



SITOLUB

SIMULATION TOOLS FOR
THE DESIGN OF SAFE AND
SUSTAINABLE LUBRICANTS

GenAI and *multi-disciplinary computational platform* to *accelerate R&D of lubricants*

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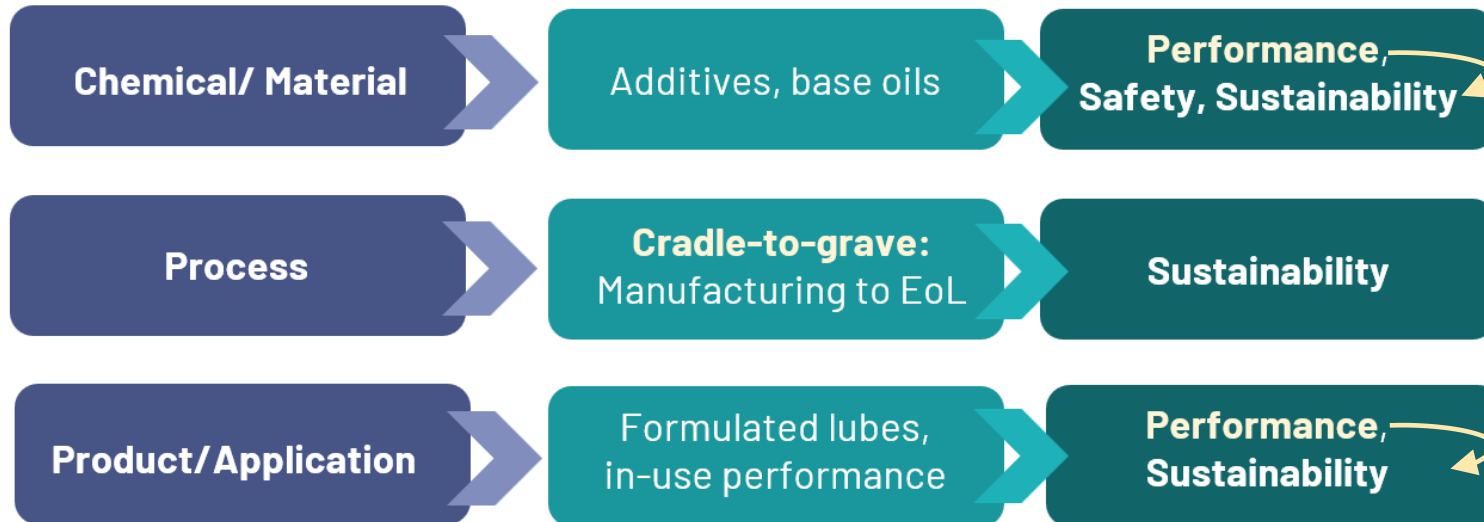
16.09.2026

- **Computational platform** development and validation
- Based on **Safe & Sustainable by Design (SSbD)** framework
- Integrated **performance** assessment

SSbD (re)design goal

SiToLub scope

SiToLub models



- *Avoid regrettable innovation*
 - *Regulatory & compliance foresight*
 - *Cost & time efficient R&D*
- *eliminate large-scale testing campaigns*



- **OPEN CALL for free external validation phase:** *January 2027 – June 2028*



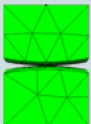
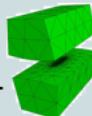
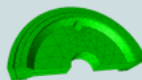
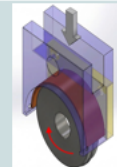
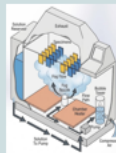
Single-Entry Point: simulations, testing, analyses, databases

Functionality ranking & application requirements fit



Objective benchmarking under application conditions

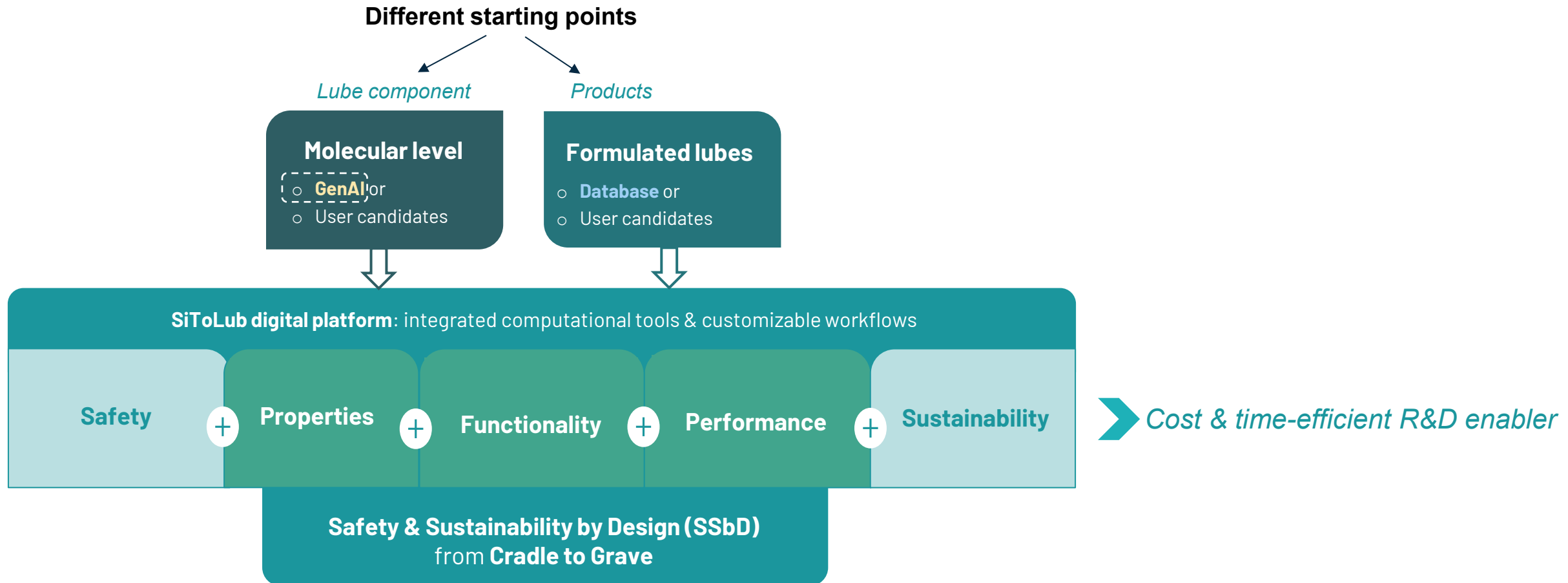


Use cases	Lubricant components	EP additives	Solid & soluble AW	Base oils	Corrosion inhibitors
Molecular level (additive & base oil)	Benchmarks	Chloroparaffins	PTFE & TPPT	PFPE	Benzotriazole
	(r)MD models	Base oil stability, Tribofilm performance, CoF, Viscosity as $f(T, p, \text{shear})$ and more			
	QSPR models	Physicochemical properties			
Application level (formulated lube, tribo-pair, conditions)	Viscosity model	Viscosity as function of (T, p, shear) simultaneously			
	FEM models	Frictional losses, Wear volume, Film thickness and more			
	Contact situation	Point - sliding - boundary regime 	Elliptic - Slide-Roll Ratio (SRR) - mixed to EHL regime 	Conformal - sliding - EHL regime 	No contact model relevance - static
	Test Rig	4-ball test 	Twin disc 	Block on ring 	Salt spray chamber 
	Applications	Metal forming	Gears	Journal Bearings	Corrosion test

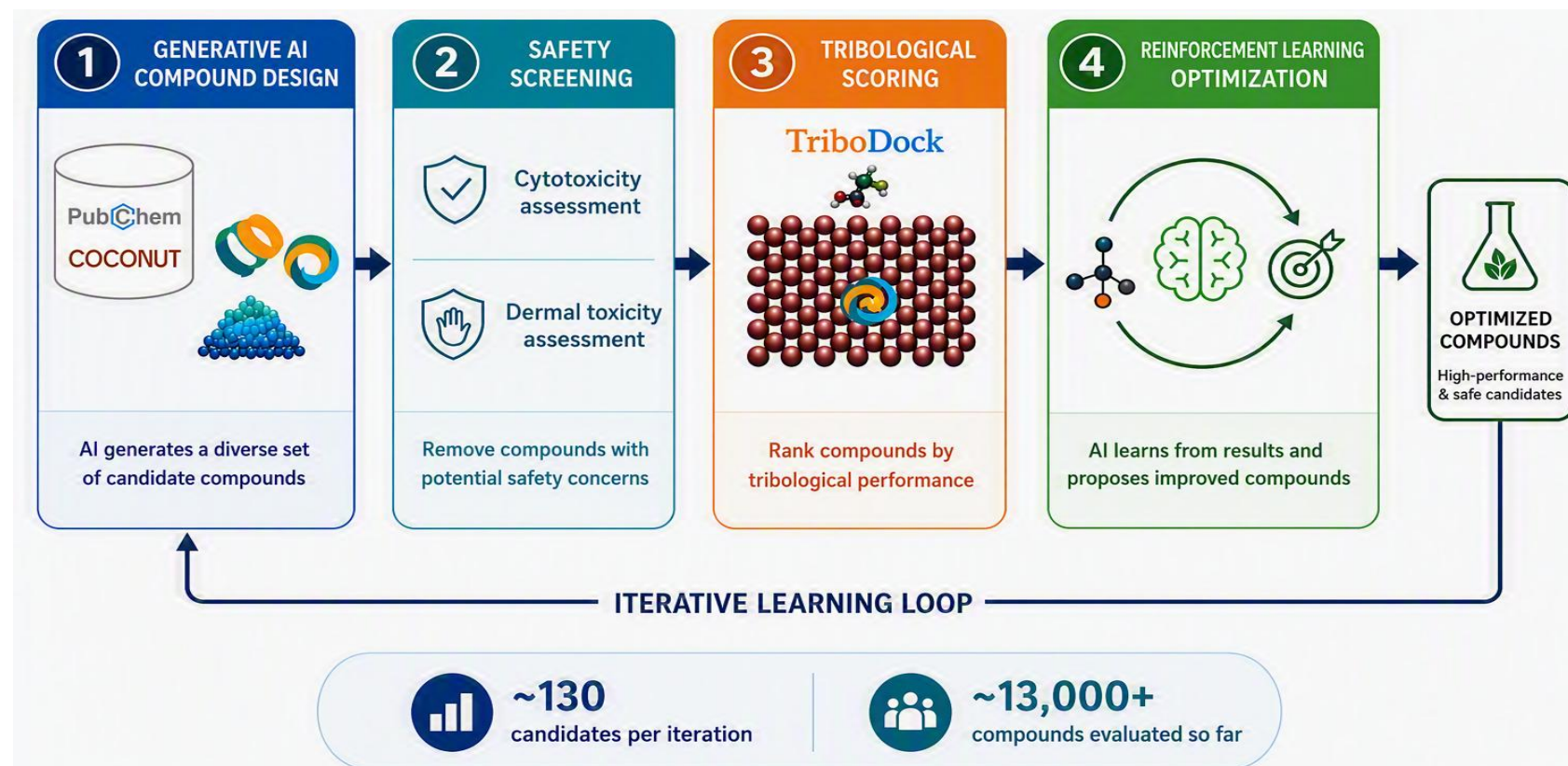


Component tests

- **Full SSbD workflow** overview
 - Starting from GenAI step



- Representative for **surface-protective additives**: EP, AW, Corrosion inhibitors (CI)
 - Safer alternatives or bio-based candidates
 - Synthesizability** and **commercial availability** of structurally similar compounds → **experimental validation step**

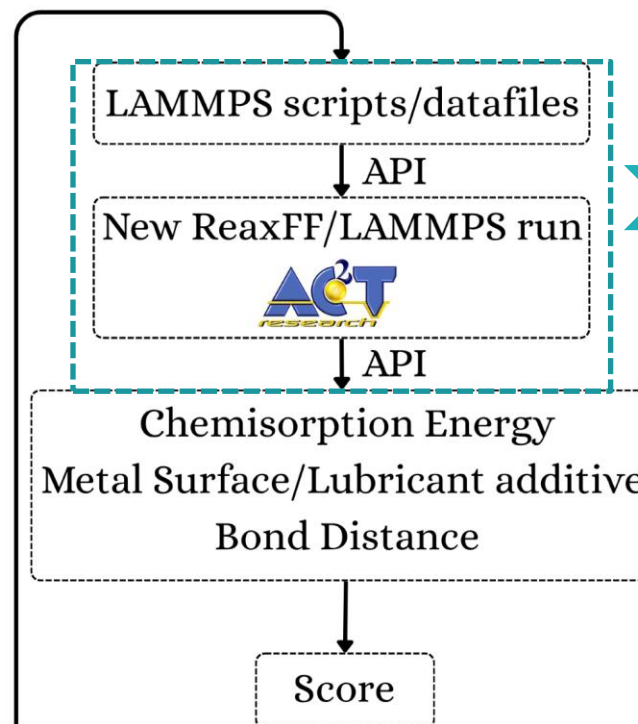
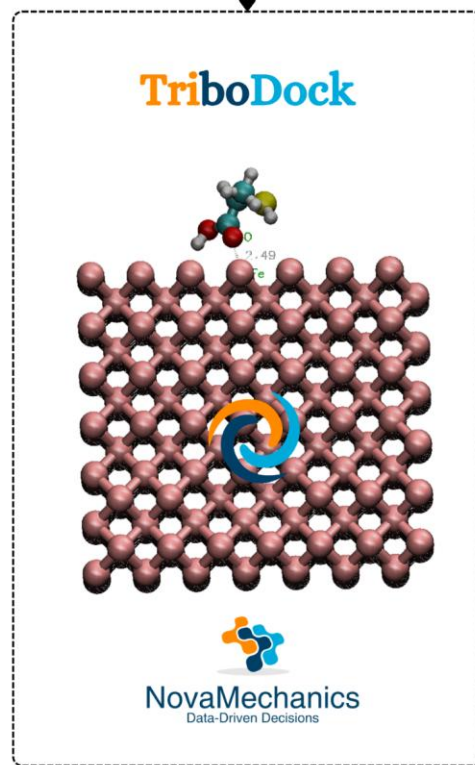


*Thousand of promising candidates to assess,
instead of handful in costly experiments*

genAI candidates

- Thorough assessment of **tribofilm forming potential**
 - Chemisorption energy** and **tribofilm density** assessment

From QSAR models



Time demanding →
as refinement loop
from rMD workflow step

Assessment in seconds →
evaluation need of
thousands of candidates

Actual functionality score

genAI candidates

- **QSAR models** for lubricant compositions
 - High-quality (QMRF validation reports)
- **(Eco)toxicity & biodegradability**
 - In-line with REACH/CLP (SDS, SVHC) and Ecolabel (VGP)
 - **Replaces** experimental data
 - **Exclude SVHC** substances

Assess safety and exclude prior sample acquisitions

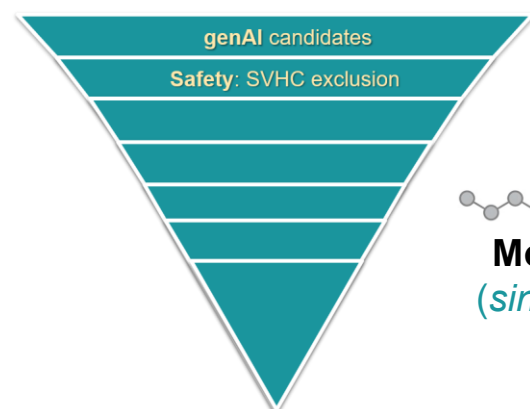


QSAR = QUANTITATIVE STRUCTURE - ACTIVITY RELATIONSHIP

Numerical, measurable data Molecular features, descriptors Biological effect, property, toxicity Mathematical correlation, model

Endpoint type	Name	Guidelines / Standards
Environmental Fate	Ready biodegradability	OECD 301
	Persistence water	OECD 309
	Persistence soil	OECD 307
	Persistence sediment	OECD 308
	Bioconcentration factor (BCF)	OECD 305-I
(Eco)toxicity	Fish acute toxicity	OECD 203
	Fish embryo acute toxicity	OECD 236
	Algae growth inhibition	OECD 201
	D. magna acute	OECD 202
	D. magna chronic	OECD 211
	Sludge inhibition	OECD 209
	Developmental toxicity	-
	Carcinogenicity	Animal/epidemiologic
	Genotoxicity (Ames Test)	OECD 471
	Genotoxicity (Hprt assay)	OECD 476
	Genotoxicity (Comet Assay)	OECD 489
	Genotoxicity (Chromosomal Aberration)	OECD 473
	Genotoxicity (Micronucleus)	OECD 474
	Skin Irritation	OECD 404
	Eye irritation	-
	Skin sensitisation	OECD 429
	Acute Oral Toxicity	-

Deep safety assessment in minutes



Molecular level
(single chemicals)

Ecolabel
REACH
Both
SVHC

Properties: 2nd step

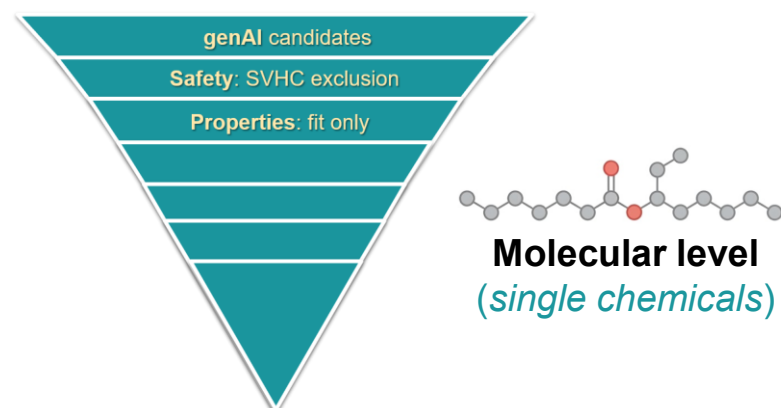
- **QSPR models** for **lubricant compositions**
 - High-quality: QMRF validation reports
- **Application requirements fit**
 - Under real operating conditions
- Relevant for **safety requirements**
 - REACH: SDS, CLP hazard labeling

*Assess application-fit
prior sample acquisitions*

QSPR=**QUANTITATIVE**-**STRUCTURE**-**PROPEERTY**-**RELATIONSHIP**
Numerical, measurable data Molecular features, descriptors Physical-chemical effect, state Mathematical correlation, model

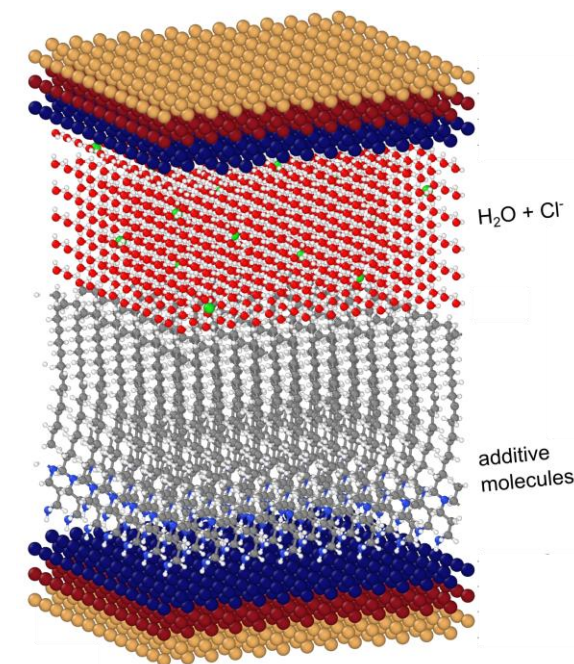
Endpoint type	Name	Guidelines / Standards
Physical state	Melting point (°C)	OECD 102
	Boiling point (°C)	OECD 103
	Vapour pressure	OECD 104
Solubility	Water solubility (log S)	OECD 105
	Partition coefficient (log Kow/ log P)	OECD 107, OECD 117
Rheology	Dynamic viscosity (mPa.s) at 40°C	OECD 114
	Dynamic viscosity (mPa.s) at 100°C	OECD 114
	Density (g/mL) at 25°C	OECD 109

Insights for application fit in minutes

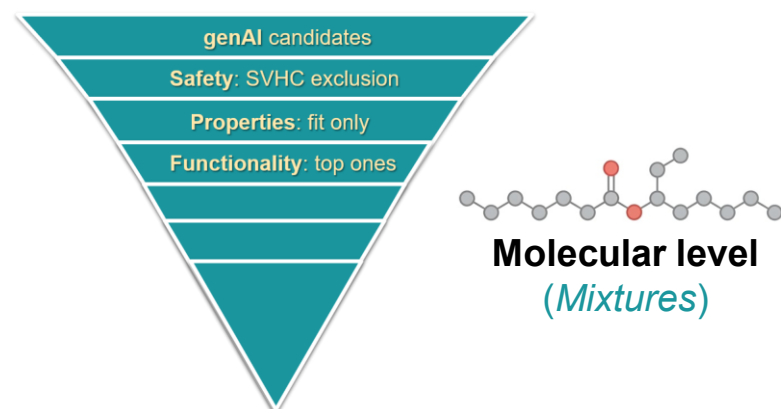


- **MD models for Application-relevant**
 - Density and Dynamic viscosity data at **T, p, shear**
 - Capabilities beyond conditions of rheometer measurements
- **rMD models**
 - Base oil stability: **thermo-oxidative & hydrolytic**
 - Onset of degradation, main degradation products
 - Surface-protective additives' performance: **EP, AW, CI**
 - Tribofilm formation, stability, CoF, CI film protection: water & salt

*Assess and rank for **actual**
(inter)molecular & surface **interactions***



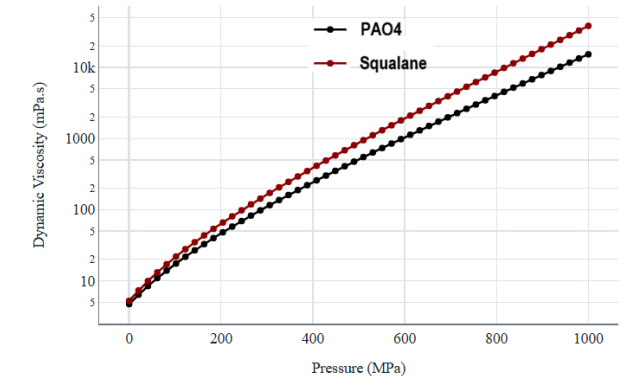
Actual molecular-based functionality



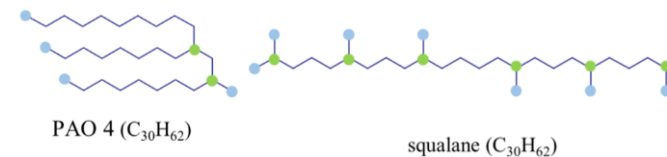
- **Lubricant-specific viscosity mapping** under real operating conditions
 - Determine **viscosity at any temperature, pressure and shear rate combination** simultaneously
 - Combined carefully selected and **validated empirical models**
 - Proper data fitting using **MD or Experimental data inputs**
 - Predict and benchmark **base oils** and **formulations: fresh or aged**
 - Essential to evaluate **load carrying capacity & frictional losses**

*Determine & rank for
base oils and formulations*

Select lubricant PAO4	Select lubricant Squalane
Select model Doolittle-Murnaghan	Select model Doolittle-Murnaghan
Fitting error (%) 6,54	Fitting error (%) 7,95



Same MW, different molecular structure



Products or Molecular level
(Unknown or known composition)

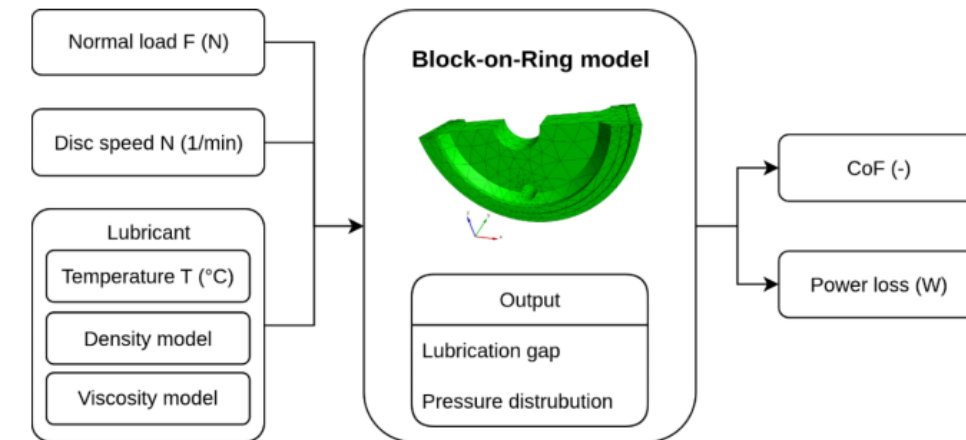
Test for free @ i-tribomat.eu

Performance in application: 4th step

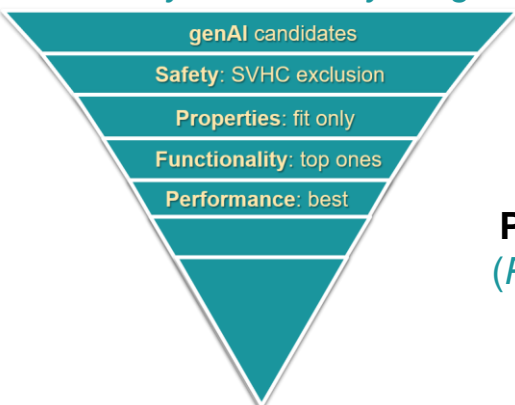
- **FEM models of actual applications for SiToLub use-cases**
 - Actual **material, geometry, surface, operating conditions** and **rheology**
 - From **boundary** to **EHL** lubrication regimes

FEM models	Frictional losses, Wear volume, Film thickness and more		
Contact situation	Point -sliding - boundary regime	Elliptic - Slide-Roll Ratio (SRR) - mixed to EHL regime	Conformal - sliding - EHL regime
Test Rig	4-ball test	Twin disc	Block on ring
Applications	Metal forming	Gears	Journal Bearings
Lubricant components, formulations /products	EP additives	Solid & soluble AW	Base oils

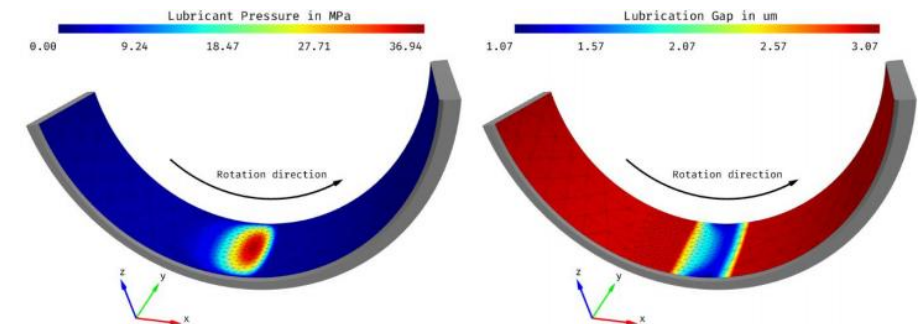
Benchmarking & optimization under application-relevant conditions



Efficiency & Durability insights



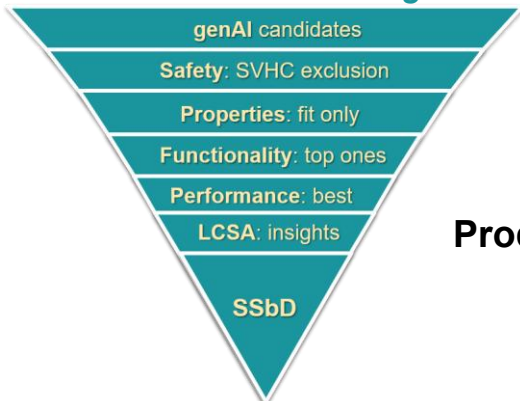
Products and Application
(Performance in application)



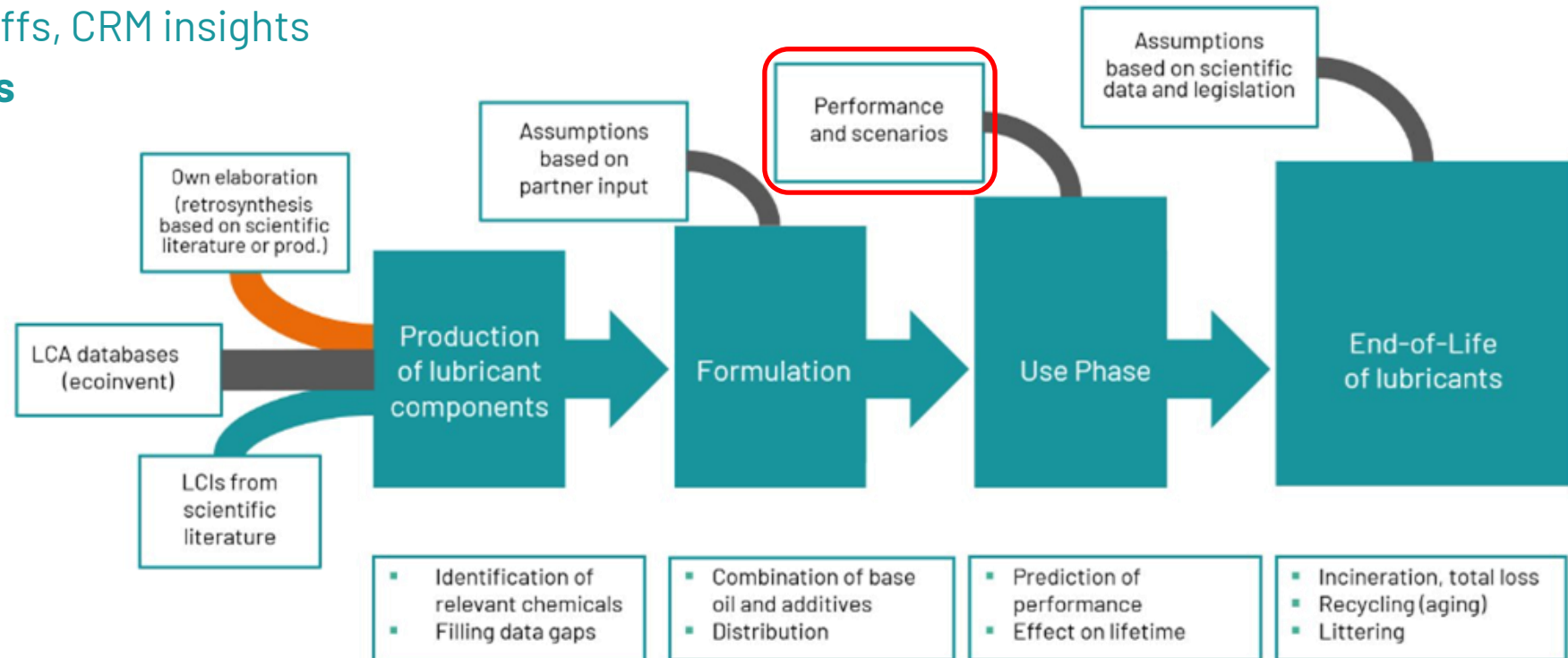
- **Comprehensive LCSA** throughout **Cradle-to-Grave** lifecycle
 - **ecoinvent** and **CarbonMinds** databases or **user data**
 - Explicit **performance** consideration
 - PCF, hot-spots, trade-offs, CRM insights
 - **Impactful optimizations**



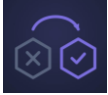
Full SSbD ranking



Product and Processes (Entire lifecycle)



ISO14067 (**PCF**), ISO-14040/44 (**LCA**), soca v3.12 (**S-LCA**), **UEIL/ATEIL** & **API** methods



J1 — Substance replacement

Replace PFAS or CRM, avoid SVHC, comply with EU Ecolabel — or swap any ingredient



J2 — Virtual candidate evaluation

Evaluate any base oil or additive — before you buy or synthesise it



J3 — Lubricant comparison & selection

Compare candidates across performance, safety, and sustainability



J4 — Application performance

Predict lubricant performance in your specific machine contact



J5 — Stability & service life

Predict how long your lubricant will last under real conditions



J6 — Sustainability & compliance

SSbD assessment, LCA, product carbon footprint (PCF), and ESPR / Digital Product Passport



 *Workflows for actual needs*

*From thousands of candidates rapidly to
high performing, safe and sustainable lubricant*

SiToLub



Catalogue of models



i-TRIBOMAT



Contact for Open Call



sitOLub

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