliaries**
6. **Design for Energy Efficiency**
7. **Use of Renewable Feedstocks**
8. **Reduce Derivatives**
9. **Catalysis**
10. **Design for Degradation**
11. **Real-time analysis for Pollution Prevention**
12. **Inherently Safer Chemistry for Accident Prevention**

Anastas, P. T. and Warner, J. C. Green Chemistry: Theory and Practice. Oxford University Press: New York, 1998, p. 30. By permission of Oxford University Press.

How Do We Use Green Chemistry?

Please watch this short video about Green Chemistry at InKemia Green Chemicals



What Can InKemia Green Chemicals Do For Your Company?

Identify an alternative green chemical that allows for enhanced performance.

Drive Formulation Performance Beyond State of the Art While Keeping Outstanding Sustainability Standards.

Improve Environmental, Health and Safety Profiles Without Compromising Technical Efficacy.

Design and Develop New Technologies and Products with Greener Chemicals.

How Do We Do It?

InKemia Green Chemicals is a trusted research & development partner for some of the most respected companies, as well as for government and academia

Unique Methodology

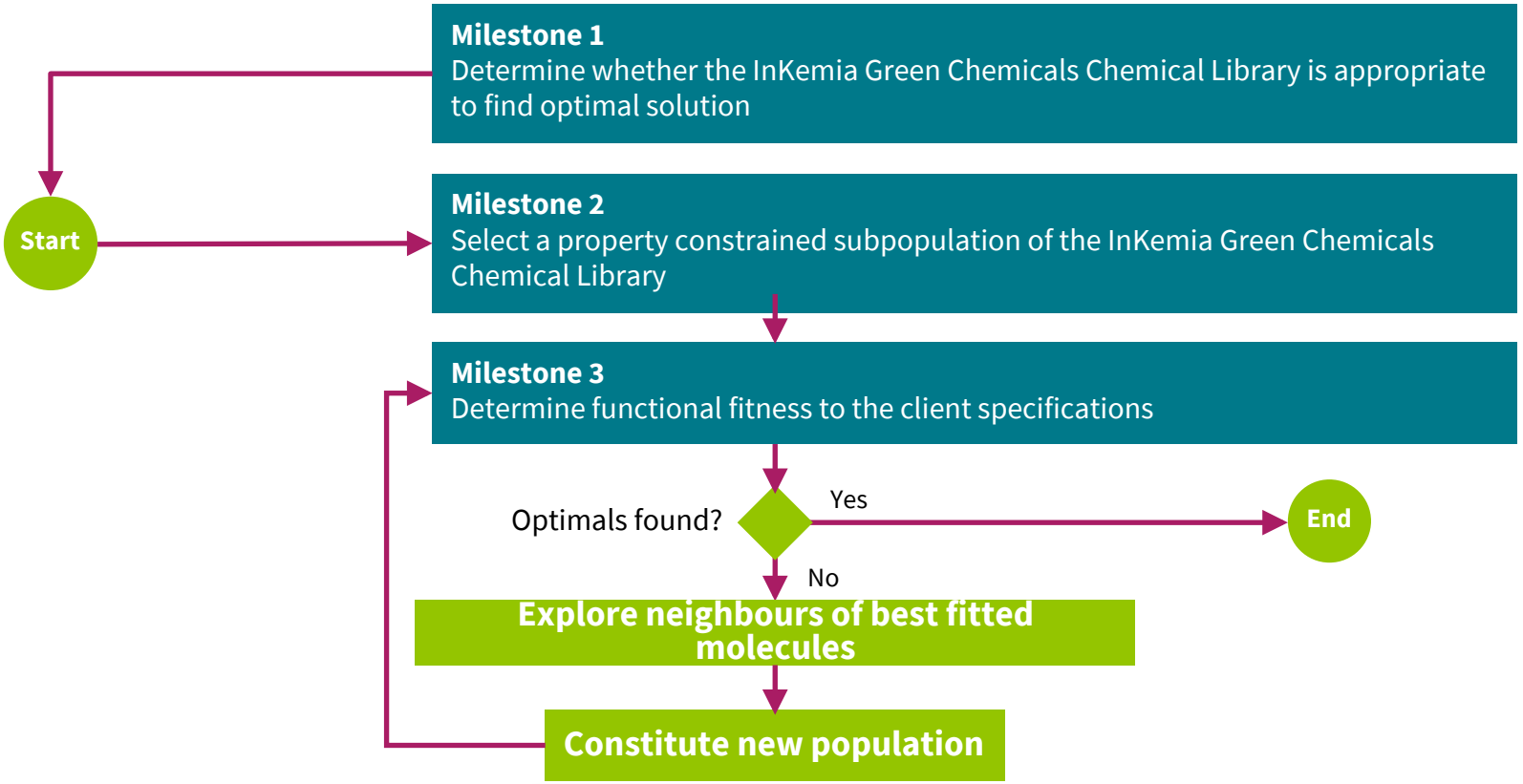
We use the most advanced computational and experimental platforms to achieve chemical design breakthroughs

Chemical Diversity

Our large and highly diverse chemical library ensures the best chance of success to find a solution

Methodology

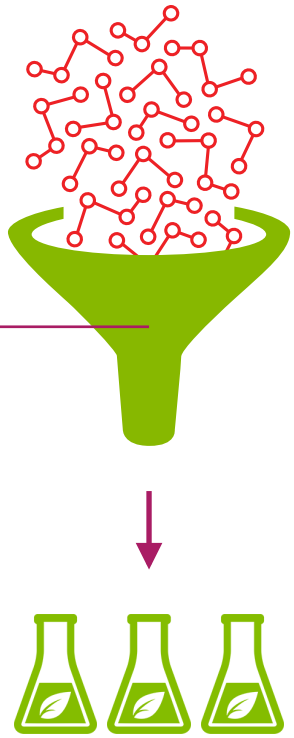
InKemia Green Chemicals partners with your R&D team to complete a low capital and highly time efficient R&D project to achieve your specific goal.



Chemical Diversity

Our highly diverse chemical library gives us the best opportunity to find an optimized solution for your company

Traditional Chemicals
80,000+



Environment, Health, and Safety Constraints + Performance Parameters

Small Number of Green Chemicals

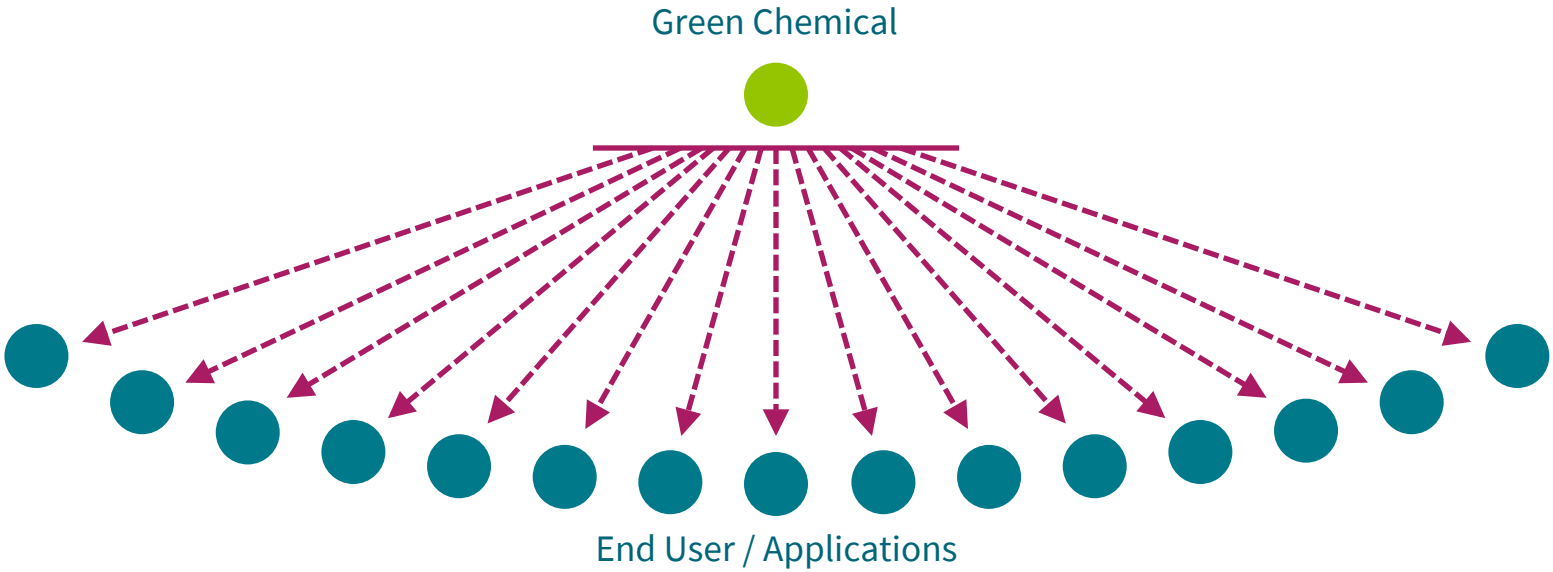
vs.

InKemia Green Chemicals has Hundreds of Green Chemicals

Old Approaches to Identifying Green Chemicals

Chemical Supplier: Commercialize one or a **few** green chemicals. The chemical is offered to **many** end/users.

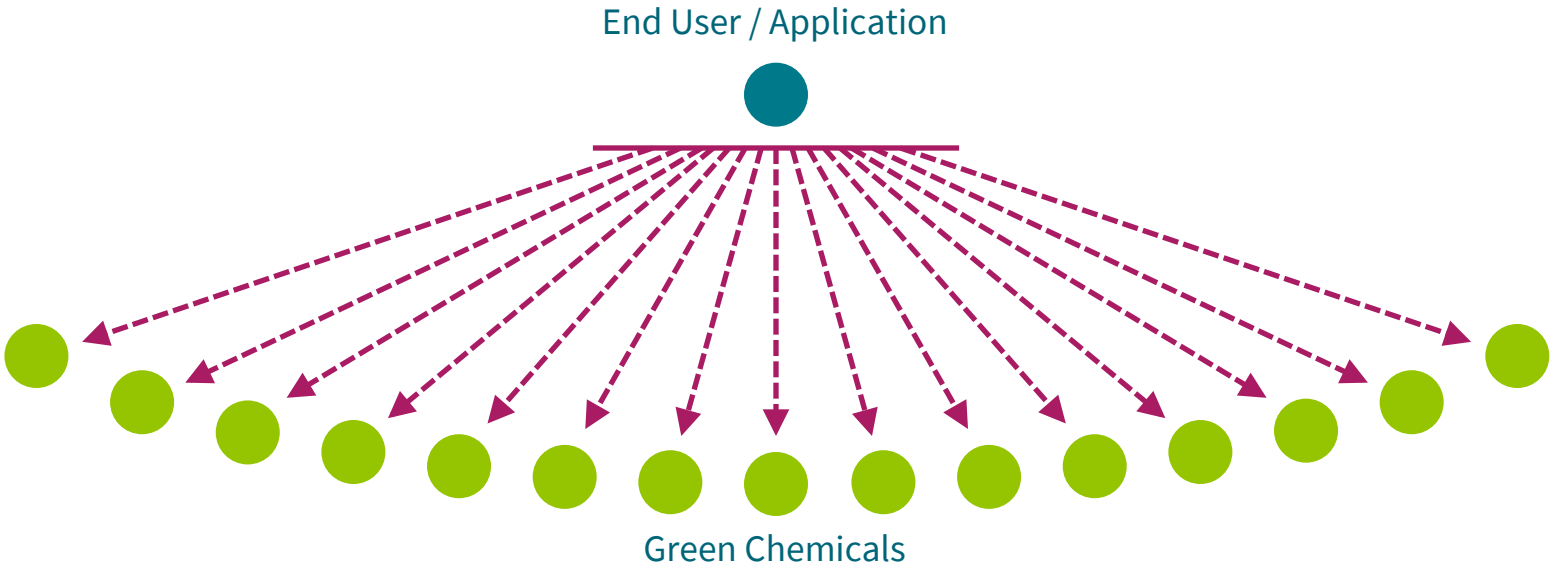
End User: Try **few** chemicals, get **poor** property match and technical efficacy is often suboptimal.



InKemia Green Chemicals Approach: Diversity + Methodology for Property Match

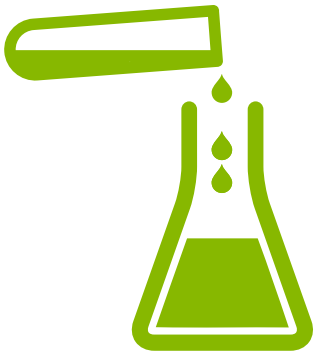
InKemia Green Chemicals: Commercialize **many** greener chemicals. A **few** chemicals are selected according to the functional specifications.

End User: Try **few** chemicals, get **excellent** property match and functional efficacy is now optimal.



Solvent Solutions

Our solvent library and unique discovery and search platform can tackle the most complex and challenging formulation problems.

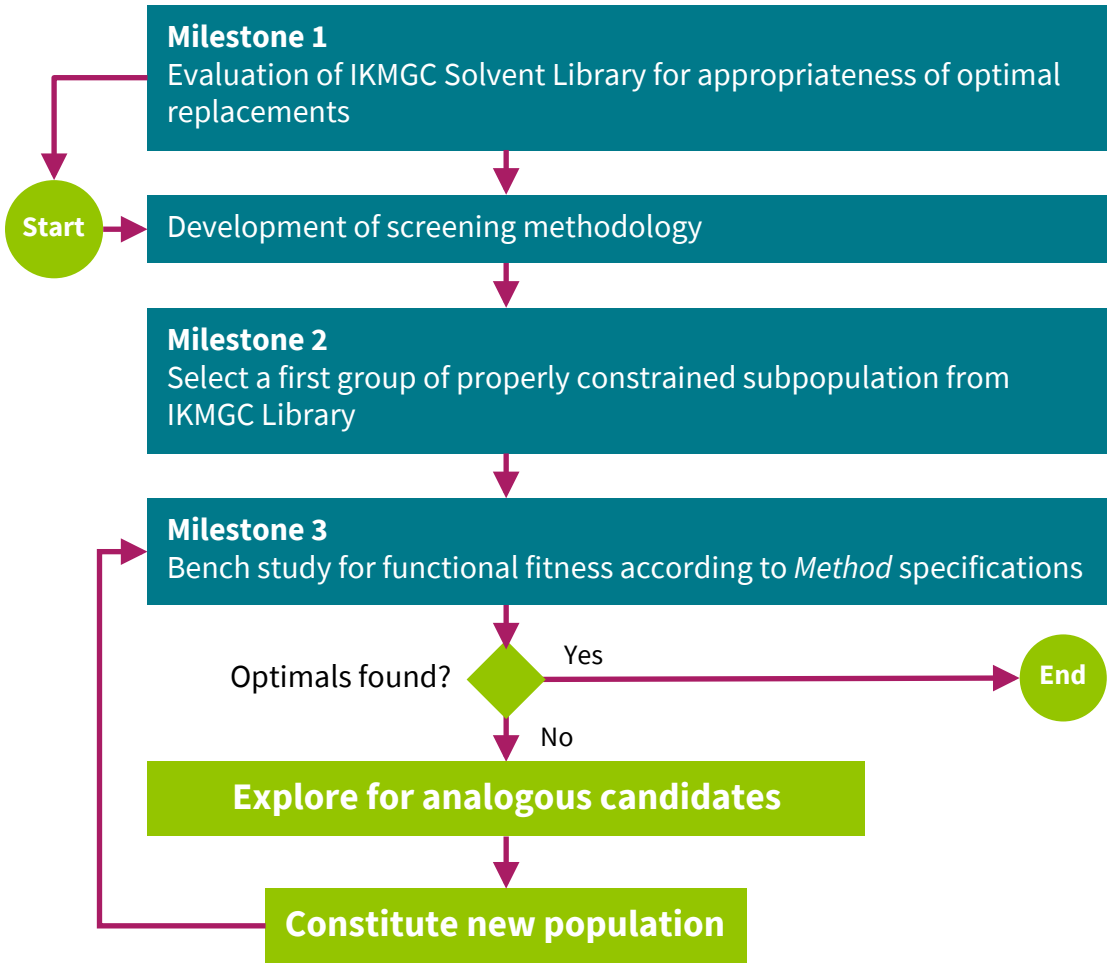


- Solvent library developed over a 20 year R&D history and composed > **250 green solvents** with more added each month.
- The solvent library + methodology leads to unique solvent solutions that differentiate the products of our clients.
- The goal of the InKemia Green Chemicals R&D solvent solutions projects is to maximize the probability of finding at least one functionally optimal solvent in the InKemia solvent library.

InKemia Approach: Project Flow Chart

The InKemia discovery strategy involves a sequential search procedure where solvent candidates are screened for functional property match.

To avoid long experimental testing campaigns in large libraries (the InKemia Solvent Library is composed of > 250 chemicals), R&D teams utilize a combination of proprietary advanced statistical experimental evaluation and learning algorithms.



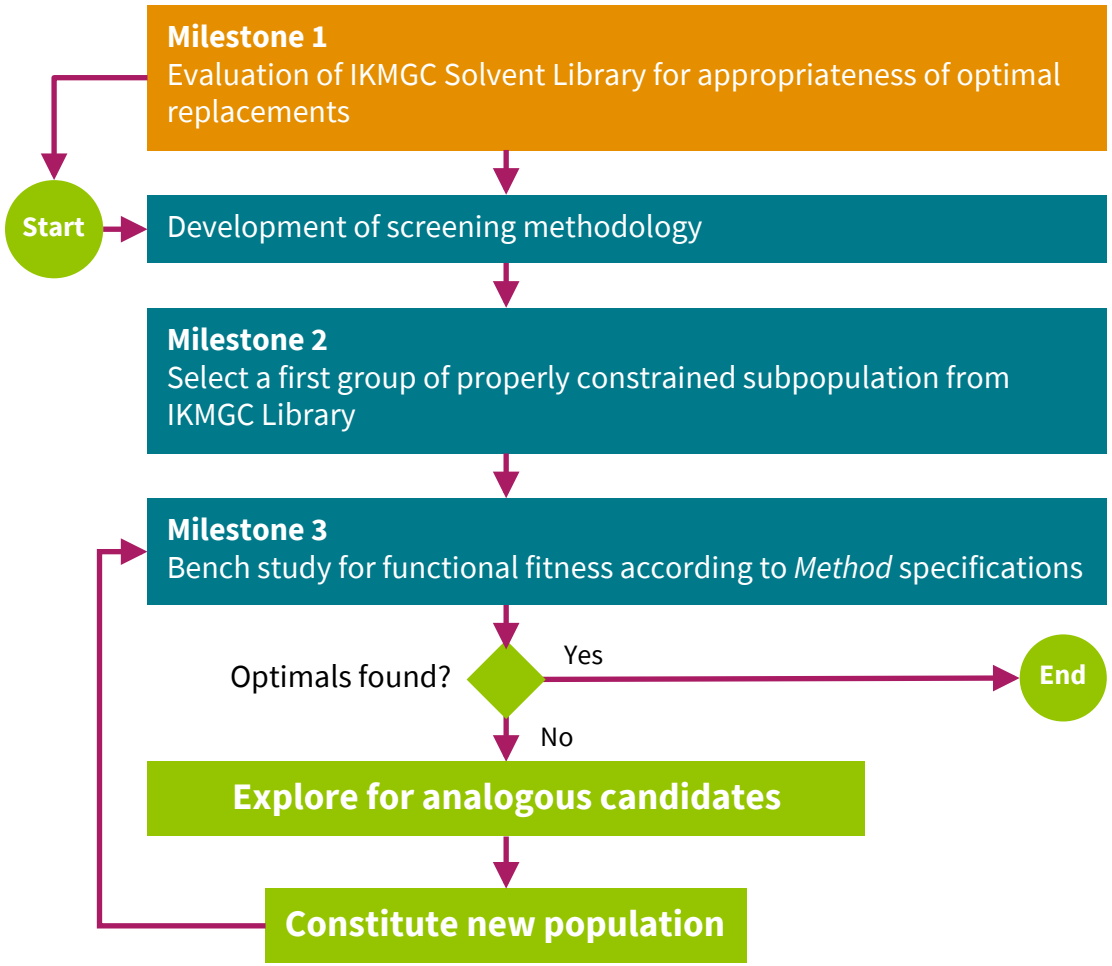
Milestone 1: Appropriatenes of IKM Library

Milestone 1:

Aimed at determining the appropriateness of the InKemia Library for each particular project.

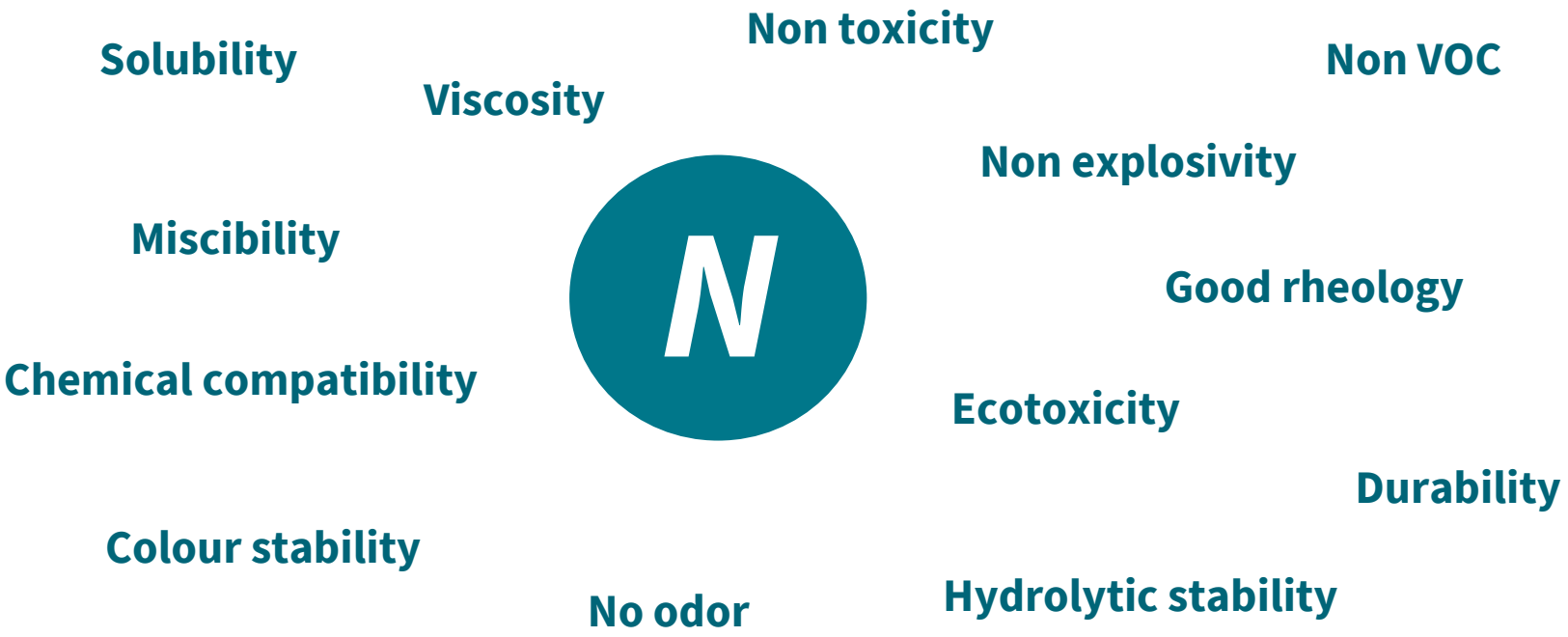
A Functional Data Sheet (FDS) is sent to the Client, filled with the required data and sent back to InKemia.

Based on the number and nature of essential functional variables, InKemia estimates the probability to find optimal solvents in the InKemia Library



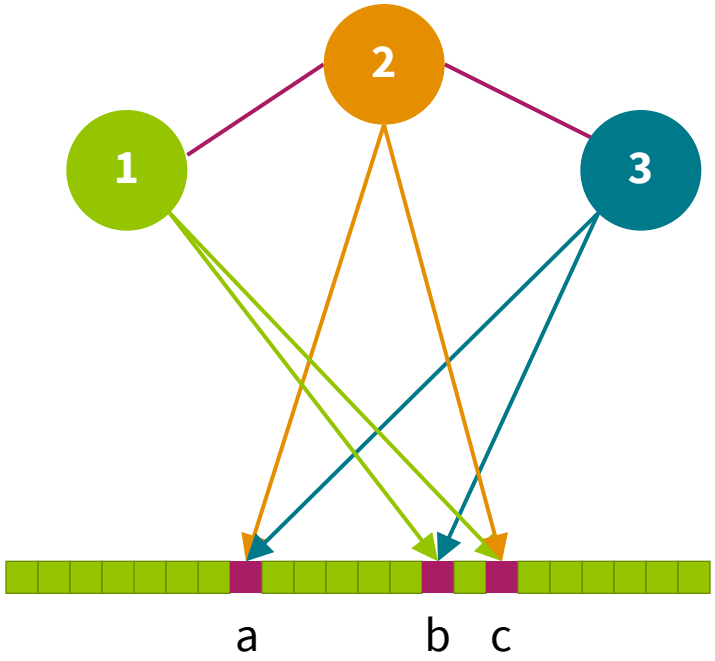
Milestone 1: Functional Variables

Chemical optimization problems in industry are complex. Multiple parameters to be optimized. Satisfying all parameters is the ultimate goal. FDS helps to determine the number and nature of the essential functional parameters, *N*.



Milestone 1: Fitness

InKemia makes a first estimation on how fitted is the InKemia Library to the complex function. Fitness, *f*, is evaluated by establishing preliminary structure-function relationships.

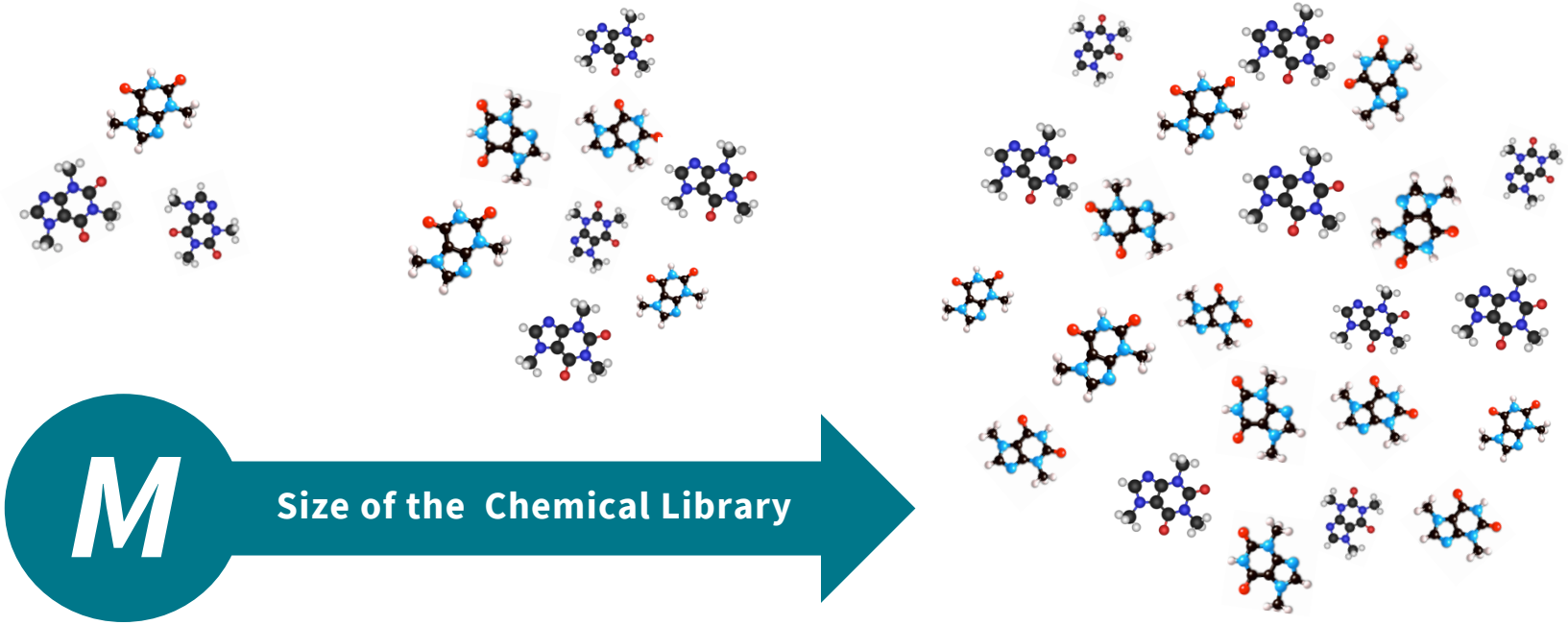


Structural Features

Functional Variables

Milestone 1: Library Size

InKemia has developed a large and diverse chemical library fitted to the functional requirements of a variety of industrial problems. The size, *M*, of the InKemia library together with *N* and *f* make it possible to calculate the probability of finding a solvent that matches the *N* functional parameters.



Milestone 1: Probability of Success (1)

The goal of Milestone 1 is to estimate an upper threshold of the probability α (1) of finding at least one functionally optimal solvent. This probability is discussed with the Client who makes a GO/NO GO decision.

$$\alpha(1) = f(N, M, f)$$

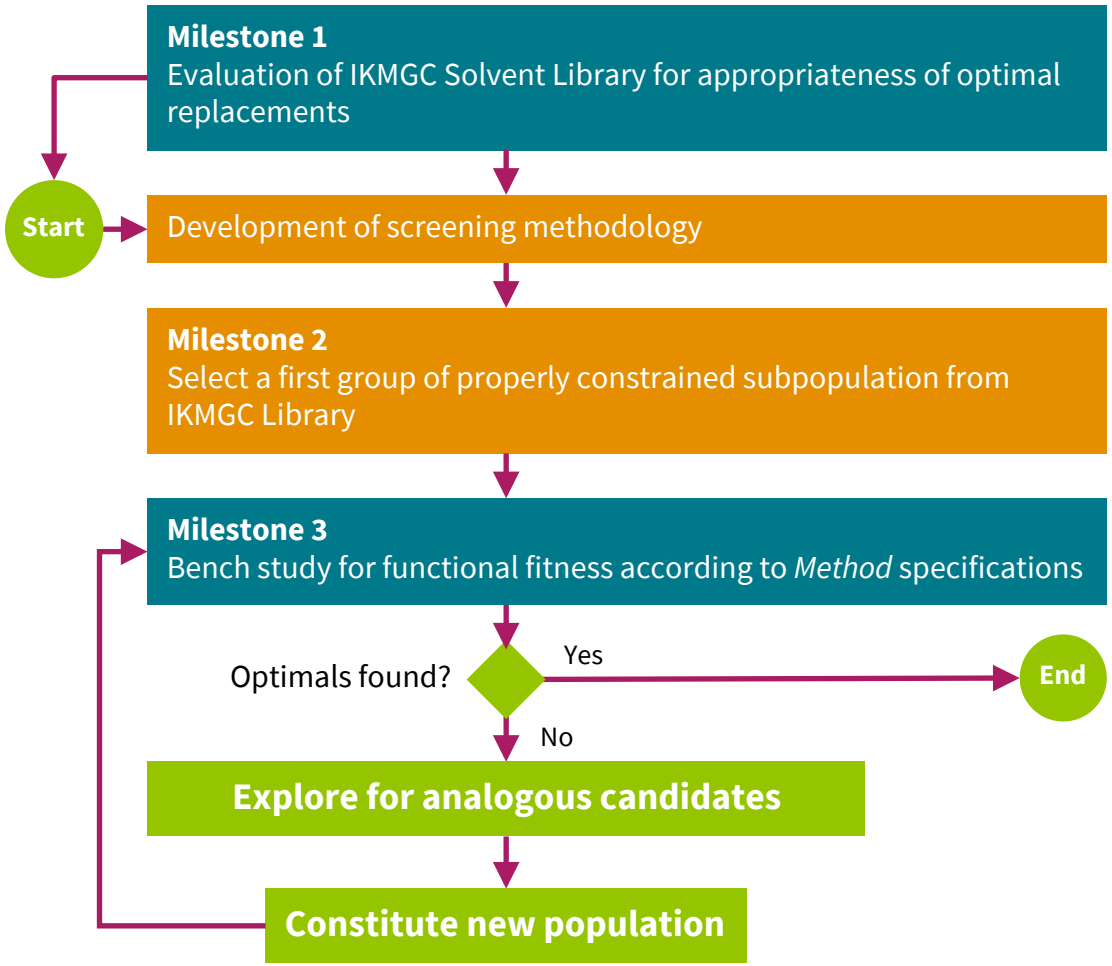
Milestone 2: Screening and Selection

Milestone 2:

A selected group of solvent candidates is selected and iteratively screened for functional performance.

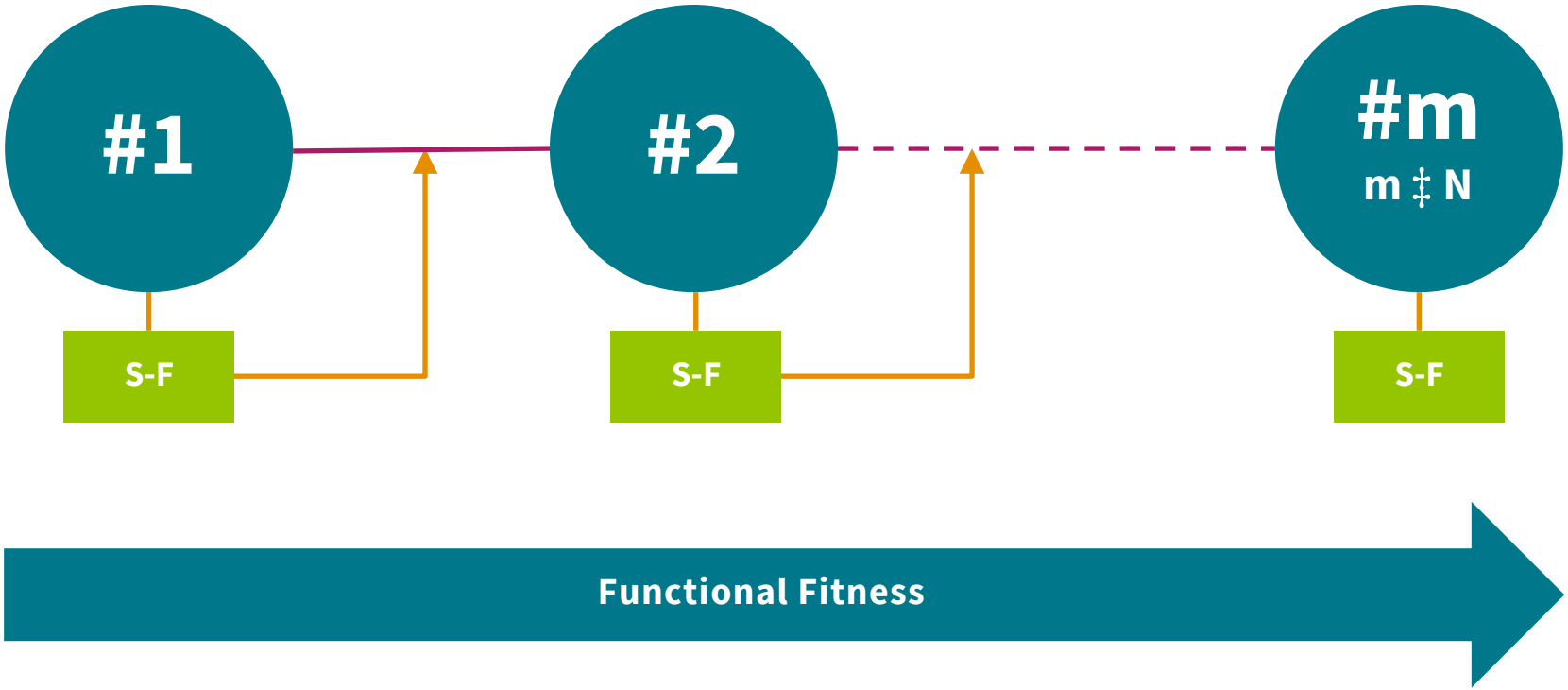
Functional property match is evaluated for each candidate using either predictive tools (if the system is sufficiently understood) or simplified laboratory screening experiments or both.

A subpopulation of optimal candidates is identified.

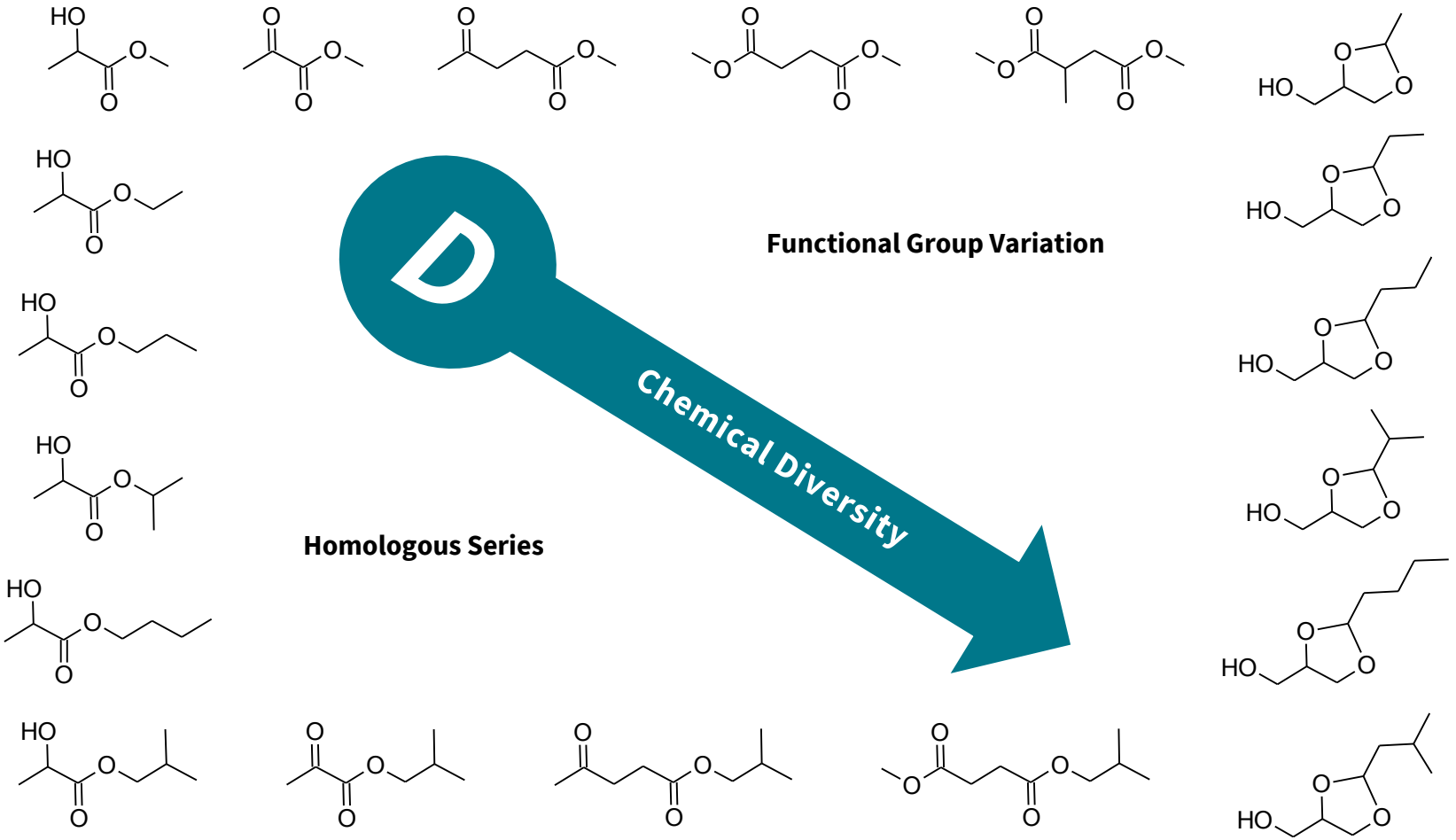


Milestone 2: Structure-Function

Predictive and experimental evidence is used to refine structure-function assumptions and climb iteratively to higher altitudes in the functional fitness landscape.



Milestone 2: Molecular Diversity



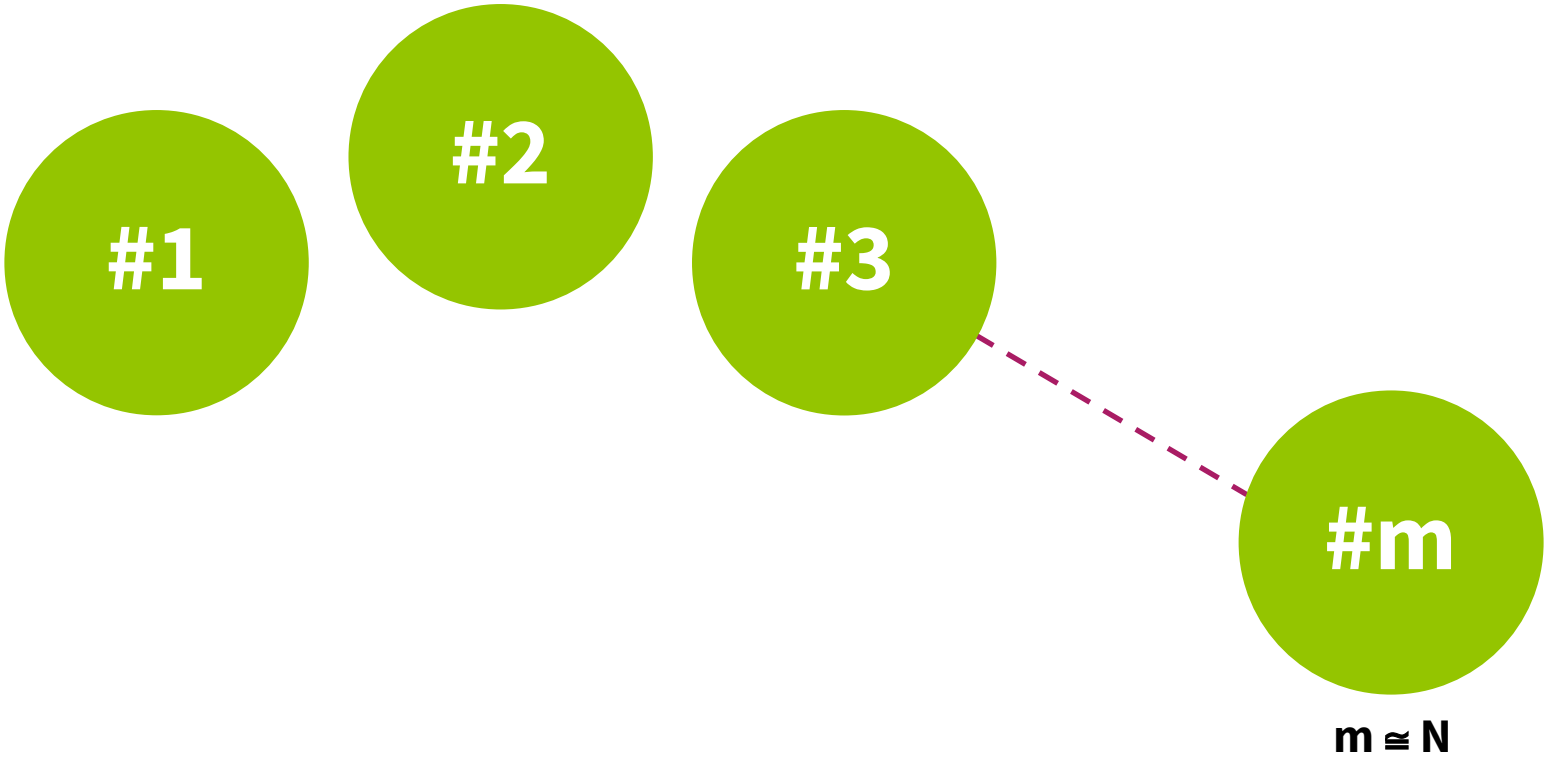
Milestone 2: Probability of Success (2)

The probability of finding an optimal solvent in the InKemia Library is refined. In particular, the information gained in the iterative screening and the molecular diversity used allows us to calculate an exact value of such probability, a (2). This probability takes into account conflicting constraints and non linearities due to synergistic and antagonistic effects. Again, this probability is continually reported and discussed with the Client who can make a GO/NO GO decision at any stage of progress.

$$\alpha(2) = f(N, M, f)$$

Milestone 2: Subpopulation Selection

The best possible candidates, those displaying very high fitness values are selected for further evaluation and validation.



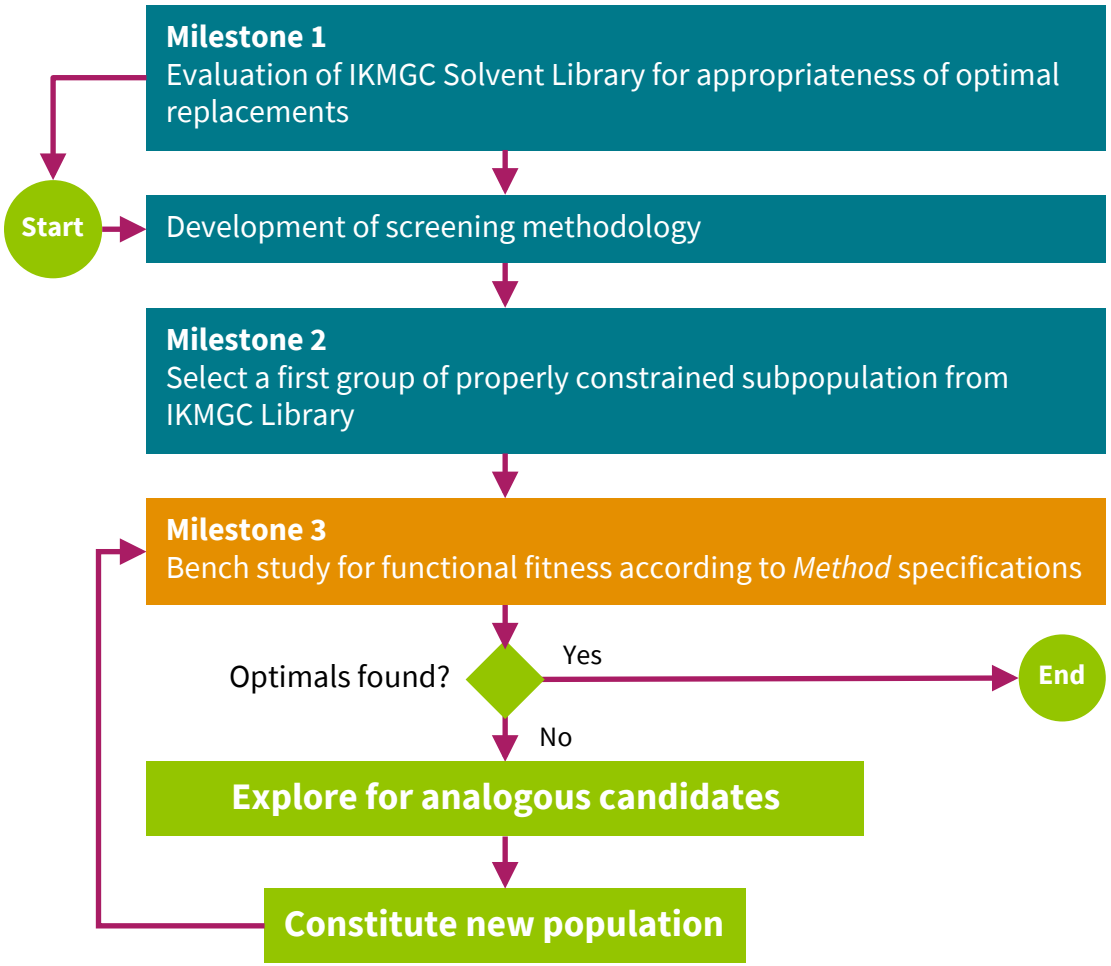
Milestone 3: Validation

Milestone 3:

The subpopulation of selected solvents is now evaluated in relevant industrial settings.

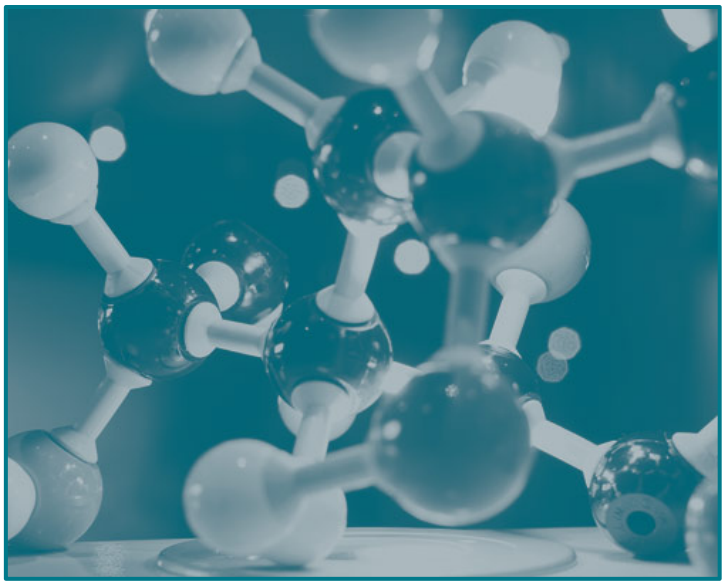
The formulations using the selected solvents are validated against official test methods (e.g., ASTM).

The best candidate is selected.



Conclusions:

- InKemia offers its rich chemical ensemble and its unique discovery and search platform to tackle the most complex and challenging formulation problems.
- The goal is to maximize the probability of finding at least one functionally optimal solvent in the InKemia solvent library.
- This is done through a sequential process and assuring that the best possible trade-off between information and cost is achieved.



Our History Of Success

We provide chemical products and services for multiple business sectors, many of which are not listed here.

Adhesives

Agricultural

Cosmetics

Paints & Coatings

Household & Consumer Goods

Electronics

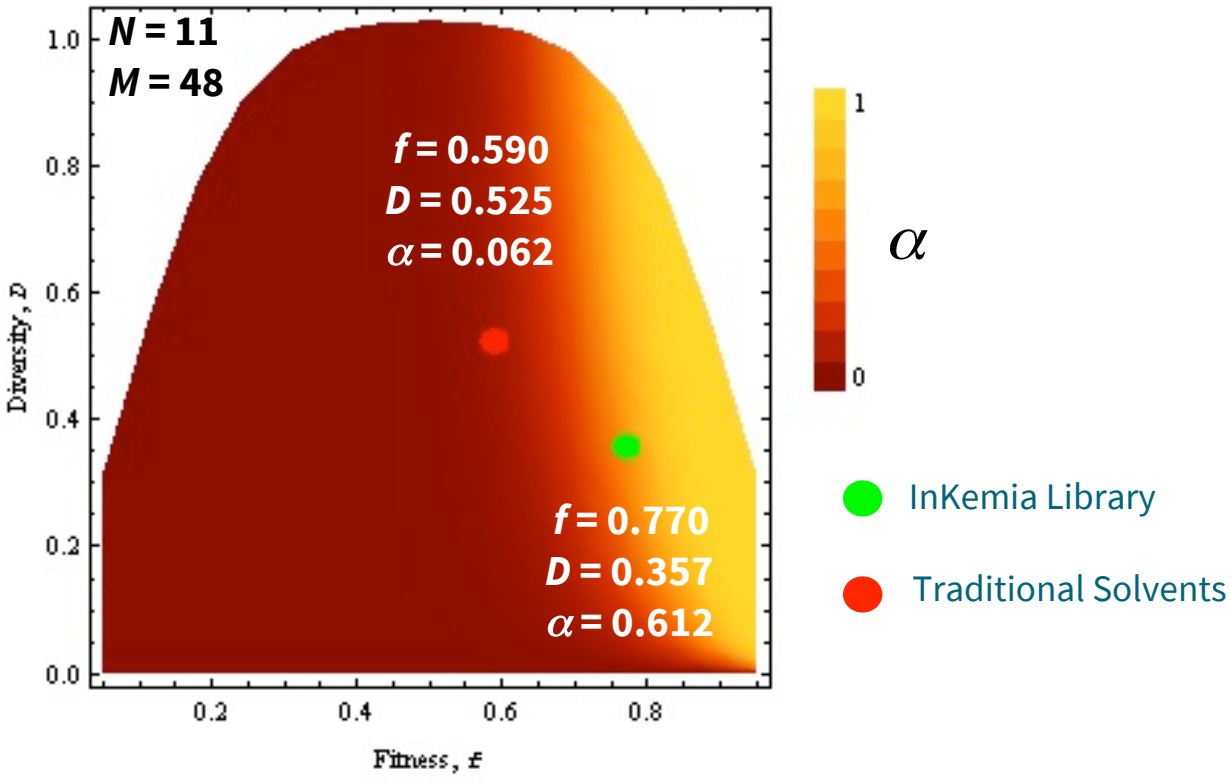
Textiles

Energy

The InKemia Solvent Library Applied to Metal Degreasing Challenge

- The Challenge: To find a replacement for trichloroethylene for the degreasing of sinterized metal parts by immersion and ultrasonication.
- Functional Specifications:
  1. Hansen dispersion solubility parameter
  2. Hansen polar solubility parameter
  3. Hansen hydrogen bond solubility parameter
  4. Surface tension
  5. Boiling point
  6. Molar Volume
- Sustainability Constraints
  7. Environmental impact: Low Environmental Hazard (Levels 0, 1 in Column Model)
  8. Human Safety: Low Health Hazard Risk (Levels 0, 1 in Column Model)
  9. Non VOC
  10. Flammability
  11. Human Exposure

The InKemia Methodology Starts With the Calculation of the Probability α of Finding an Optimal Solvent



Sinterized Metal Parts

Operating Environment

Ultrasonic Degreasing at 58ºC

Time: 0 min 40 min 90 min

Optimal Conditions for Complete Degreasing

Immersion, 3 h @ 22°C
Incomplete degreasing

Ultrasonication, 3 h @ 58°C
Complete degreasing

Summary Metal Degreasing

- Three solvents found to display excellent removal efficiencies for metal protectors under ultrasonication conditions.
- The low vapor pressure of the solvents make them suitable for immersion or spray open systems.
- The operating procedure involves the recovery and reutilization of the solvent.
- The inherent safety of the solvents derisks the working place.

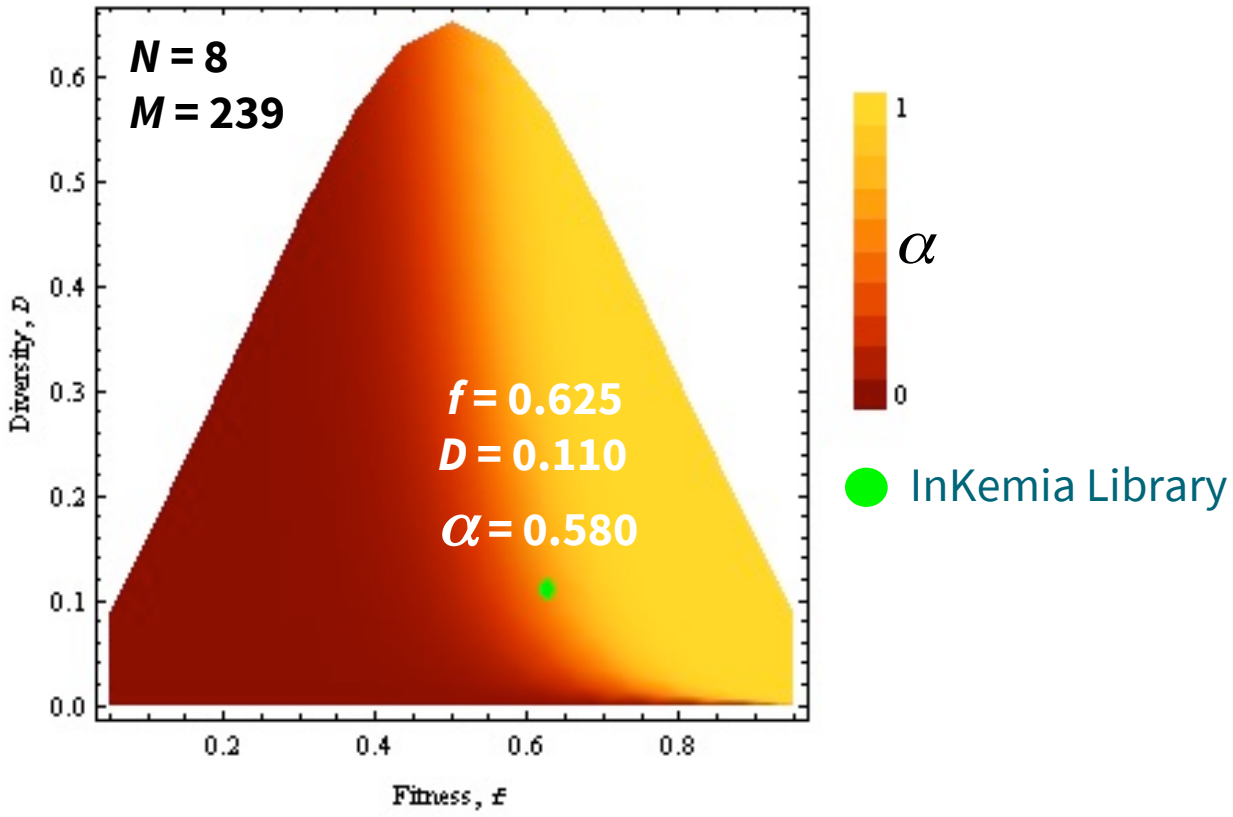
The InKemia Solvent Library Applied to an Herbicide “Tank Mix” Composition

- The Challenge: Replacement of aromatic hydrocarbons by a non-VOC safer solvent

- Functional Specifications:
  1. Solvent hydrolytic stability
  2. Chemical compatibility
  3. Emulsion stability
  4. Leave coverage
  5. Active ingredient uptake
  6. Selective phytotoxicity

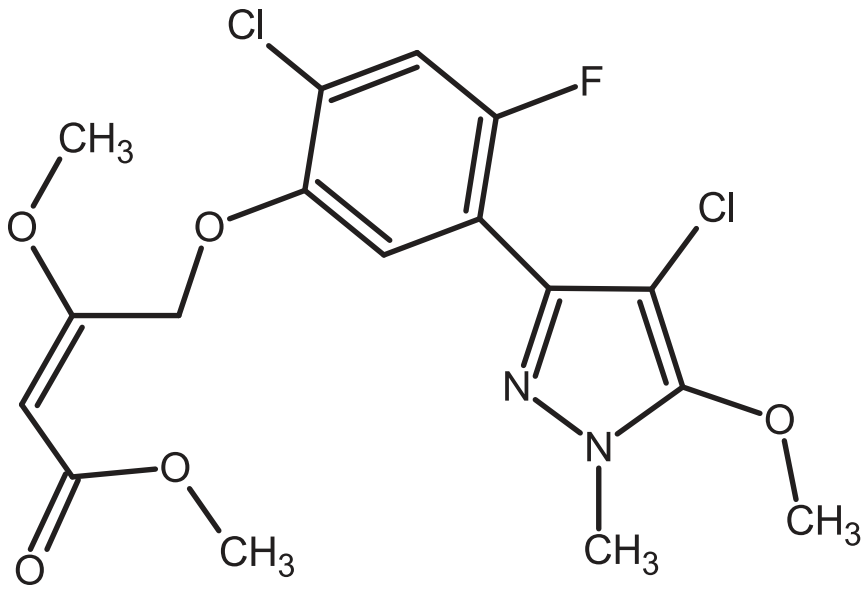
- Sustainability Constraints
  7. Health hazard (Column Model Level 0 or 1)
  8. Environmental impact (Column Model Level 0 or 1)

Probability α of Finding Optimal Solvent in the InKemia Library



Experimental Herbicide of the Class of the Protoporphyrinogen Oxidase Inhibitors

The active ingredient is combined with the solvent and the emulsifier component to form a stable emulsifiable concentrate, then the farmer adds water to form a microemulsion



Field Trials

Post-emergence control of *Gallium aparine* treated with PPO inhibitor

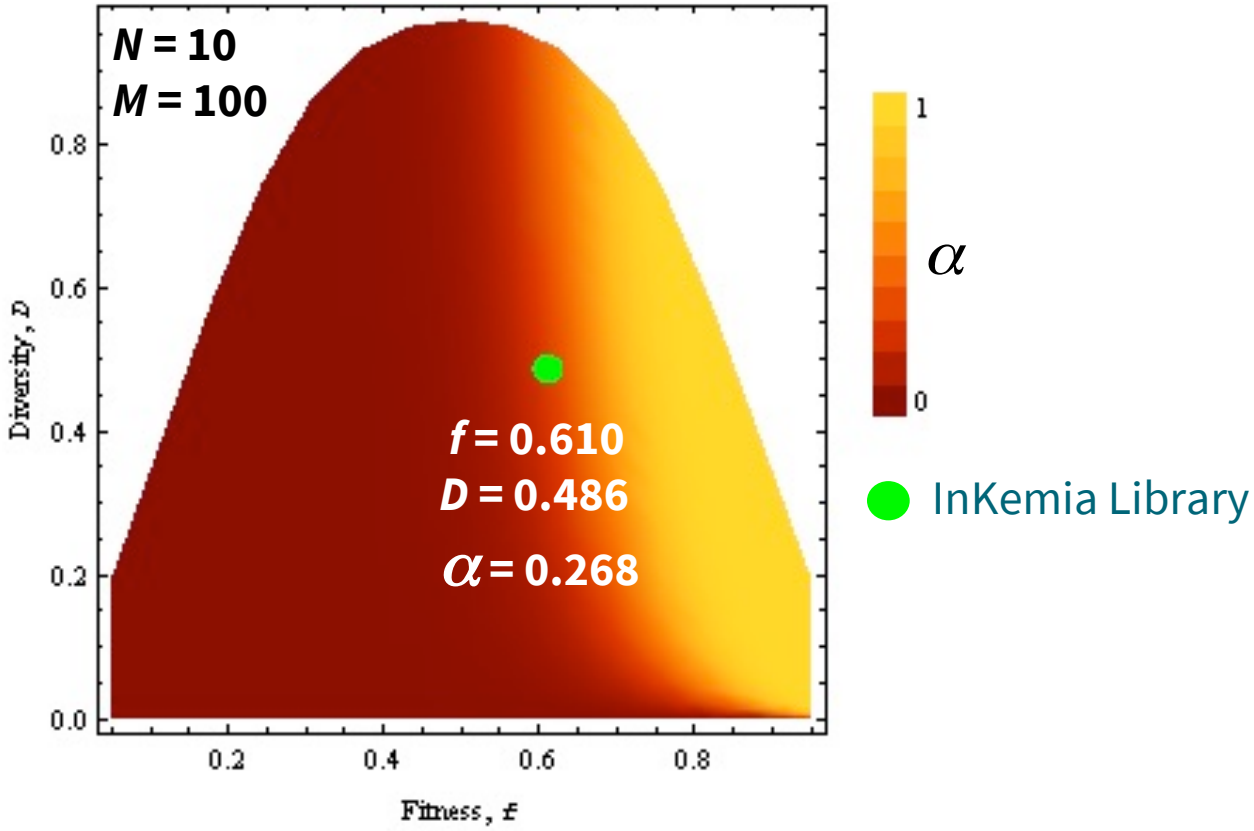
Summary: Herbicide Composition

- The standard solvent used in the formulation of PPO inhibitor is Solveso 100, a solvent consisting of a mixture of aromatic hydrocarbons.
- The formulation with Solveso 100 cannot reduce phytotoxic effects towards the crop.
- Long chain alkyl esters from InKemia Library offer much more selectivity, eliminating the adverse effects on crops.
- The green solvent increased the biological effects of the herbicide which in turn allowed to reduce the application rate in order to obtain the same selectivity towards crops.

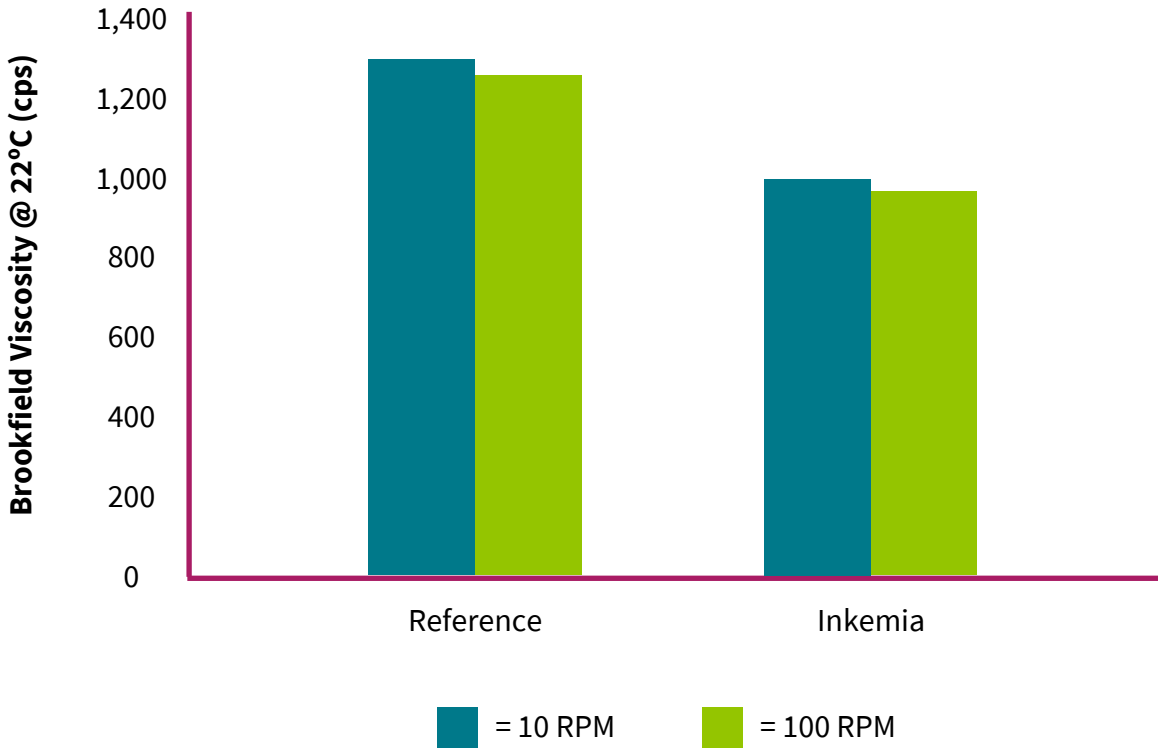
The InKemia Solvent Library Applied to a Marine Paint Formulation

- The Challenge: Replacement of a VOC hydrocarbon solvent (White Spirit) by a non-VOC reactive diluent in a marine paint formulation
- Functional Specifications:
  1. Viscosity
  2. Film formation and levelling (appearance)
  3. Colorimetric stability (no yellowing)
  4. Drying time
  5. Hardness (Persoz)
  6. Gloss
  7. Adhesion to metal and wood
  8. Chemical resistance
- Sustainability Constraints
  9. Health hazard (Column Model Level 0 or 1)
  10. Not classified Volatile Organic Compound (VOC)

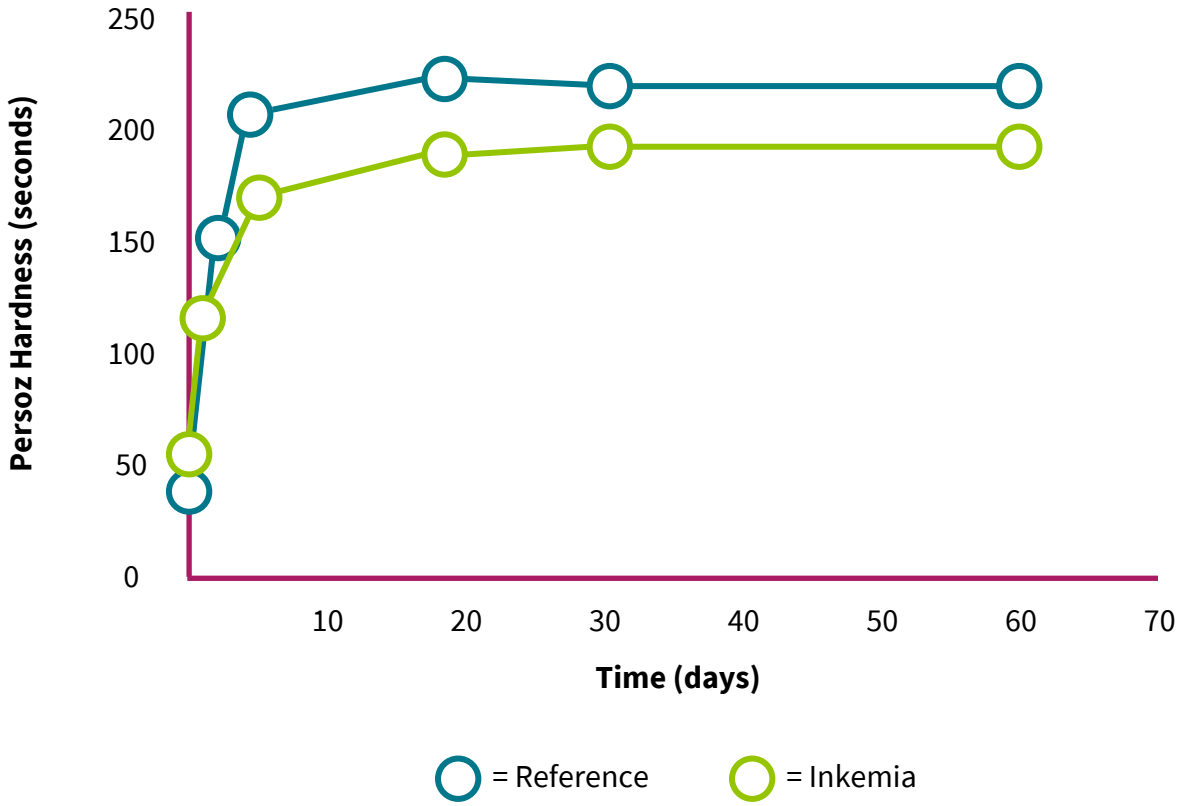
Probability α of Finding Optimal Solvent in the InKemia Library



Viscosity of the Paint Formulation is Significantly Reduced



Hardness is Acceptable and Comparable to the Reference Solvent



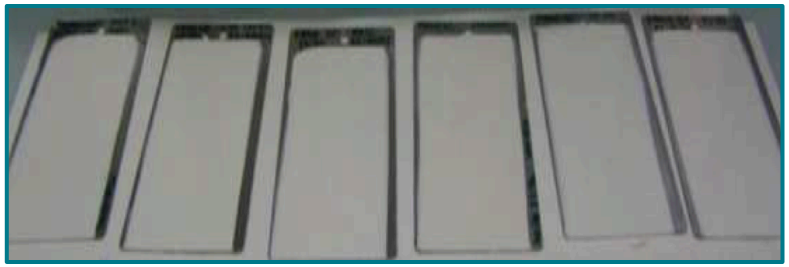
Good Film Formation and Leveling

Alkyd-Urethane in Iroko Wood

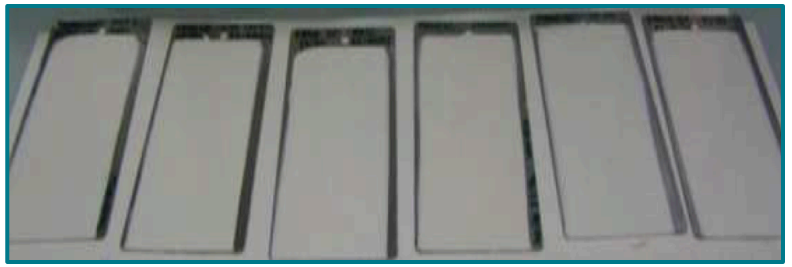
Reference

InKemia

Alkyd-Urethane in Metal Substrates

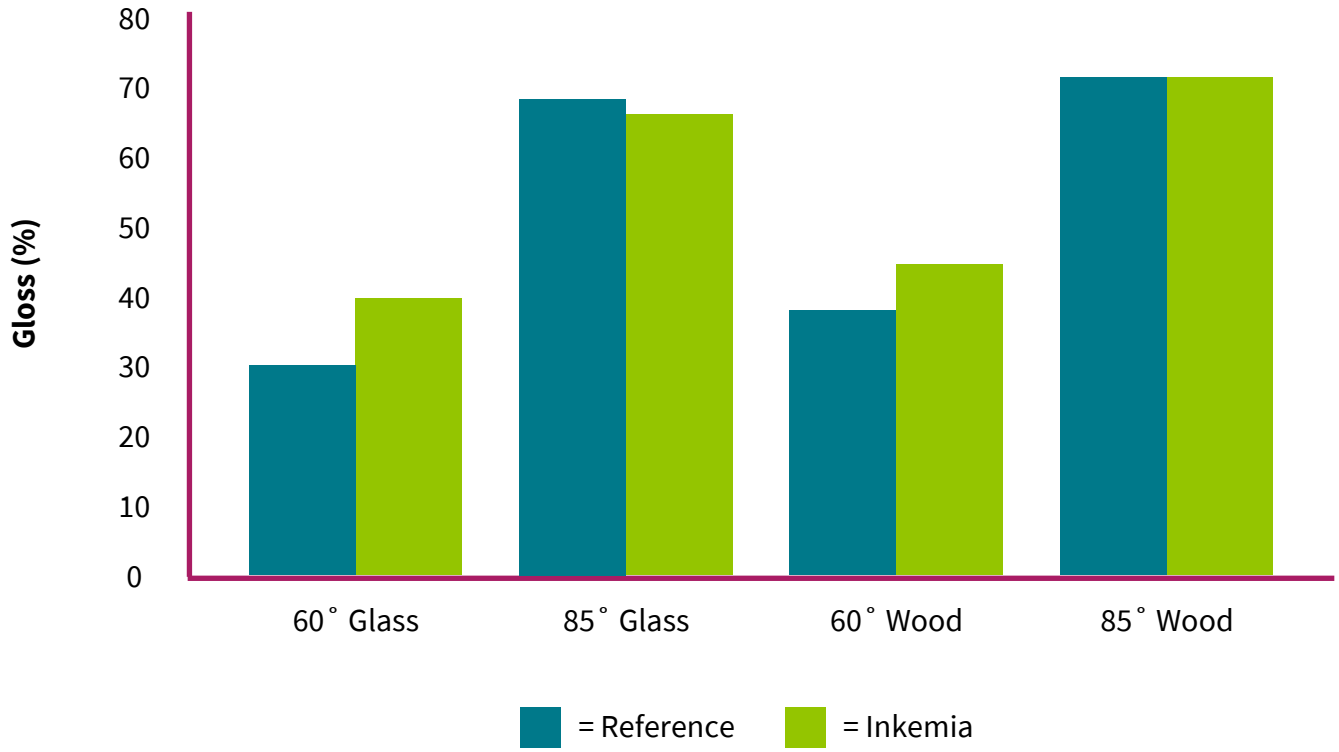


Reference



InKemia

Viscosity of the Paint Formulation is Significantly Reduced



Very Good Adherence and Substrate Wetting

Adherence cross-cut test indicates a very good adherence on wood with clear cutting and no detachment of small flakes.

Classification according to EN ISO-2409 standard

Reference: Class 0-1

InKemia: Class 0-1

Similar Chemical Resistance

Chemical Resistance ISO2812 // ISO4628	Reference	InKemia
Water 24 h // Recovery after 24 h	0 // 0	0 // 0
Ethanol 24 h // Recovery after 24 h	3-4 // 4	3-4 // 4
Hand cream 24 h // Recovery after 24 h	4 // 3	4 // 3

- Class 0: Excellent, without damage
- Class 3: Some damage is observed depending on the viewing angle, although it is suitable.
- Class 4: Considerable damage is observed, independently on the viewing angle. It is not suitable.

No Yellowing Is Observed

	Spectrometry CIELAB	Reference	InKemia
Iroko Wood	L*	94.76	95.39
	a*	-0.39	-1.07
	b*	5.55	4.53
	dE	-	***1.27***
Steel	L*	94.31	95.02
	a*	-0.48	-1.31
	b*	4.84	5.67
	dE	-	***0.96***

Target: dE below **2.00**

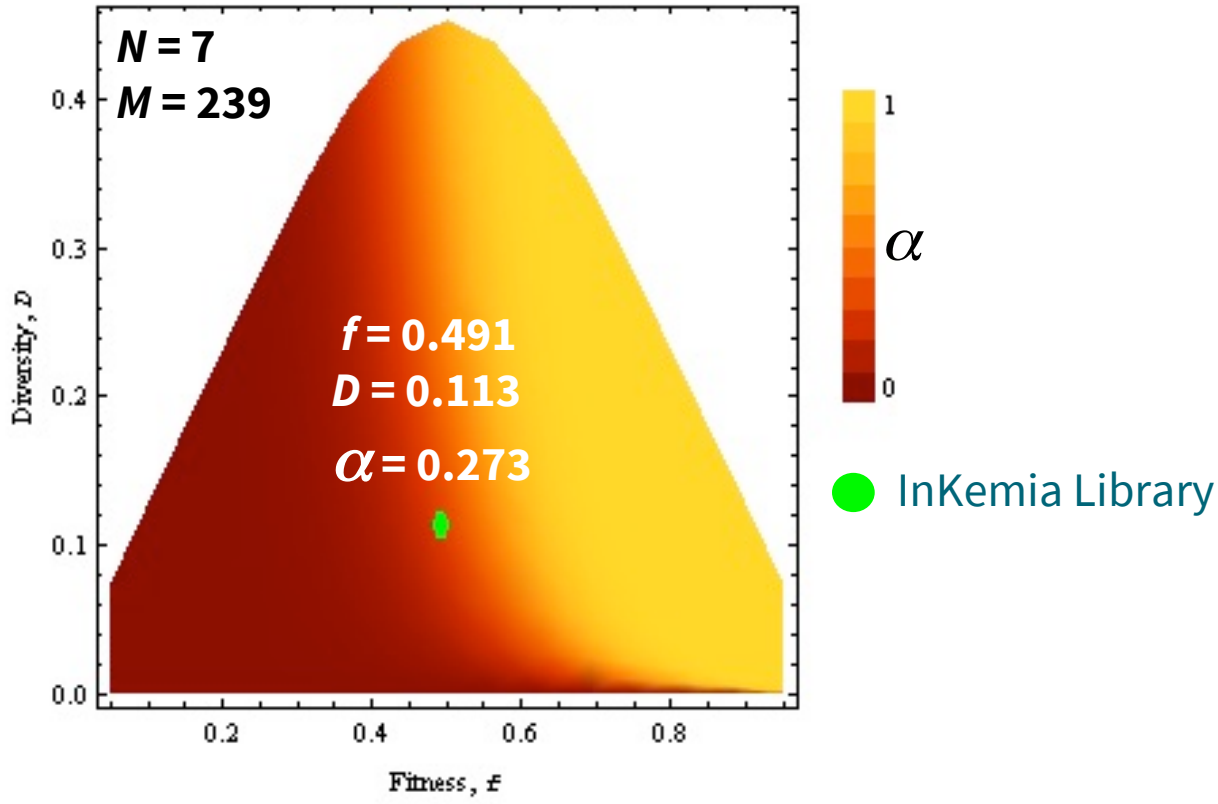
Summary Marine Paint

- One solvent found optimal in a subset of 100 solvents of the InKemia Library
- The InKemia solvent replaces a VOC hydrocarbon solvent meeting 8 functional specifications. It also displays reduced health and environmental hazards. In particular:
  - Significantly lower paint viscosity when compared to the industrial reference solvent
  - Slightly higher gloss, some adjustment using little quantities of matting agents should be done
  - Suitable drying
  - No yellowing, perfect white colour is developed
  - Good aspect: levelling and film formation
  - Good chemical properties and natural ageing (outdoor conditions)
- Synthesized via enzymatic catalysis from cheap and renewable feedstocks

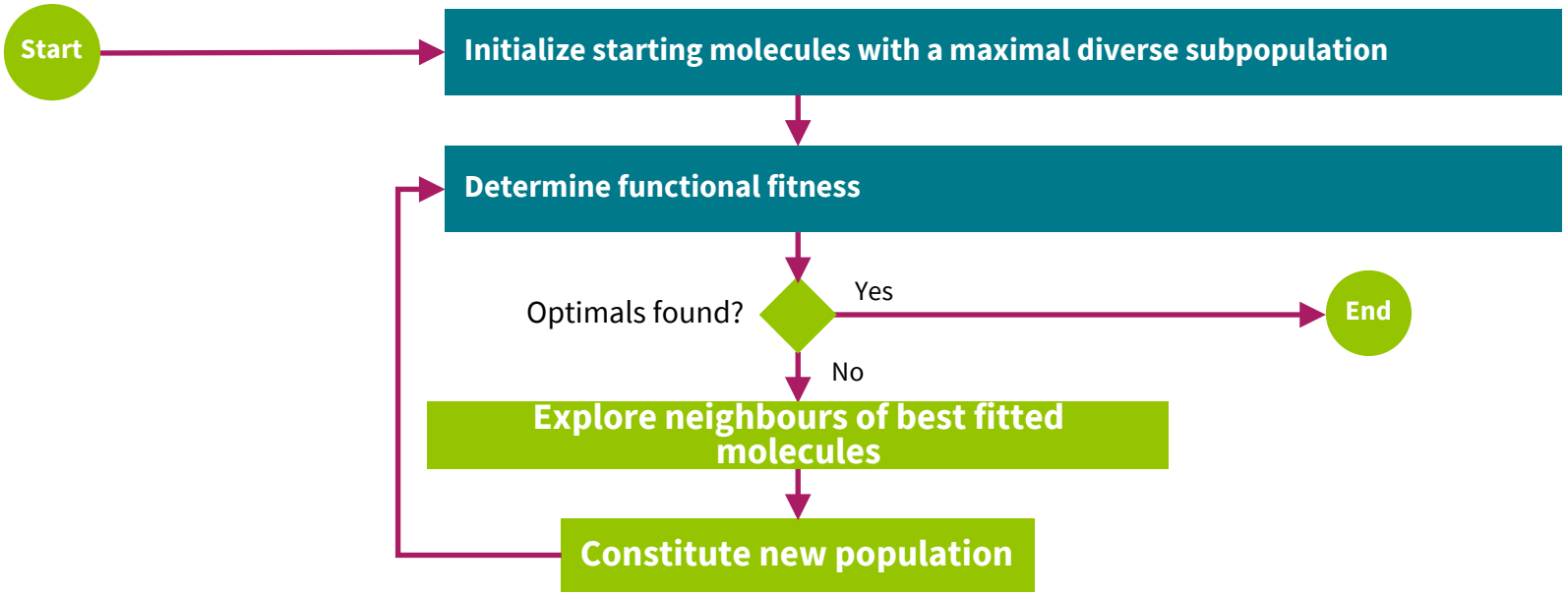
The InKemia Solvent Library Applied to Cosmetic Formulation Challenge

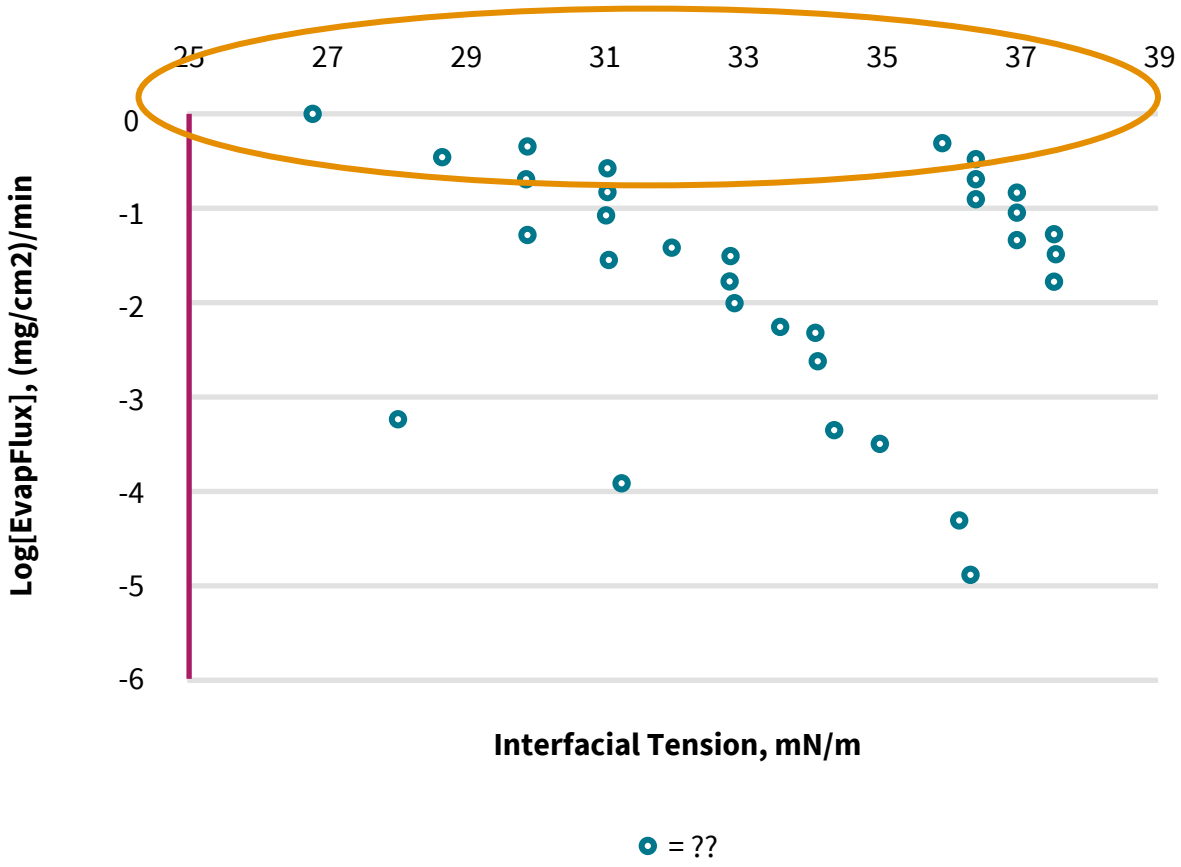
- The Challenge: To find a safer solvent for a rinse-off cosmetic formulation that meets simultaneously 7 functional and sustainability requirements.
- Functional Specifications:
  1. Transparency in blend
  2. Solubility of a hard-to-dissolve ingredient
  3. Evaporation rate in a narrow window
  4. Interfacial tension water/oil higher than threshold
  5. Odorless
- Sustainability Constraints
  6. Environmental impact: Low Environmental Hazard (Levels 0, 1 in Column Model)
  7. Human Safety: Low Health Hazard Risk (Levels 0, 1 in Column Model)
- Exclusion List: A list of 24 solvents that were known to fail one or more specifications was given to InKemia Green Chemicals.
- Cost: Any solution should have a cost lower than a specified target.

Probability α of Finding Optimal Solvent in the InKemia Library



Search Algorithm




25
27
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31
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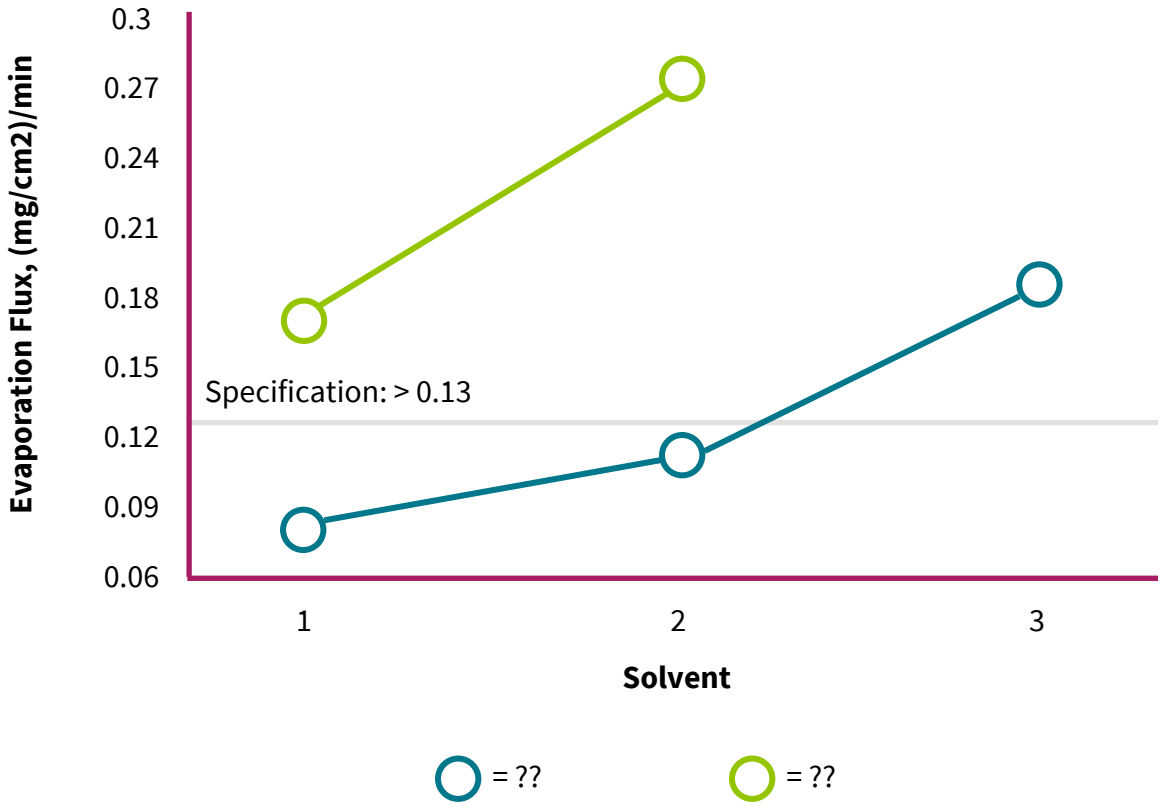
-3
-4
-5
-6
Log[EvapFlux], (mg/cm2)/min
Interfacial Tension, mN/m
= ??

Two Optimal Solvents Were Found



Summary: Cosmetic Formulation

- The Inkemia Library solved one of the hardest solubility problems in the field.
- The almost odorless and transparent solvent conferred excellent spreadability to the formulation.
- The reduced health hazard made the solvent suitable for personal care applications.

Contact

InKemia Green Chemicals is your partner in finding green chemical solutions. Please contact us to find out what we can do for you.

Come Say Hi

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1-713-909-7717

info@inkemiagreen.com

Office Hours

Monday: 9am-5pm
Tuesday: 9am-5pm
Wednesday: 9am-5pm
Thursday: 9am-5pm
Friday: 9am-5pm