GC3 Webinar Series

Green Solvents: Design, Selection, and Commercial Use

Thursday September 28, 2017

GC3 GREEN CHEMISTRY & COMMERCE COUNCIL
Business Mainstreaming Green Chemistry

What is the GC3?

- Cross-sectoral, B2B network of over 120 companies and other organizations
- Formed in 2005
- Collaboratively advances green chemistry across sectors and supply chains

Over 120 members across sectors and value chain

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DELL
ACS Green Chemistry Institute
TARGET
CVS Health
Walmart
EASTMAN
DOW
L'ORÉAL
Timberland
Steelcase
THE HOME DEPOT
GC3

Today's Speaker

Carles Estévez

Scientific Director
***InKemia* IUCT Group**

Ground Rules

- Due to the number of participants in the webinar, all lines will be muted
- If you have a question or comment, please type it in the "Questions" box located in the control panel
- Questions will be answered at the end of the presentation

inKemia
green chemicals

Industrial Application of Green Solvents

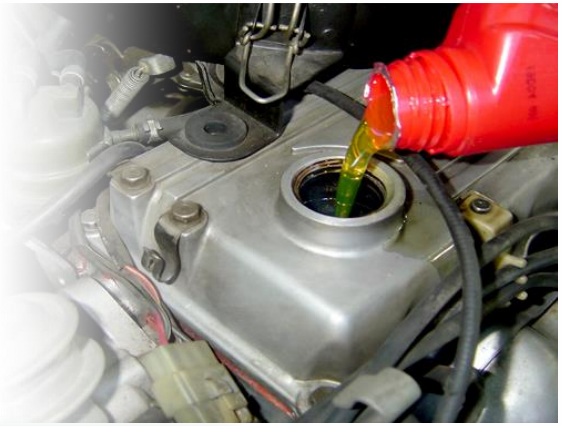
Carles Estévez
Chairman, CSO

September 28, 2017

The Green Chemist's Dream…

…is a world economy sustained by chemicals that do not pose any hazard to people and preserve the environment in its natural state.

Chemicals Enter the Economy to Fulfill a Variety of Essential Functions



(InKemia) Definition of Green Chemical

A green chemical is one that provides higher performance and functionality while being more environmentally benign throughout its entire life-cycle.

Paul Anastas

Green Chemical:
(InKemia) Operational Definition

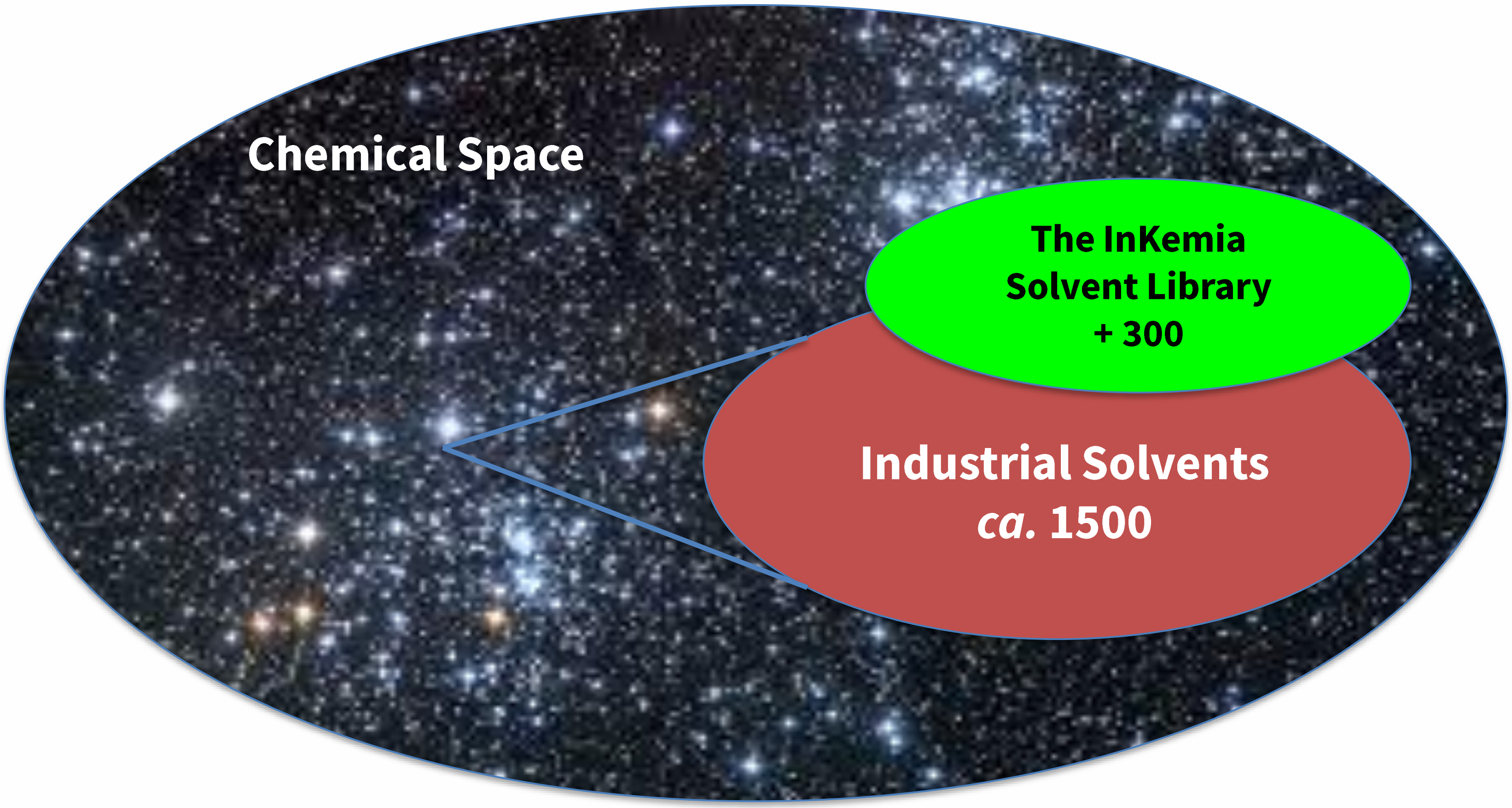
Primary selection criteria is based on Global Harmonized System codes and the Column Model hazard levels.

- *34 health end points*
- *8 environmental impact categories and*
- *24 safety parameters.*
- *Column Model → Negligible or Low Hazard*

Secondary selection criteria

- Tropospheric ozone creation potential

The InKemia Solvent Library



The InKemia Solvent Library

- The InKemia library is composed of 300+ pure solvent candidates (existing + novel)
- More than 20 000 solvent properties calculated
- 268 physico-chemical properties experimentally measured
- 30+ building blocks or chemotypes
- 189 variants generated from 20+ different building blocks
- Variant to building block ratio = 7.87

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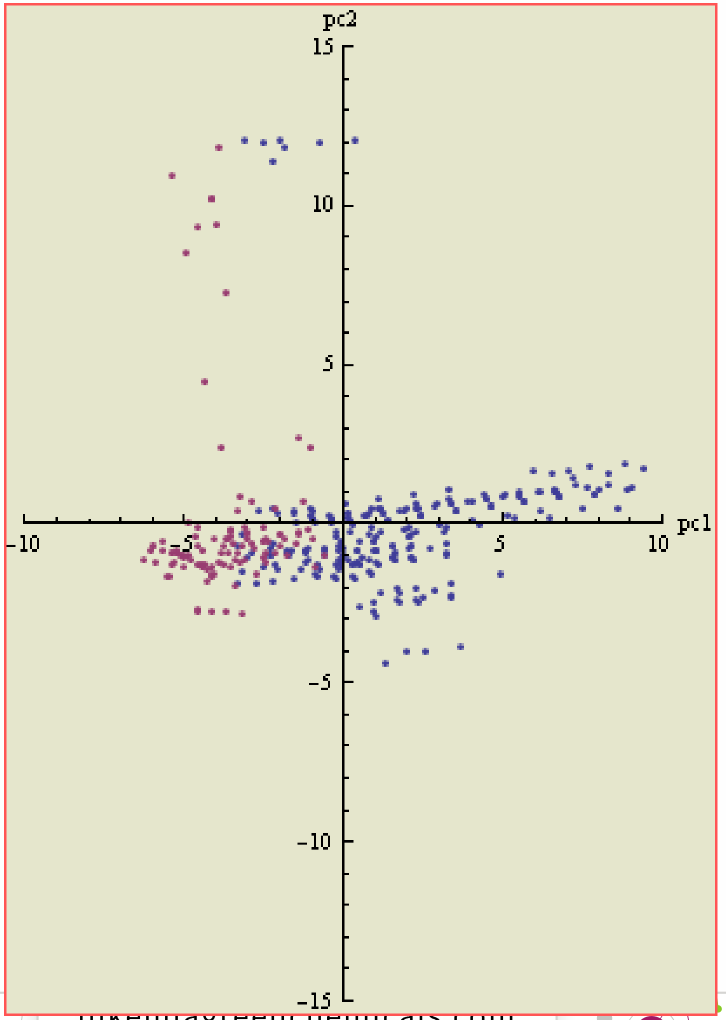
Principal components analysis of the structural characteristics of InKemia (blue dots) and traditional solvents (red dots)



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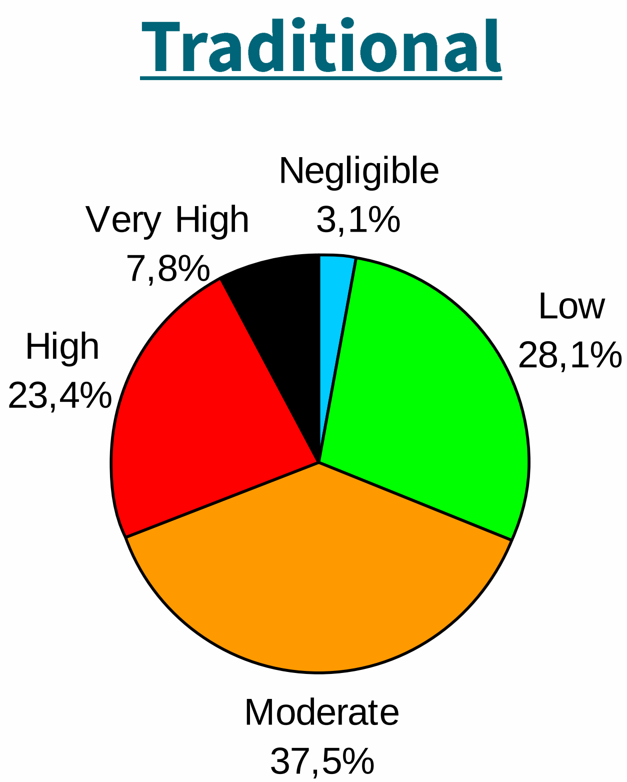
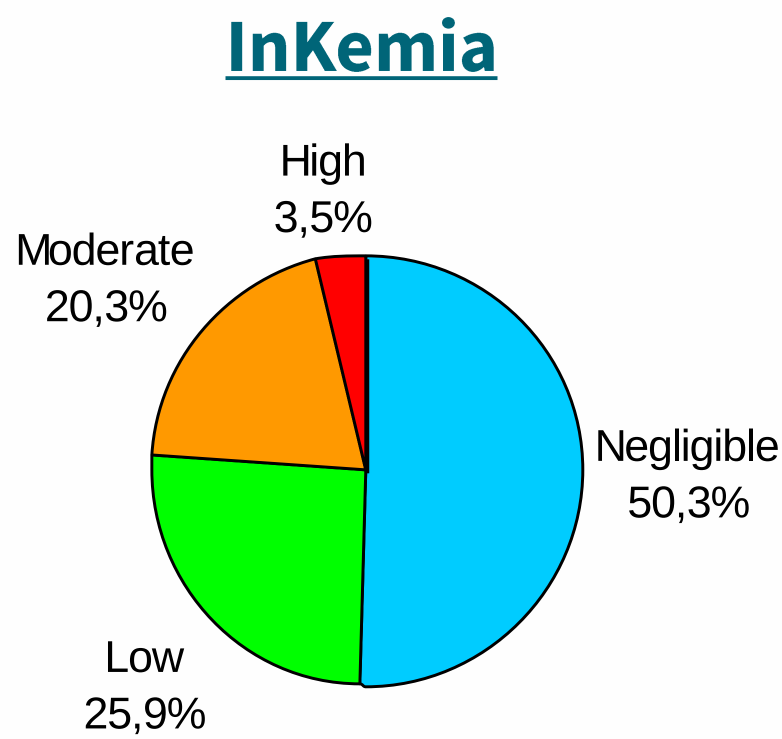
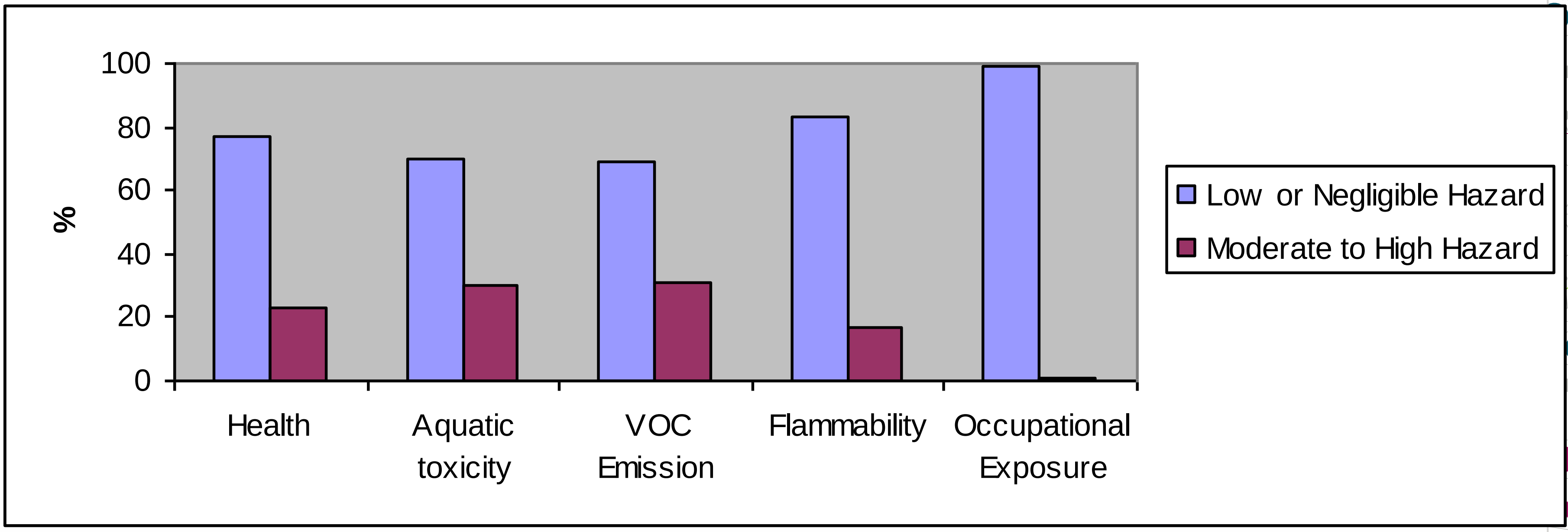
The Health Hazard Distribution of the InKemia Solvent Library





Summary of EHS Properties



The InKemia Solvent Library Applied to Cosmetic Formulation (I)

- The Goal: 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)

Further Requirements and Methodology

- 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.
- Experimental evaluation for screening purposes at InKemia laboratories with materials supplied by Client.

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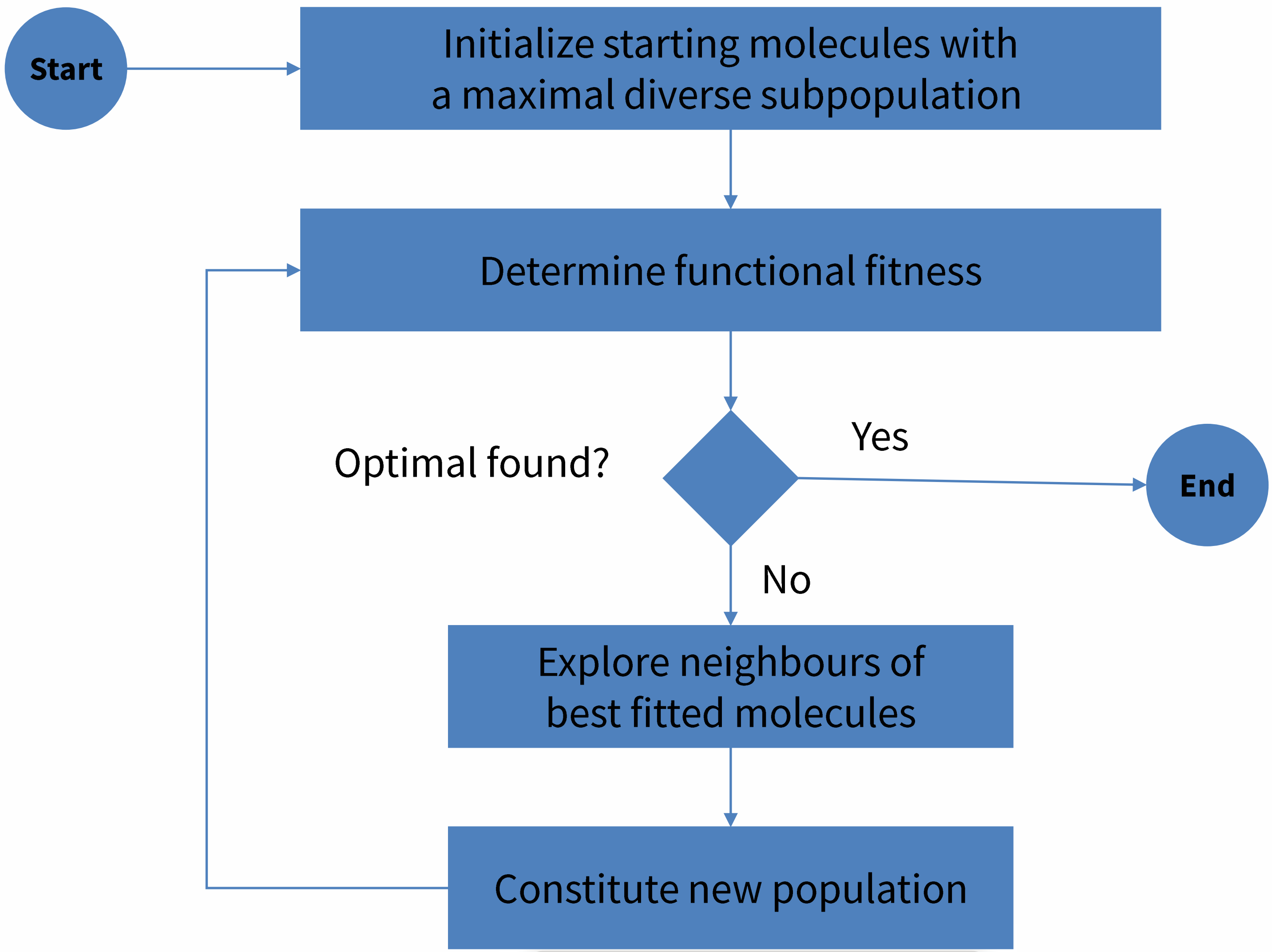
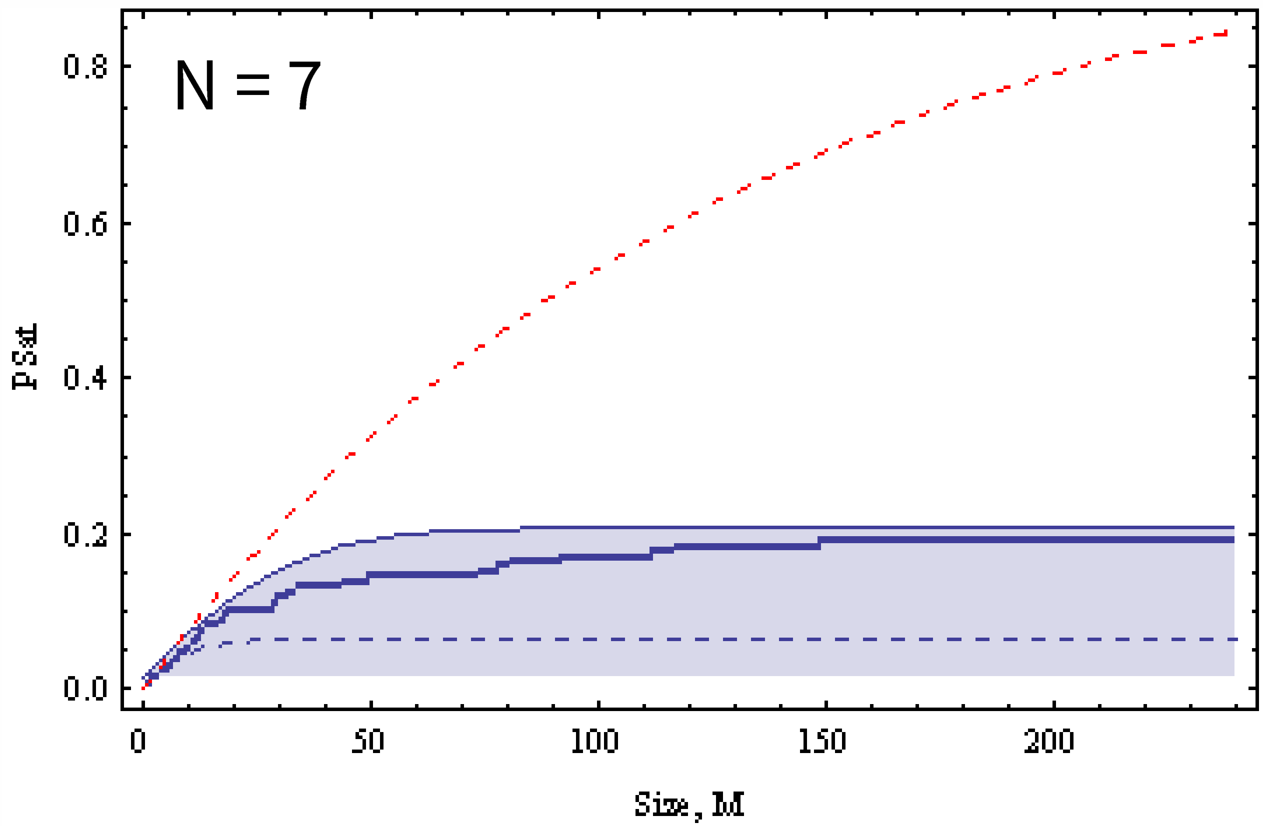
Search Algorithm



PSat in the Experimental Search of a Solvent in the InKemia Library



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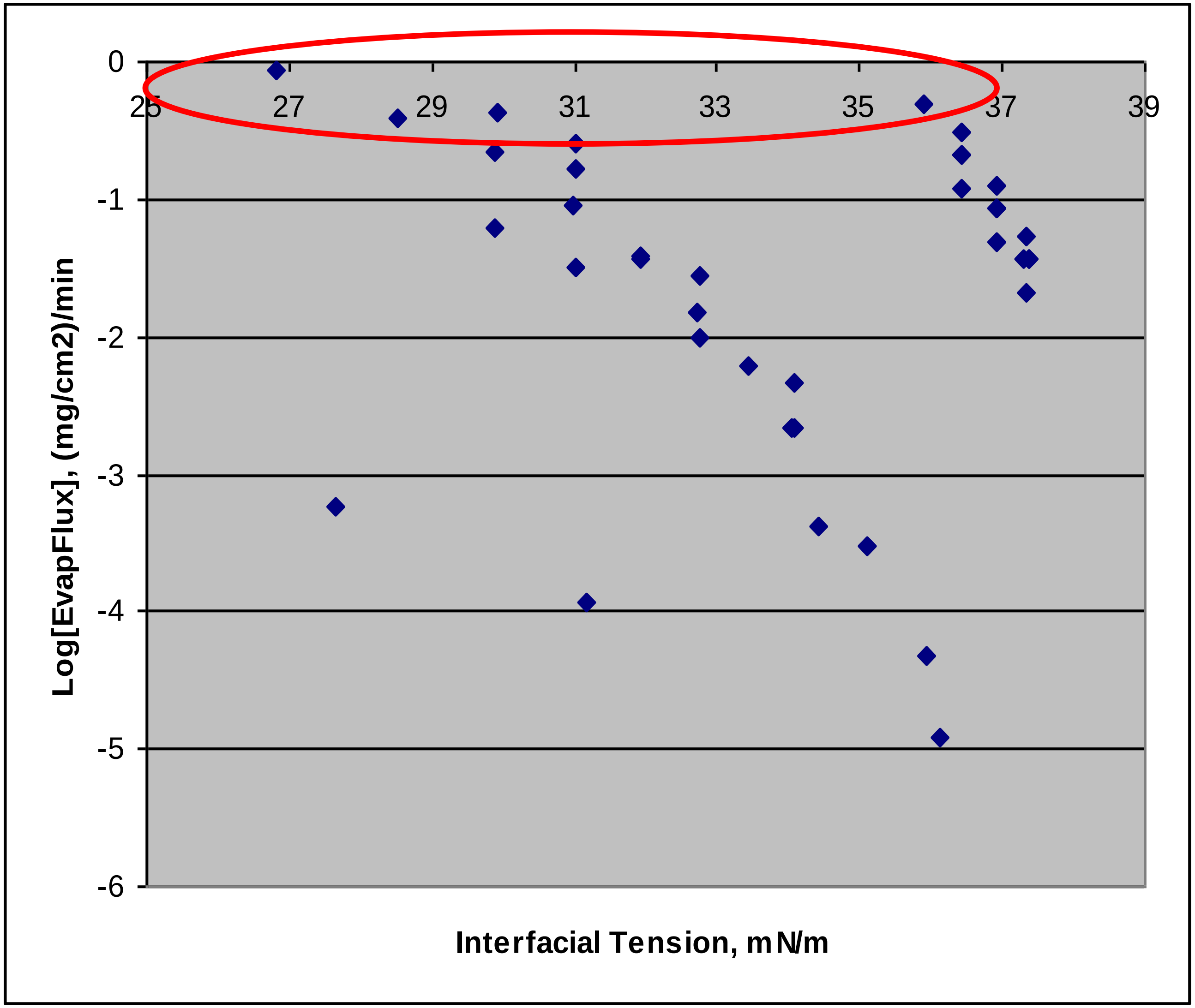
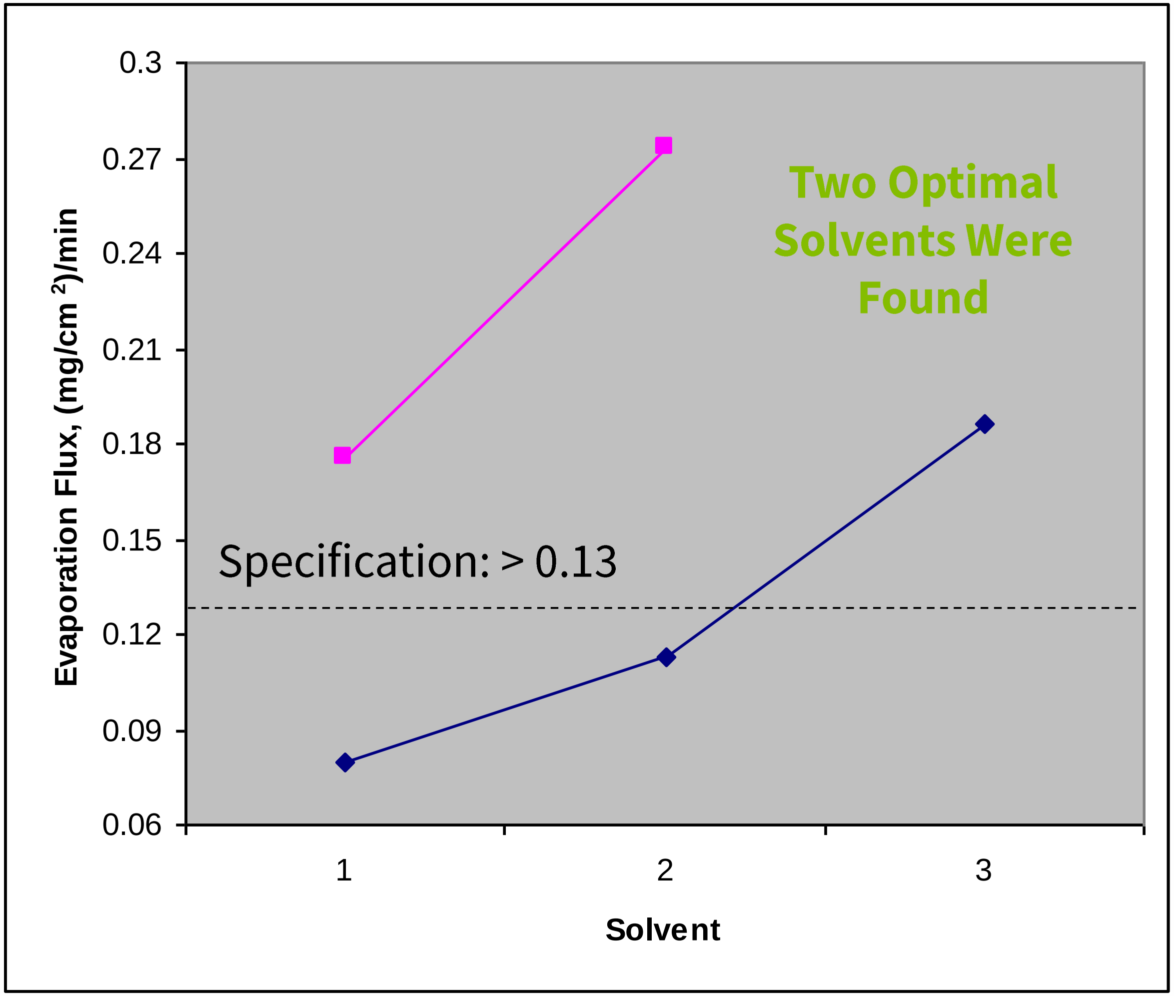
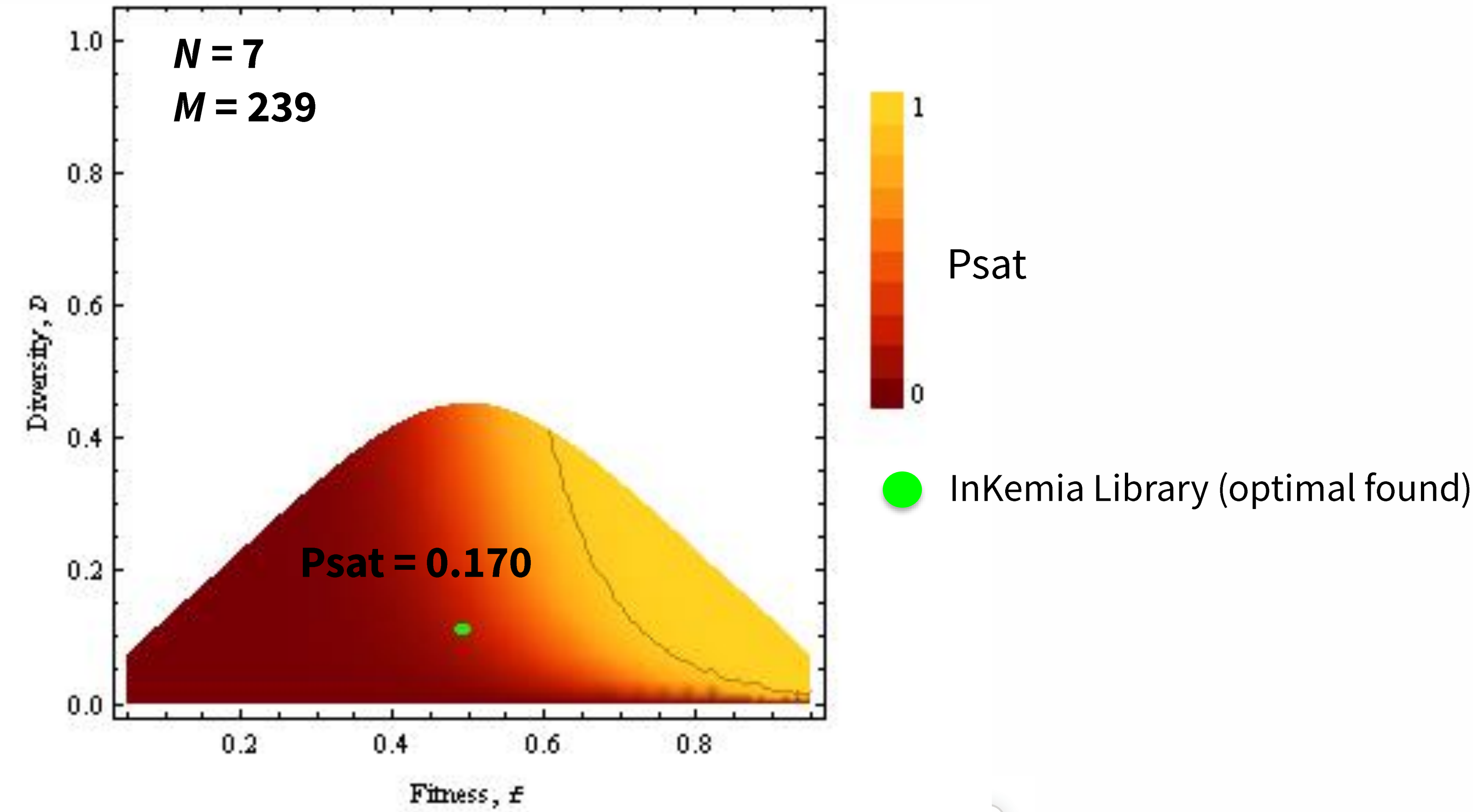



0.3
0.27
0.24
0.21
0.18
0.15
0.12
0.09
0.06
Evaporation Flux, (mg/cm 2)/min
Two Optimal Solvents Were Found
Specification: > 0.13
1
2
3
Solvent

Probability Psat of Satisfying 7 Functional Constraints



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.

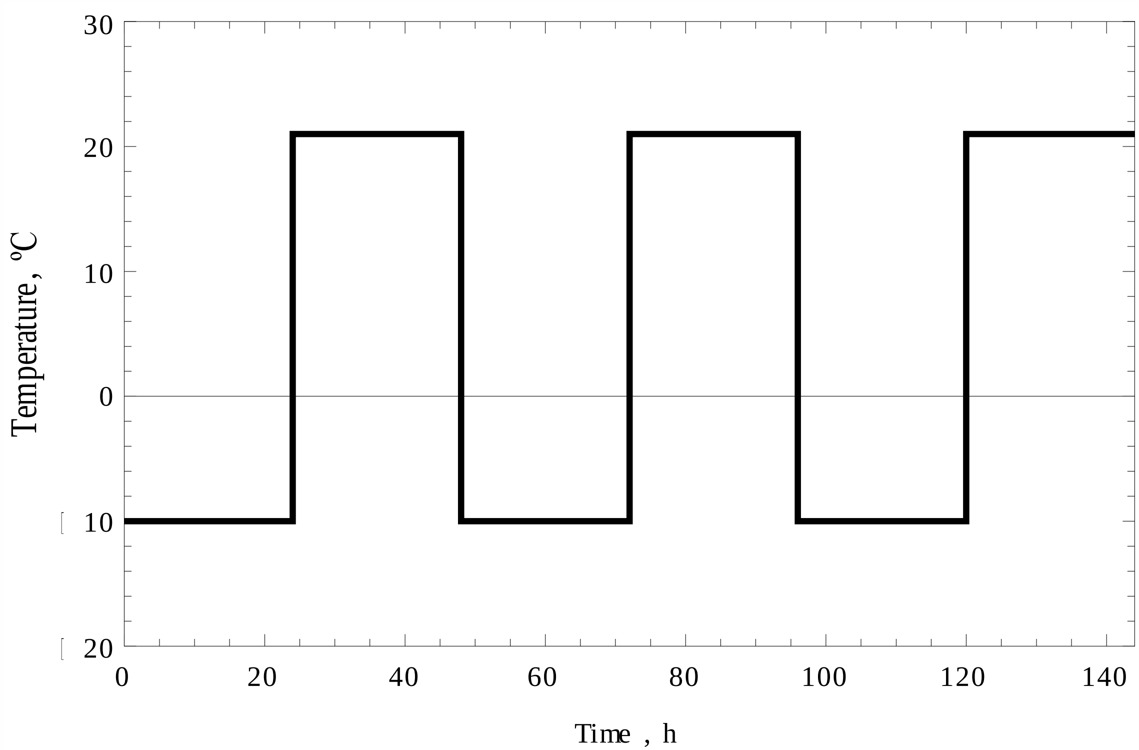
The InKemia Solvent Library Applied to Cosmetic Formulation (II)

- The Goal: To improve the safety of a skin care formulation through the replacement of an EHS-suboptimal solvent.
- Functional Specifications: The solvent must meet simultaneously 10 functional, regulatory and EHS requirements.

1. Solubility of ingredients 3 ingredients of the base formulation
2. Turbidity and phase separation after 3 freeze-thaw cycles
3. Crystallization after 3 freeze-thaw cycles
4. Discoloration at high temperature
5. Long term chemical stability at high temperature
6. INCI registration
7. Cost
8. Human health hazard
9. Environmental hazard
10. Physical hazard

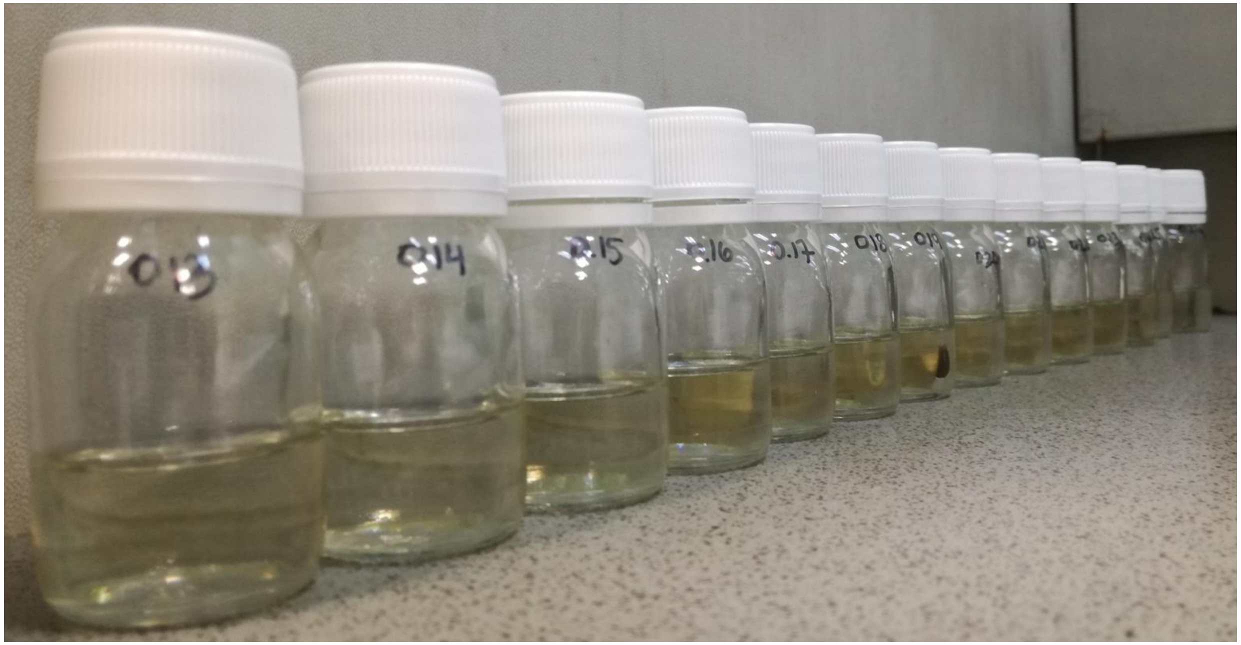
Freeze-Thaw Cycle

Formulations containing the candidate solvents were submitted to a freeze-thaw cycle in order to determine the satbility of the blend

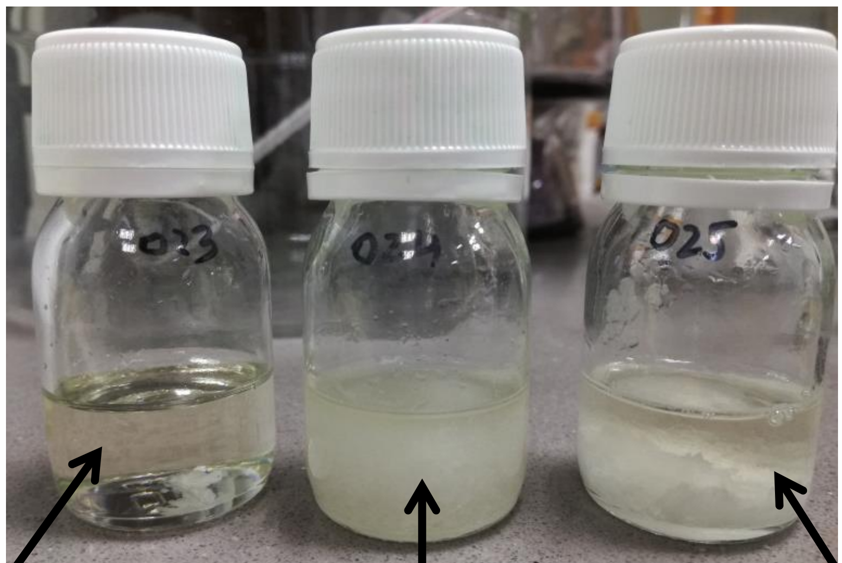


Selection of the first solvent set for *Fitness* evaluation

14 solvents were initially selected under the criteria of maximum structural diversity



Stability evaluation after FT cycle

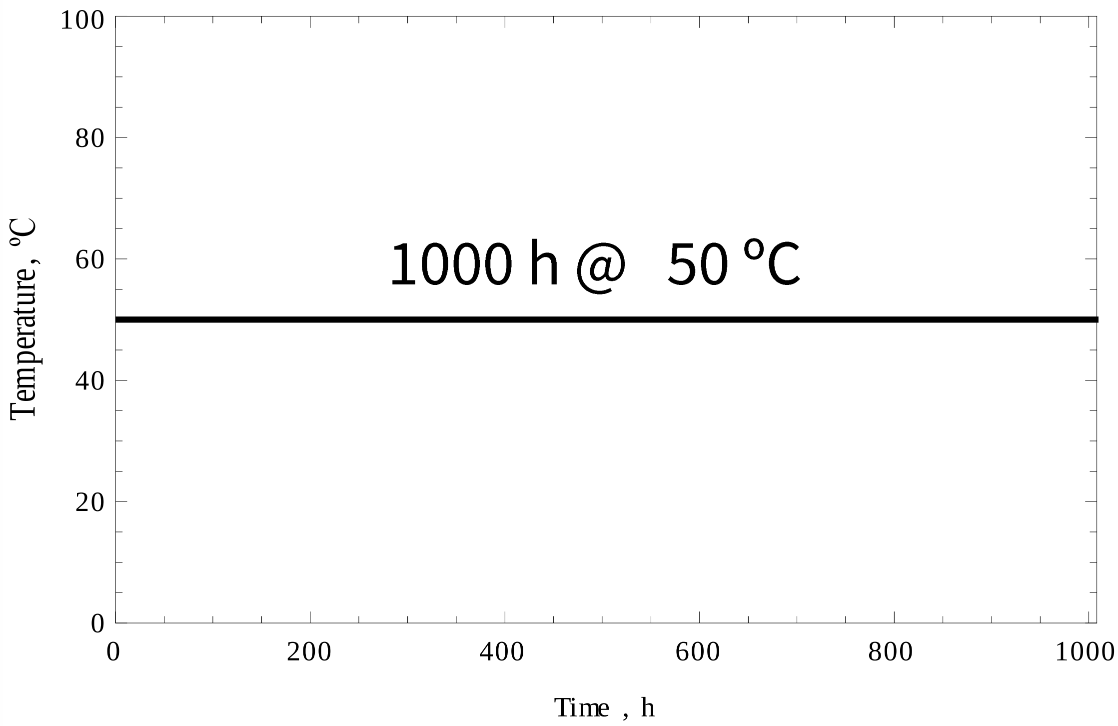


Transparent

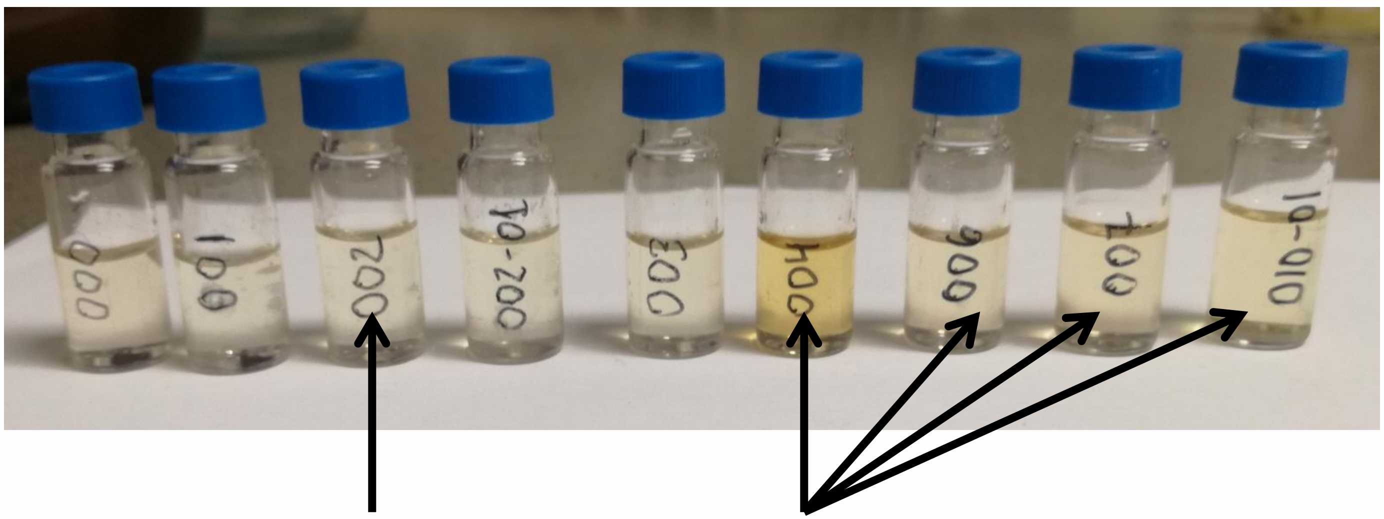
Turbidity and phase separation

Crystallization

Long term stability evaluation



Evaluation of long term stability



Hydrolysis of solvent

Yellowing

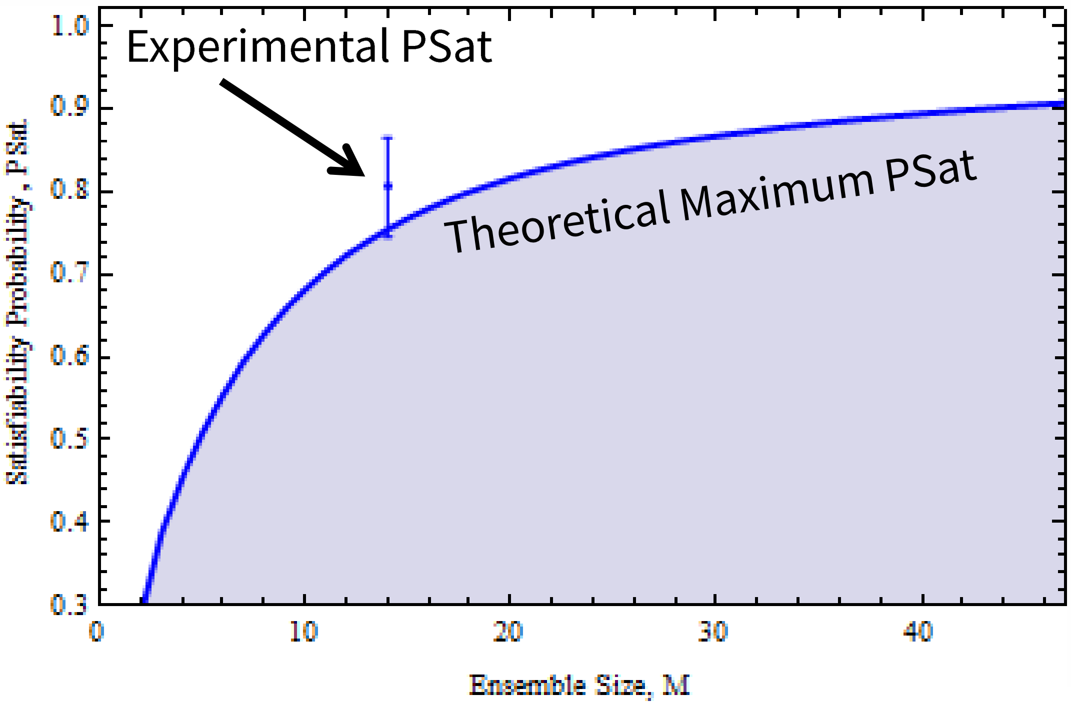
Estimation of the probability PSat of satisfying 10 functional specifications

Within the set of 14 solvent candidates, we identified an optimal solvent that enabled the formulation of a cosmetic product that met simultaneously 10 functional specifications.

Furthermore, the results obtained with the first set allowed us to compute the probability of finding additional optimal solvents with better characteristics than the one found in the initial set.

PSat Computation

The high computed Psat of the 14-set, 75%, is a consequence of the high fitness of the solvent set to the specific problem. The predicted probability indicates that the functional diversity of the set is very good (near the maximum probability curve). Furthermore, it is expected a further increase of the probability by increasing the ensemble size.



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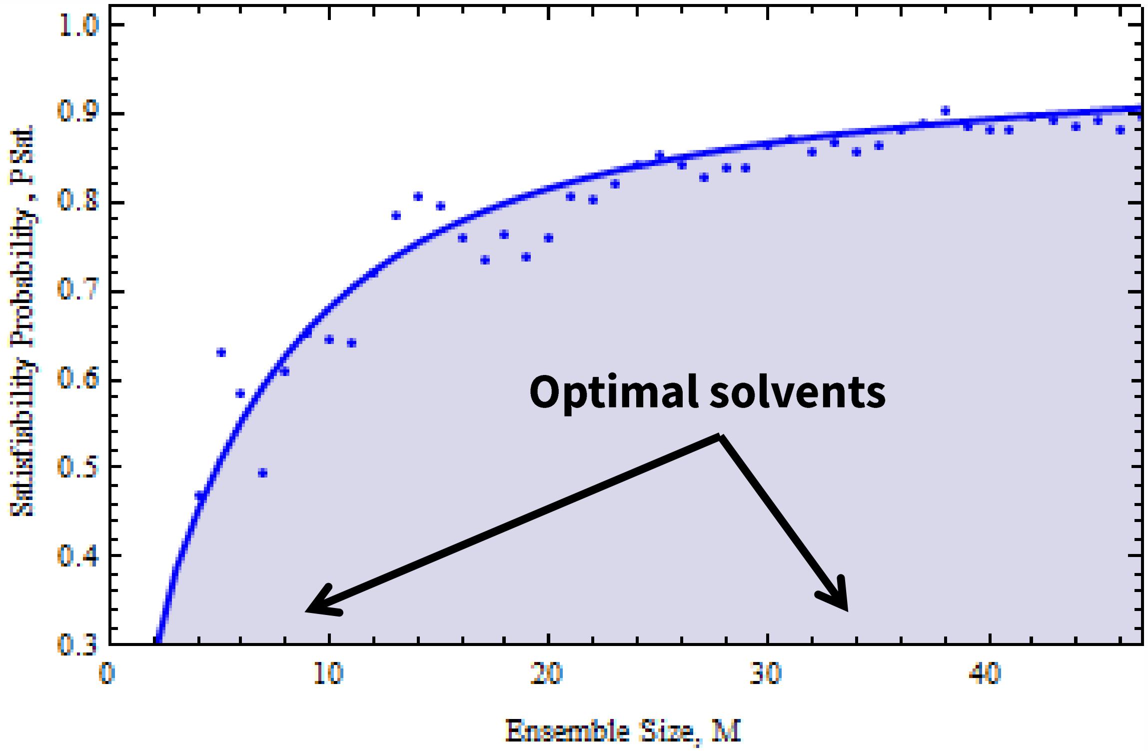
Expansion of the ensemble size to 47 solvents

Experimental PSat of the 47-solvent set

The predicted probability matches perfectly with the experimentally determined PSat. A total of two different solvents were found optimal in the set of 47 solvent candidates.



The InKemia Solvent Library Applied to Metal Degreasing

- The Goal: 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

Sinterized Metal Parts

Operating Environment

Ultrasonic Degreasing at 58°C

Time	0 min	40 min	90 min

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Optimal Conditions for Complete Degreasing

Immersion, 3 h @ 22ºC
Incomplete degreasing

Ultrasonication, 3 h @ 58ºC
Complete degreasing

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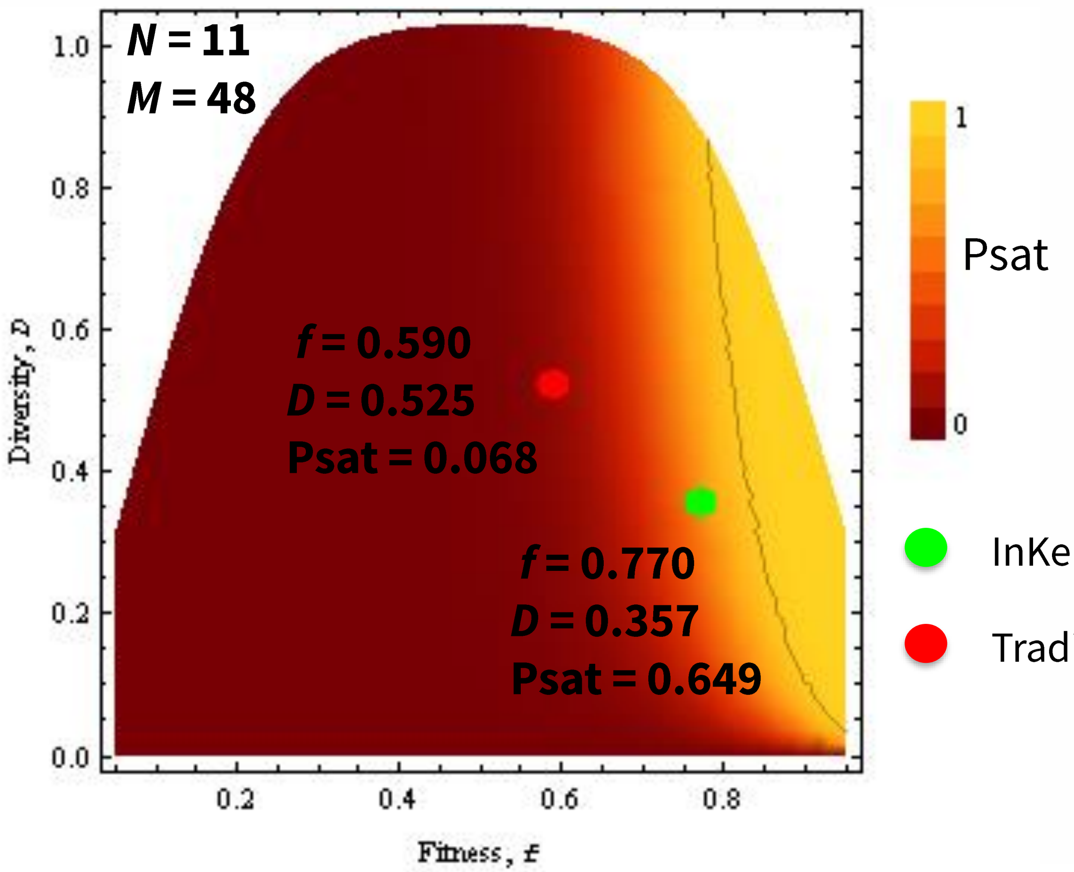
Probability Psat of Satisfying 11 Functional Variables



InKemia Library (optimal found)

Traditional Solvents (no optimal found)

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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.

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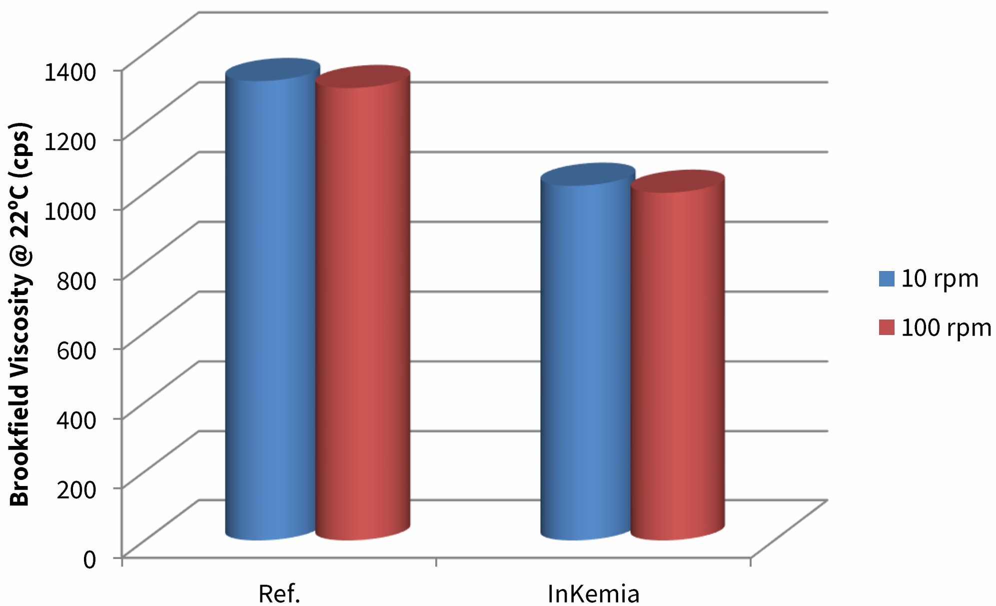
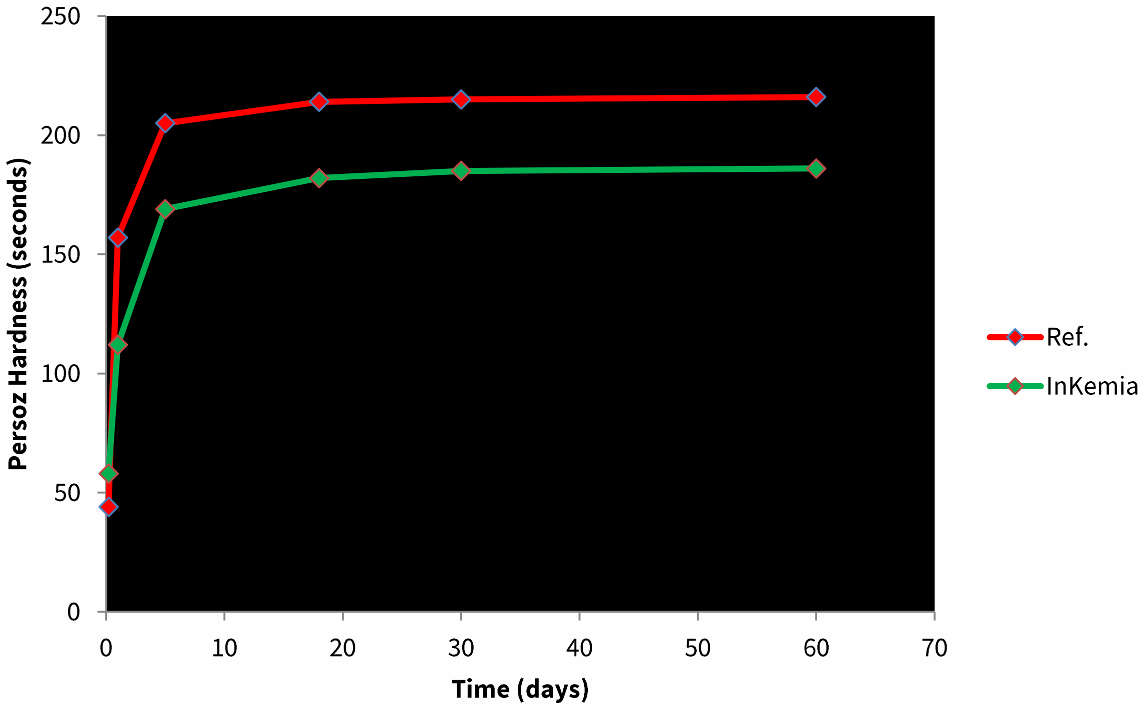
The InKemia Solvent Library Applied to a Marine Paint Formulation

- The Goal: 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
    1. Health hazard (Column Model Level 0 or 1)
    2. Not classified Volatile Organic Compound (VOC)

Viscosity of the Paint Formulation is Significantly Reduced



Hardness is Acceptable and Comparable to the Reference Solvent



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Good Film Formation and Leveling

Alkyd-Urethane in Iroko Wood

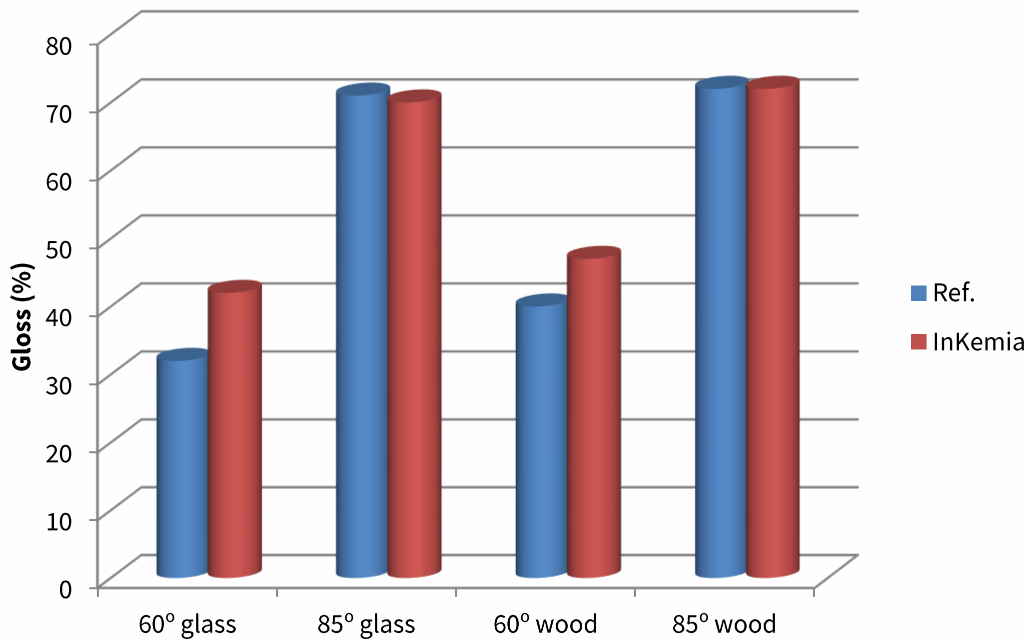
Reference

InKemia

Alkyd-Urethane in Metal Substrates

Reference InKemia

Comparable Values for Gloss



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

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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

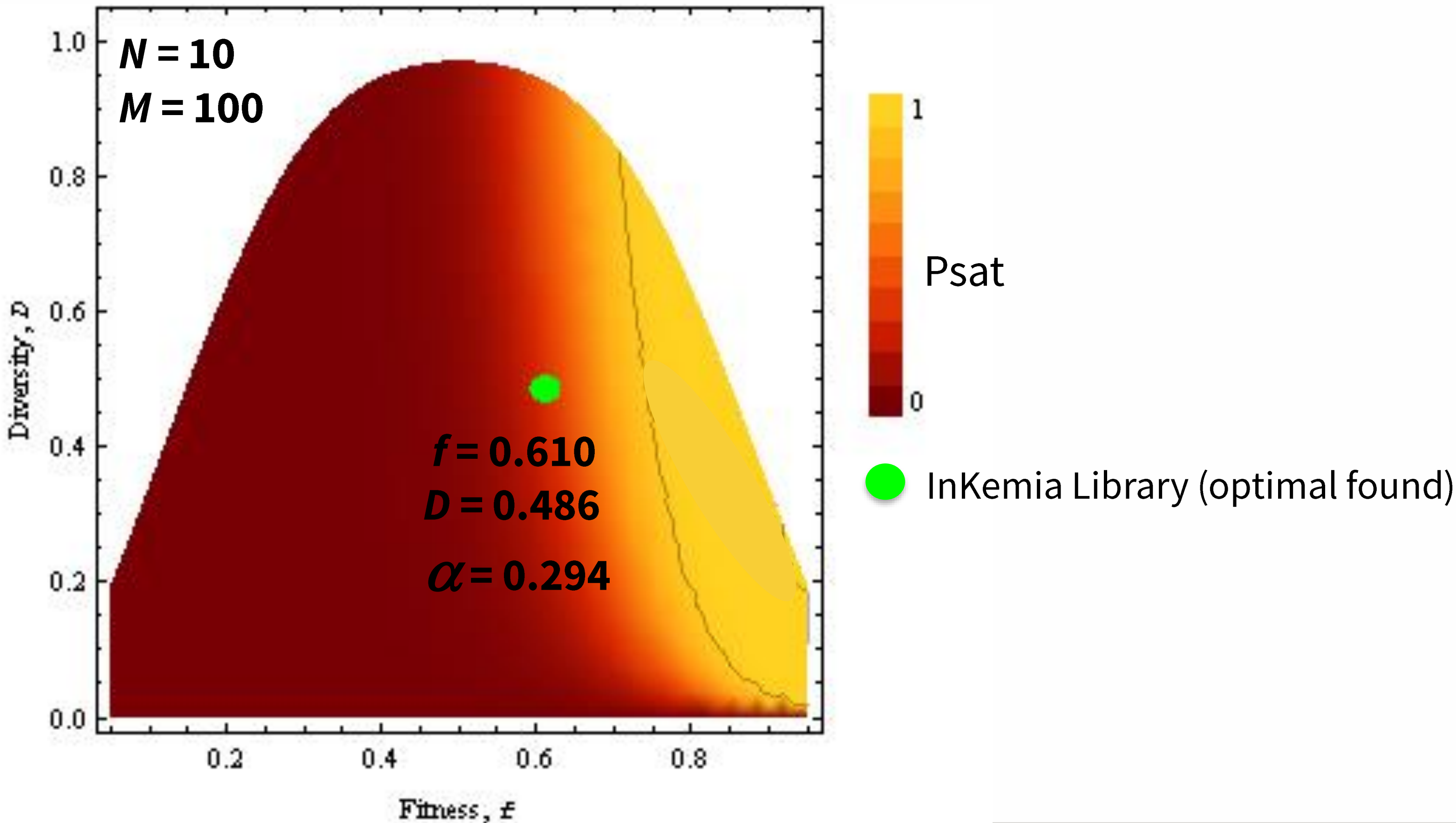
Class 0: Excellent, without damage
Class 3: Some damage is observed depending on the viewing angle, although it is suitable.
Class 4: Considerable damage is observed, independently on the viewing angle. It is not suitable.

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***

Probability Psat of Satisfying 7 Functional Variables



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

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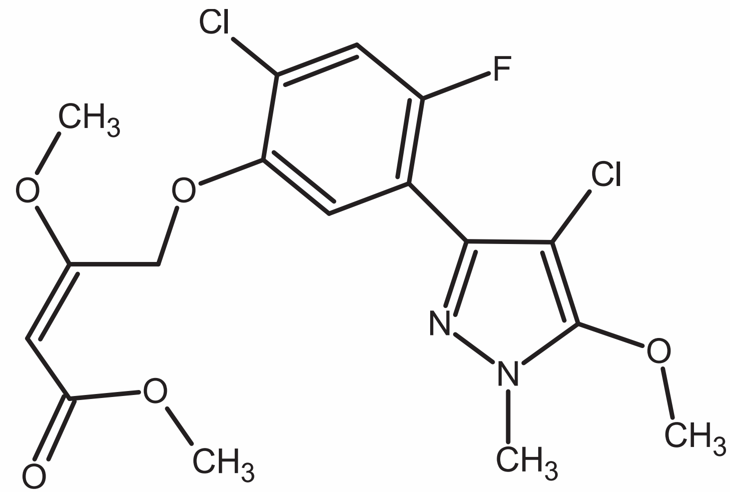
The InKemia Solvent Library Applied to an Herbicide “Tank Mix” Composition

- The Goal: 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)

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



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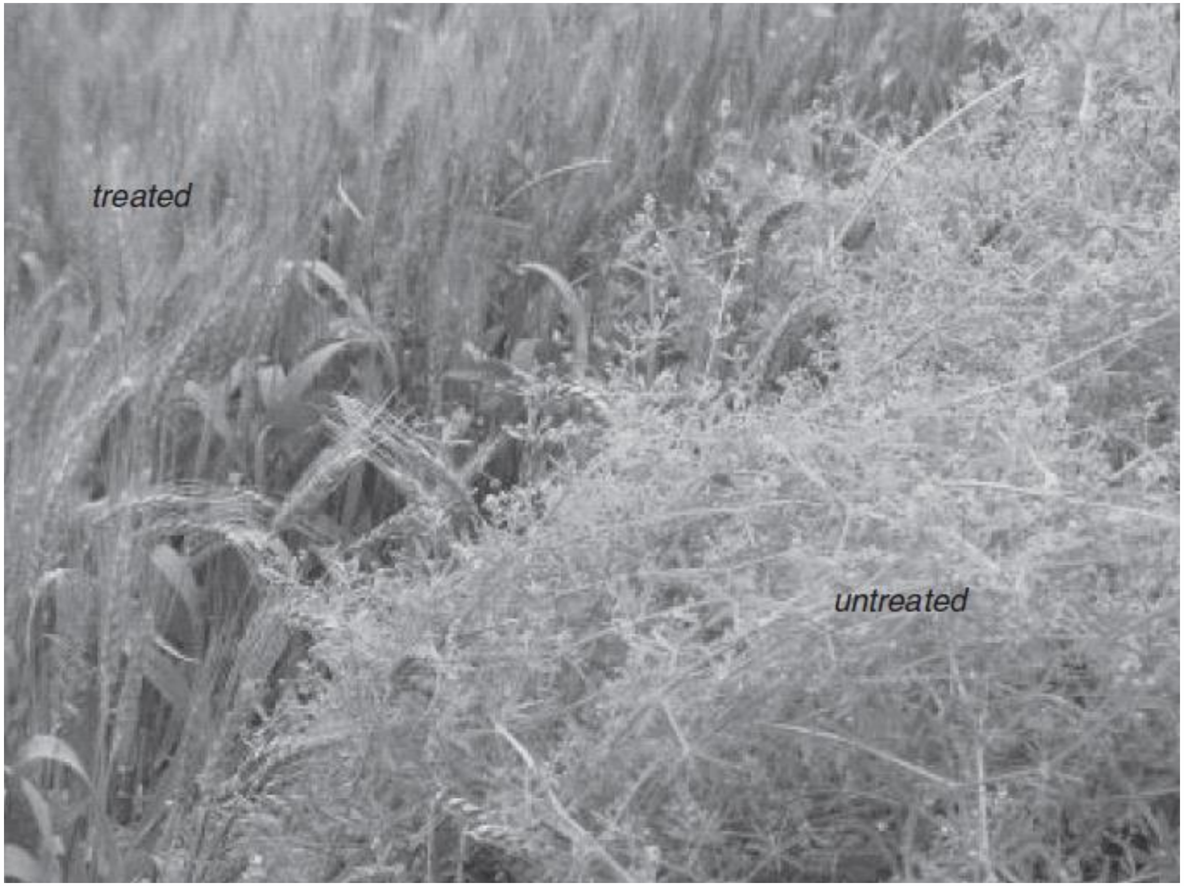
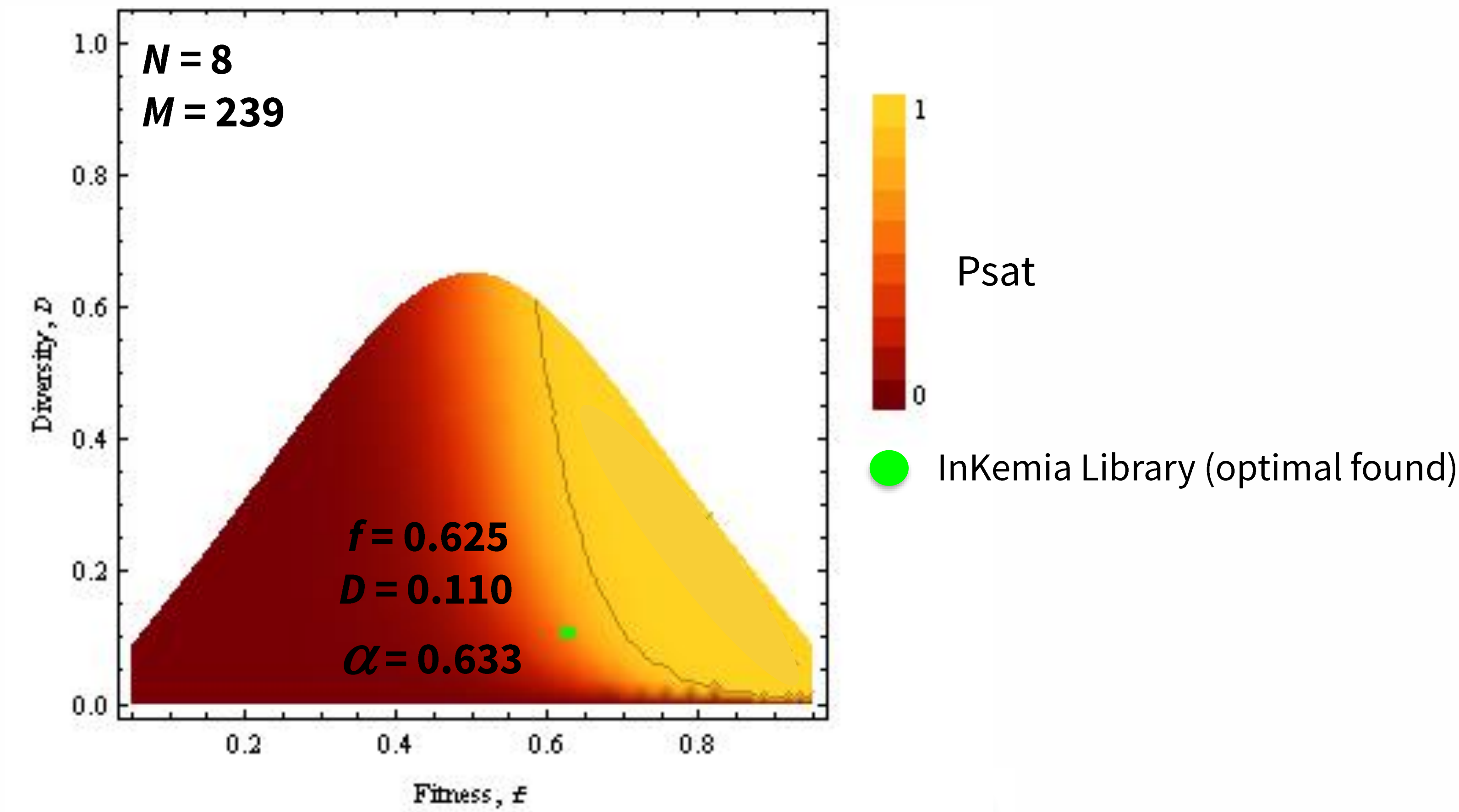
Field Trials

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



Probability Psat of Satisfying 8 Functional Variables



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.

Chemicals & Functions

Ingredients

Formulation

Application

Function

Function

Formulation Properties

- Density
- Viscosity
- Physical stability
- Chemical stability
- Compatibility between ingredients

Application Attributes

Appearance
- Natural looking
- Opacity
- Color matching

Applicability
- Spreadability
- Slip
- Non pore clogging

- Rheology
- Adhesion
- Colorimetric stability

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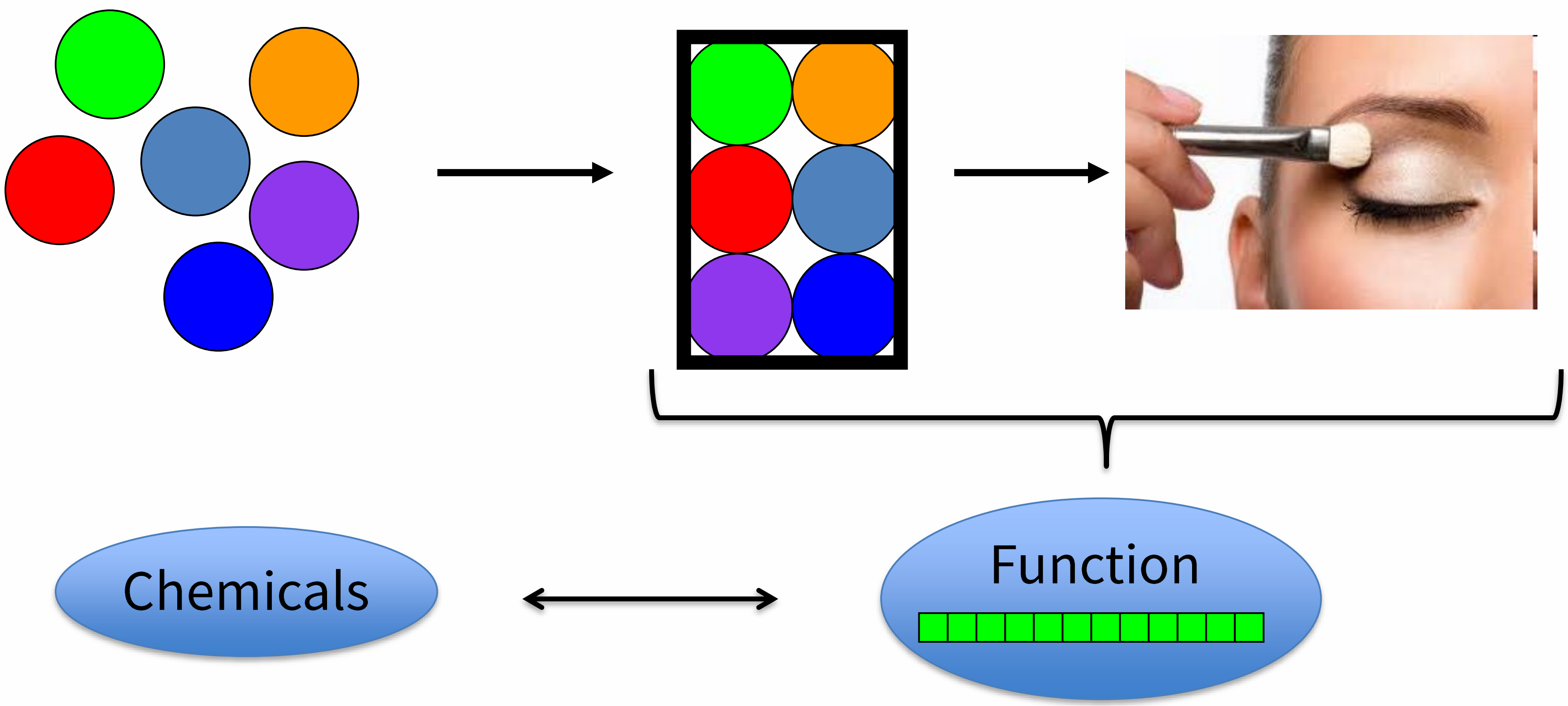
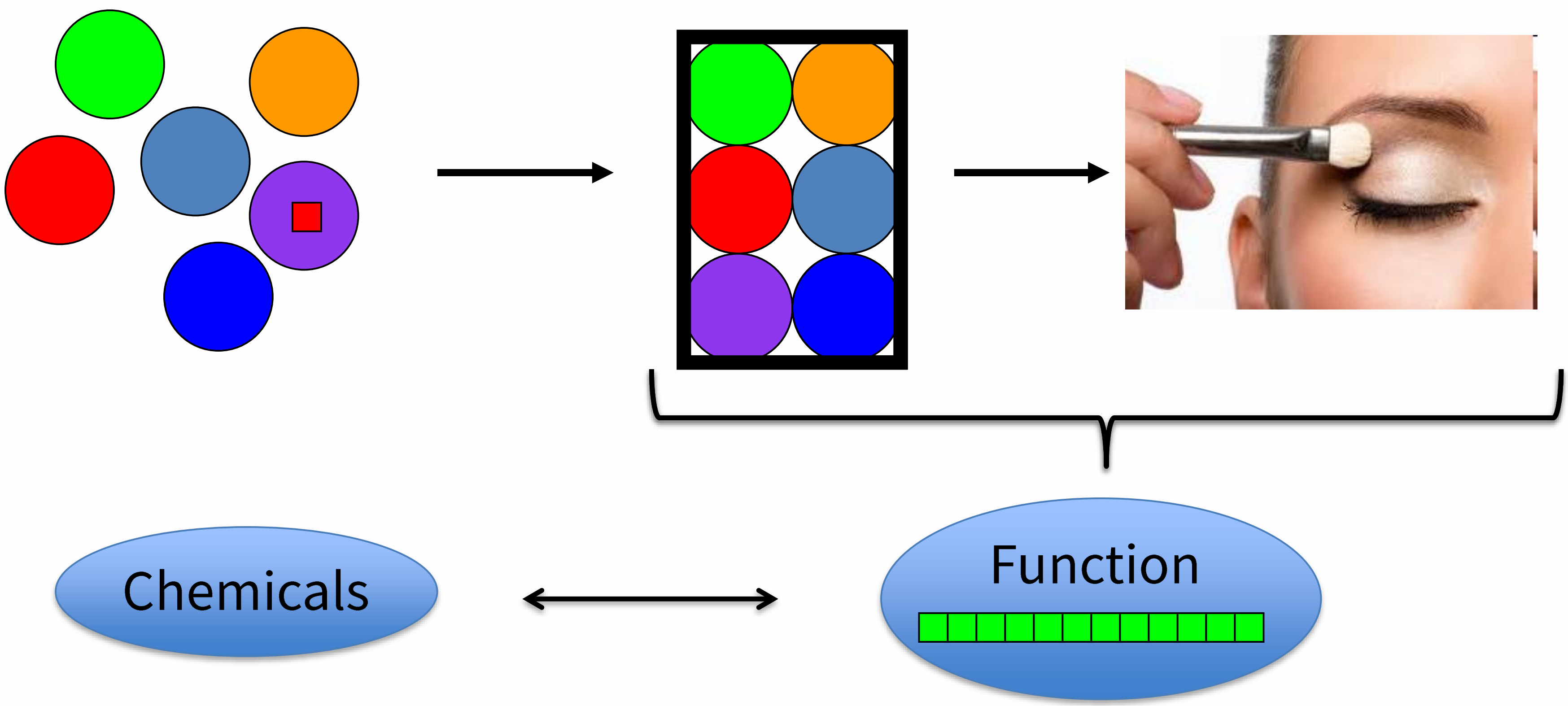
Structure and Function Relationship



Structure and Function Relationship



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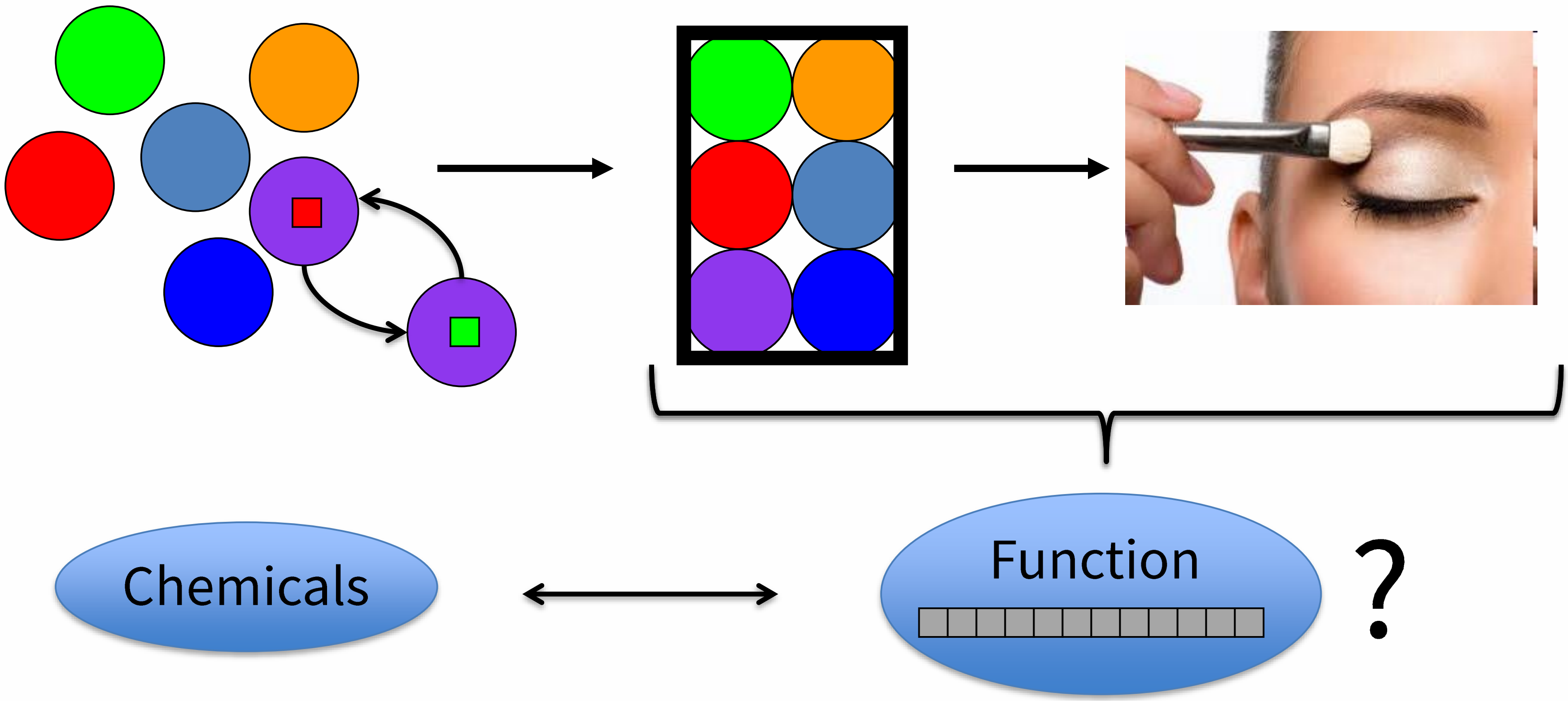
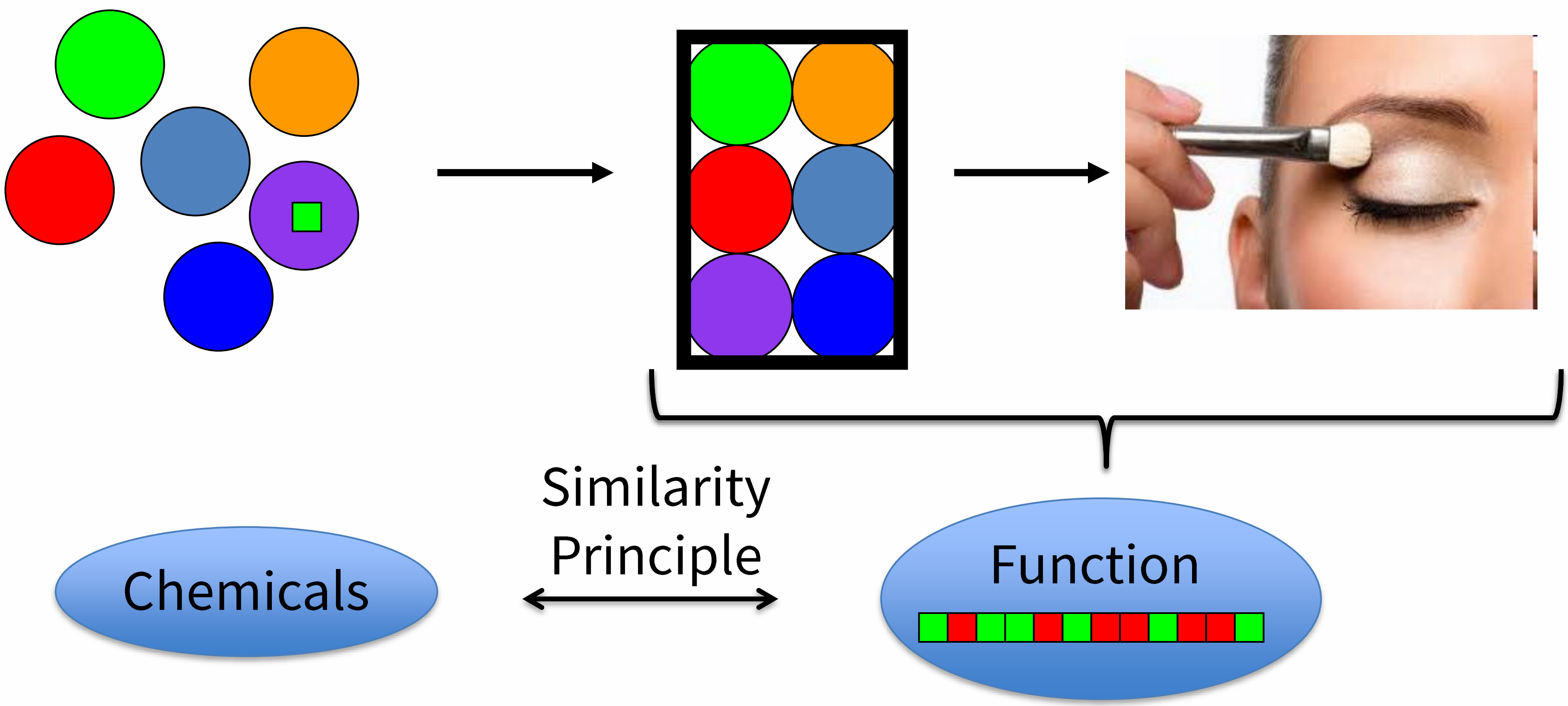
Structure and Function Relationship



Structure and Function Relationship



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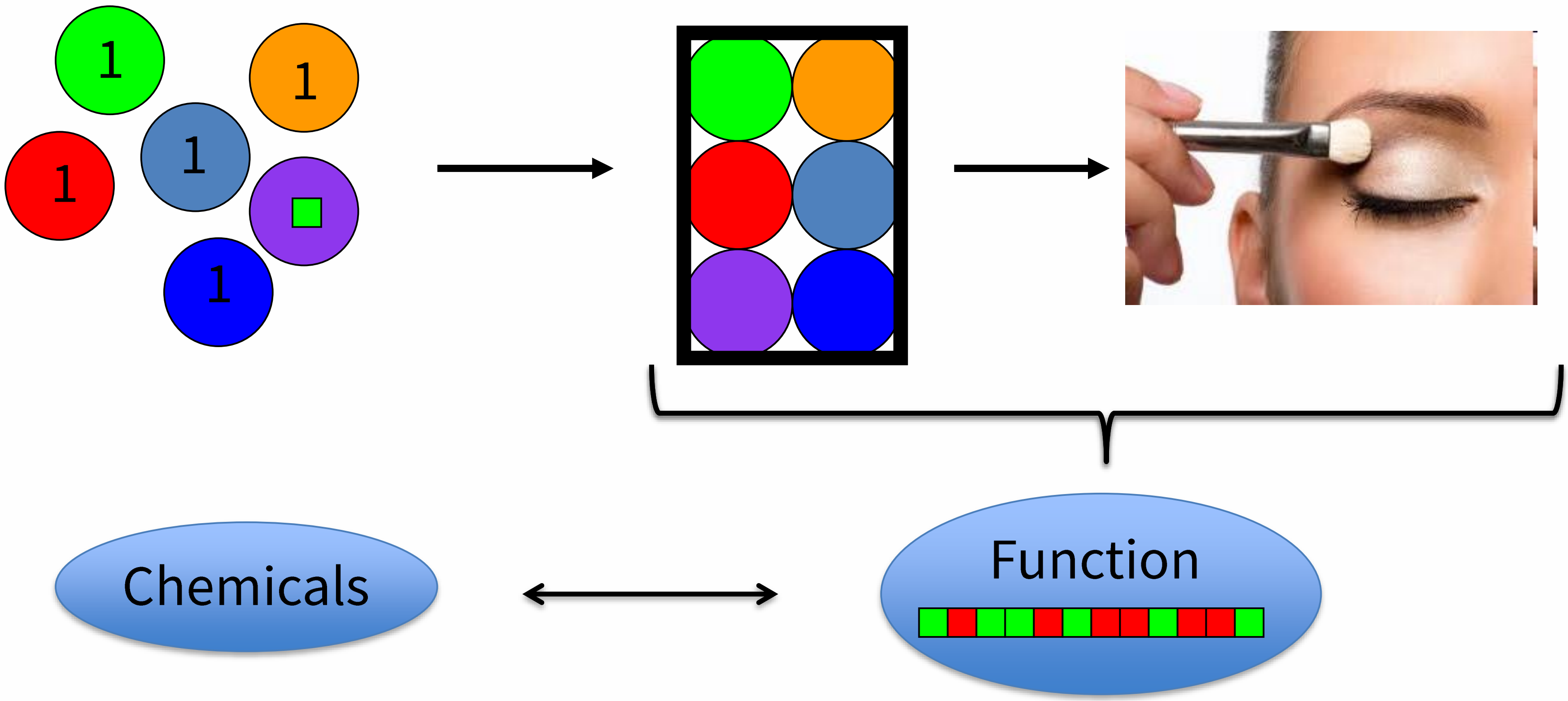
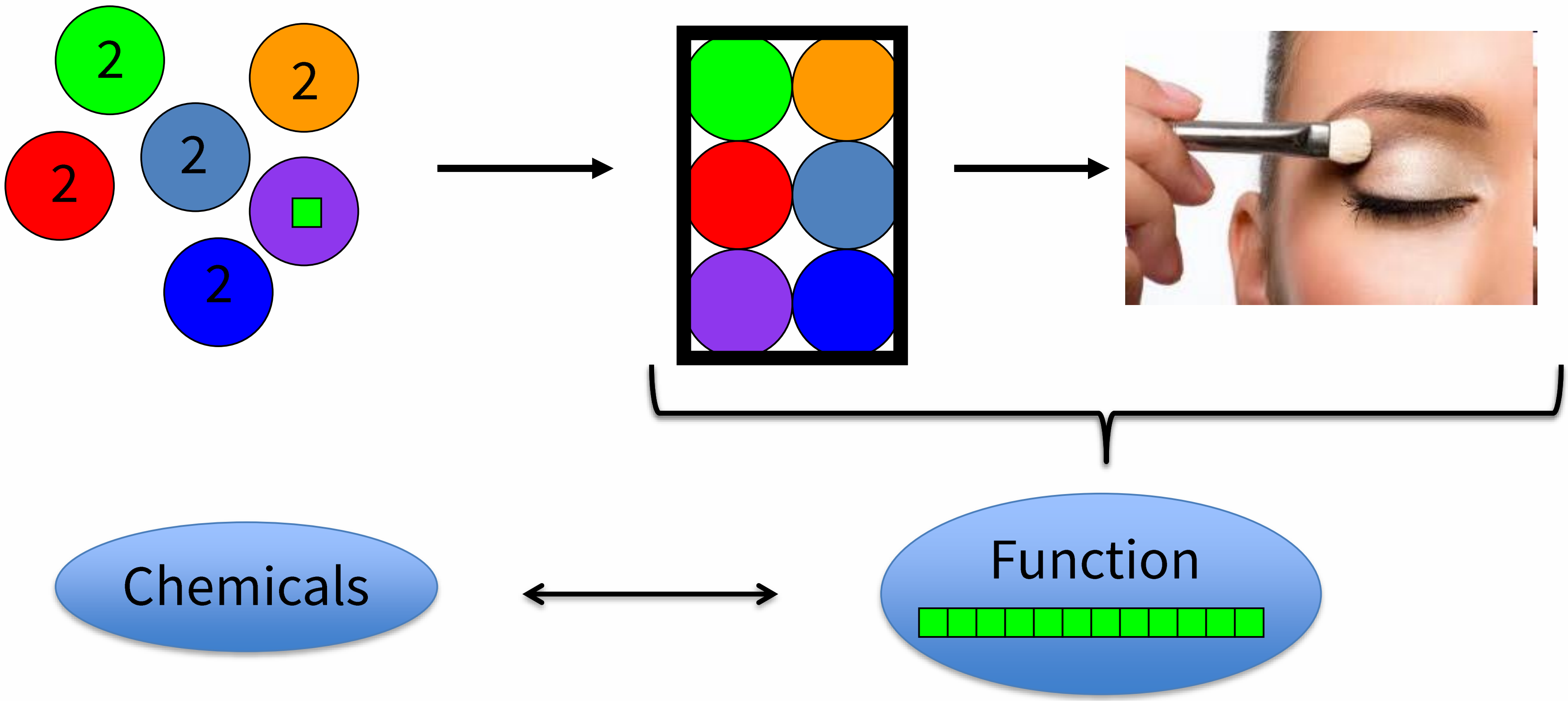
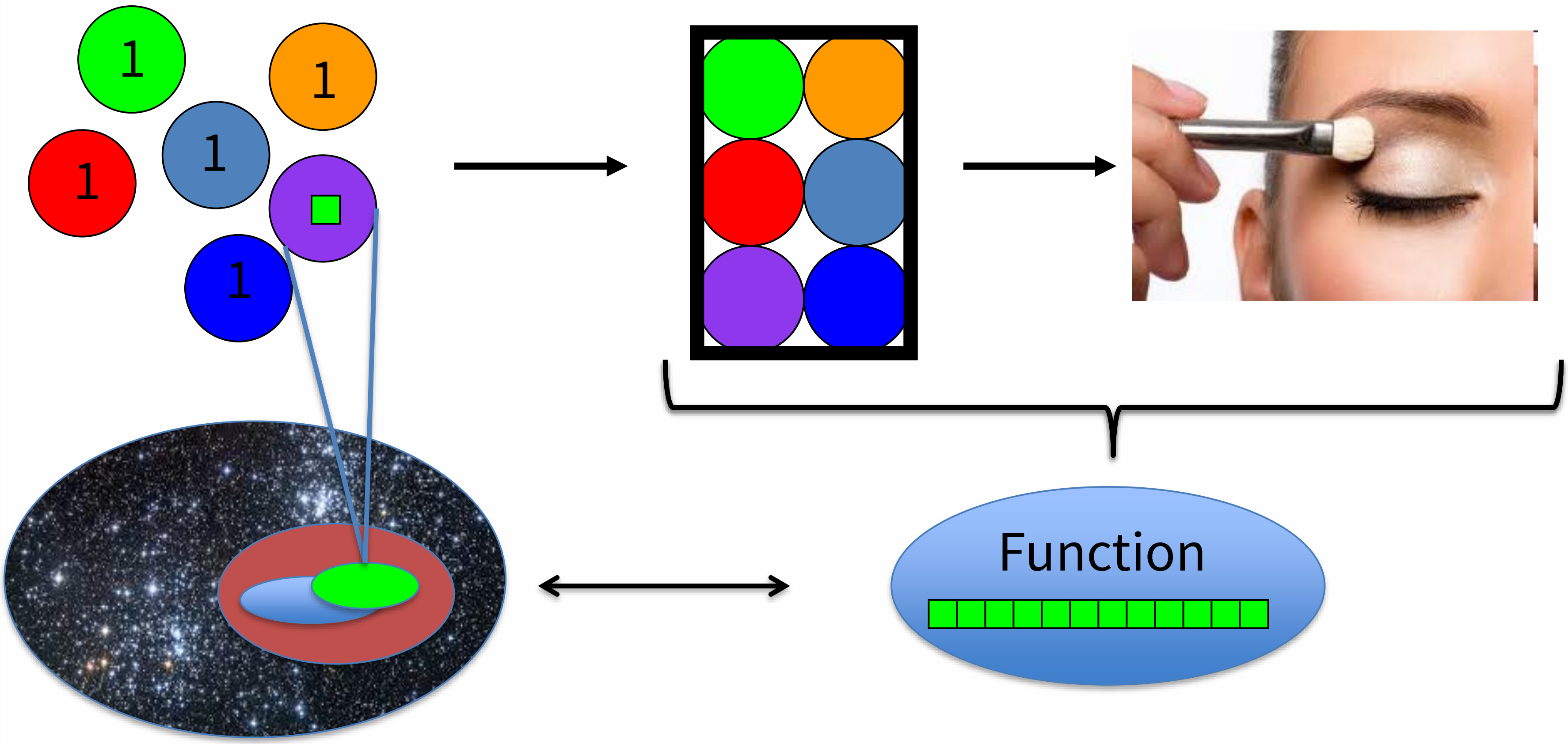
Structure and Function Relationship



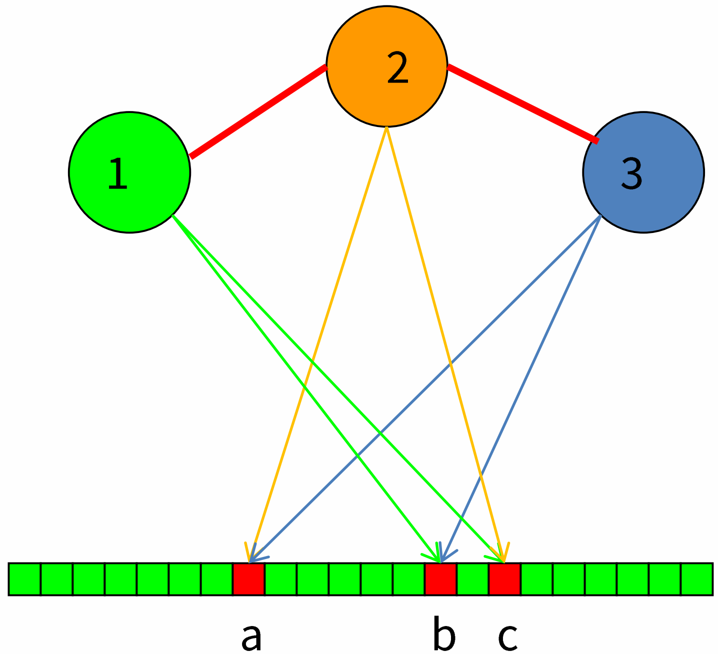
Structure and Function Relationship



Structure and Function Relationship



Understanding Structure and Function Relationships in Complex Functional Landscapes

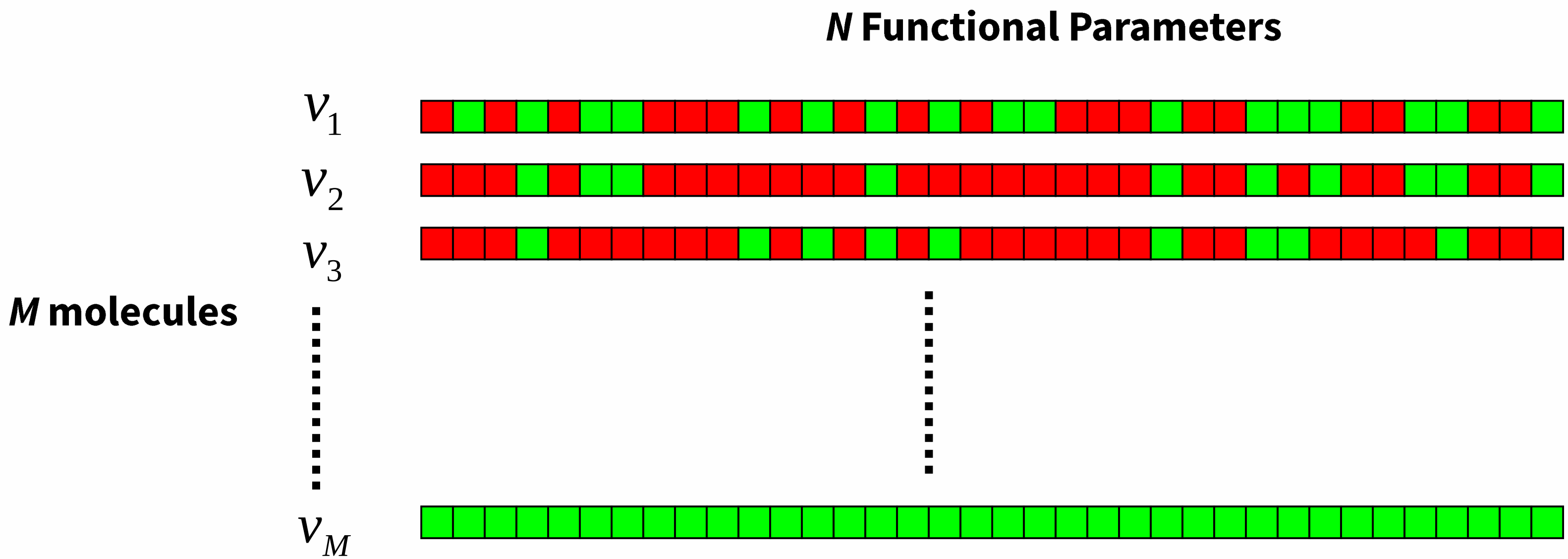


3 structural features in two possible configurations {0,1}

Corresponding states for functional variables a, b and c.

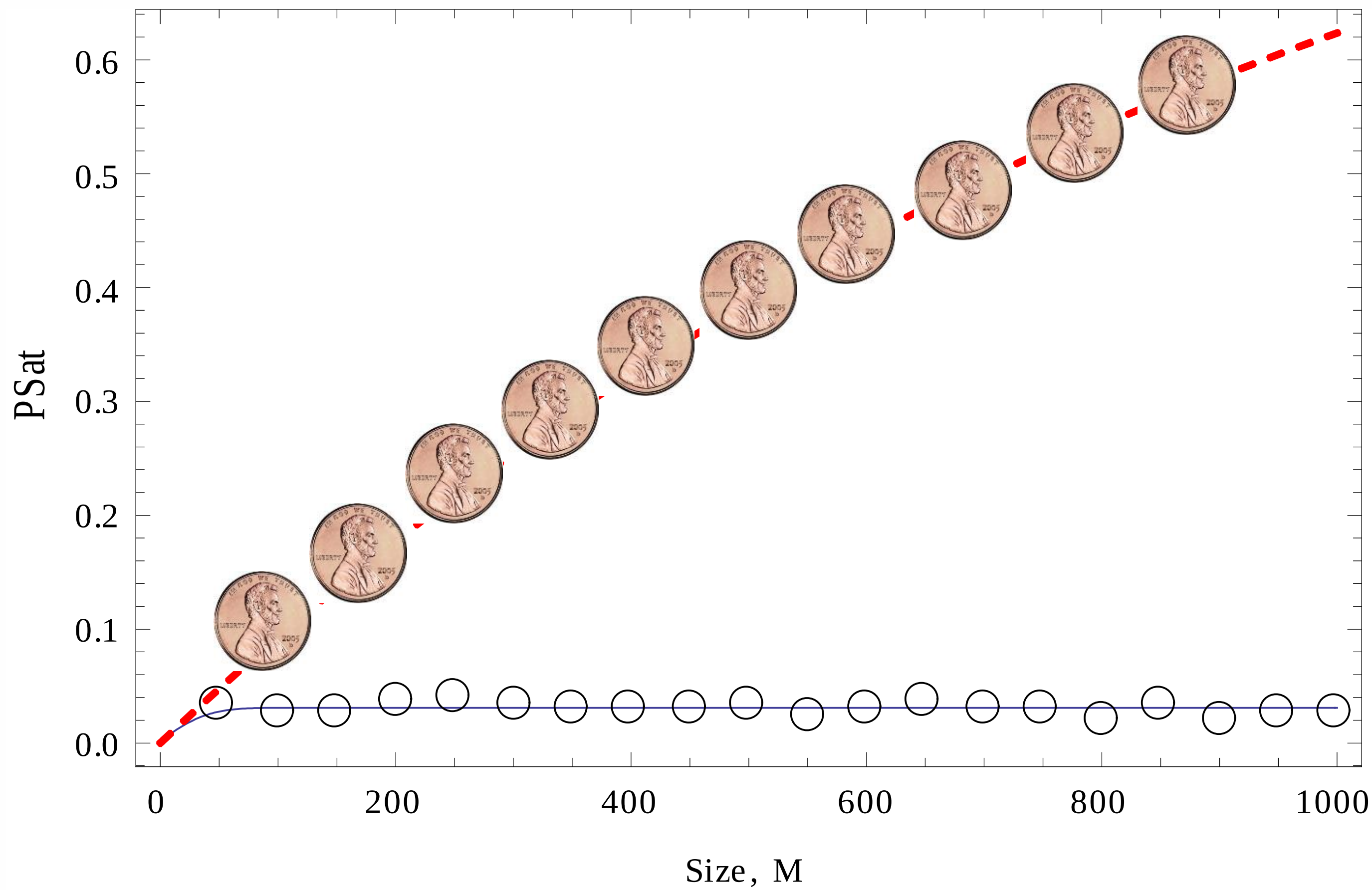
Functional States: What is the Space State

- 0, Functional variable out of specifications (red)
- 1, Functional variable within specifications (green)

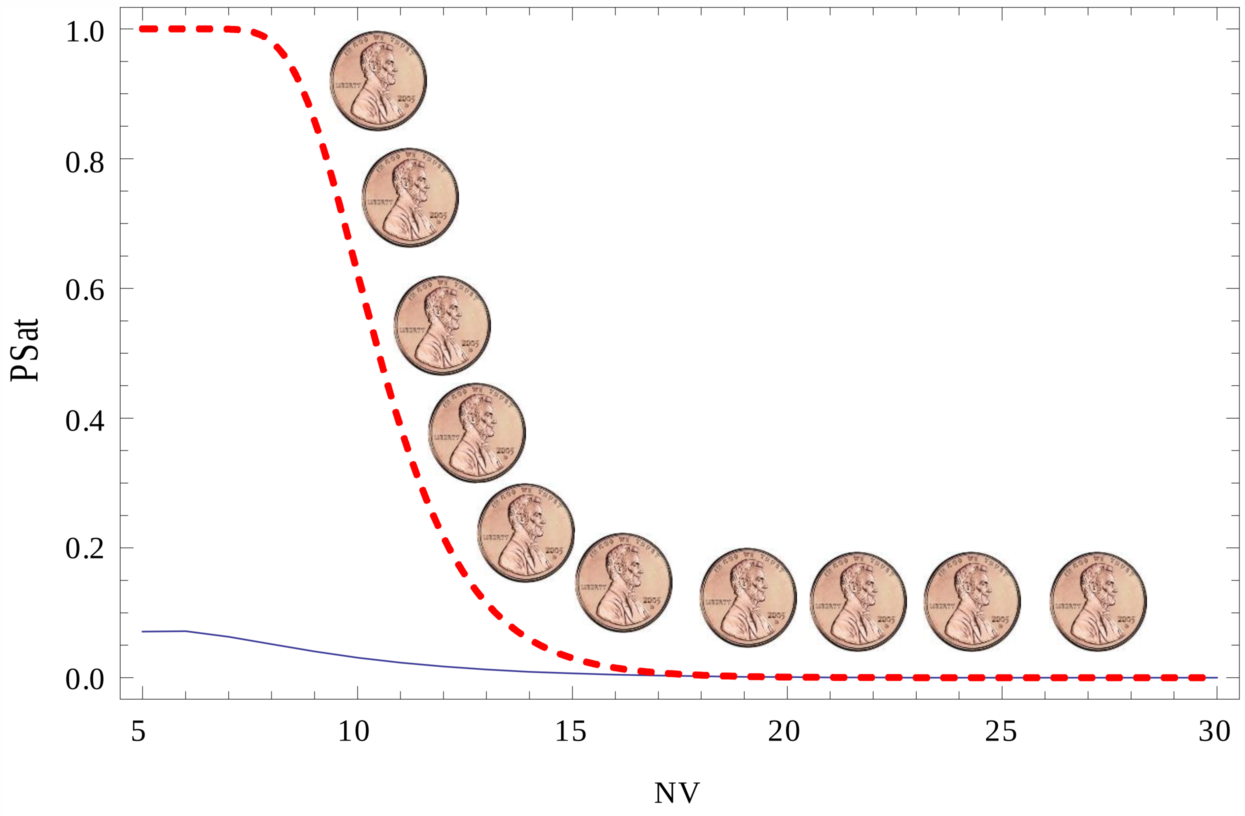


Psat = Probabilty of finding at least one chemotype that satisfies the *N* functional constraints.

PSat



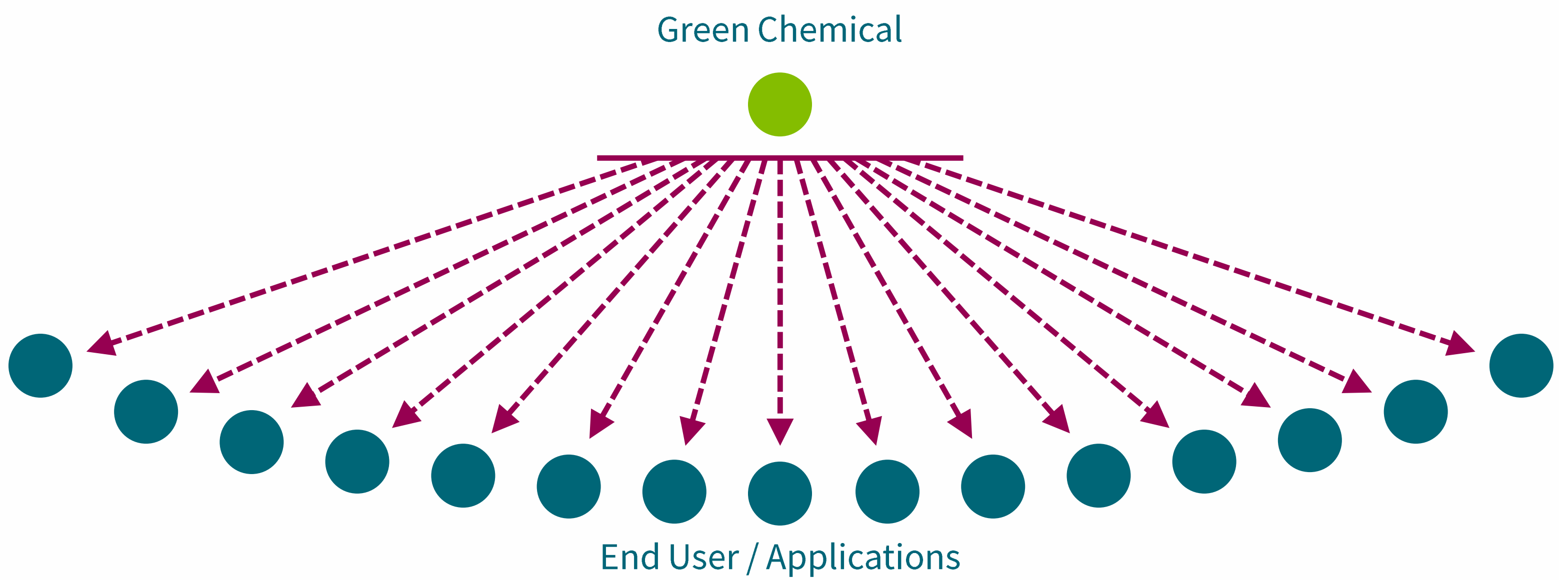
PSat



Old Approaches to Identifying Green Solvents

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

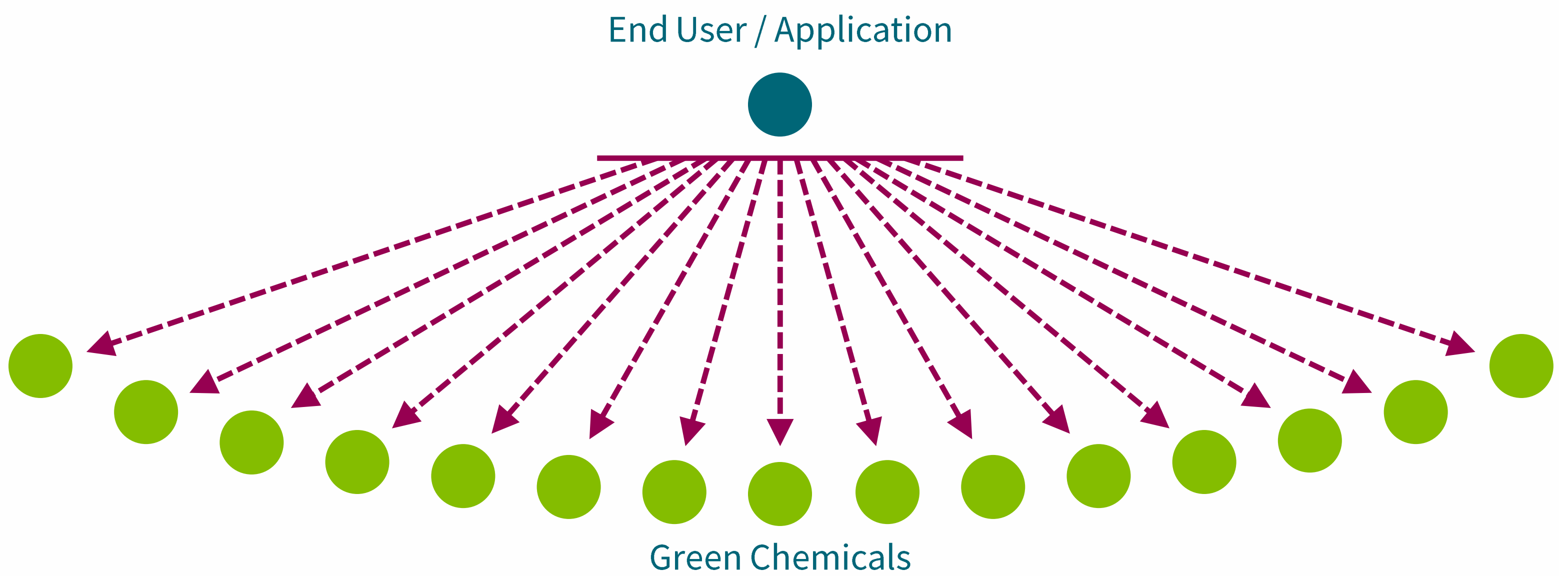
End User: Try **few** chemicals, get **poor** property match and technical efficacy is often suboptimal.



InKemia Approach: Diversity and Methodology for Property Match

InKemia: 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.



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The Team!

Paul Anastas
Chief Scientific Advisor

Lauren Zarama
CEO

Xavier Castells
Board of Directors & CFO

Lorenzo Herrero
CTO

Josep Castells
Board of Directors

Carles Estévez
President & CSO

Question & Answer

- If you have a question or comment, please type it in the "Questions" box located in the control panel
- Questions will be answered in order as they are received.

GC3 Networking Event in Boston on November 7th

NOV
07

GC3 Networking Event at Greenbuild in Boston, Nov. 7 at 7:30 pm

by Green Chemistry & Commerce Council (GC3)

Location: University of Massachusetts Club, One Beacon Street, 32nd Floor, Boston, MA 02108, with stunning views of the Boston skyline

If you are interested in attending, please email us at:
gc3info@greenchemistryandcommerce.org

GC3

Thanks for joining us!

For more information about the GC3:
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