

Corporate

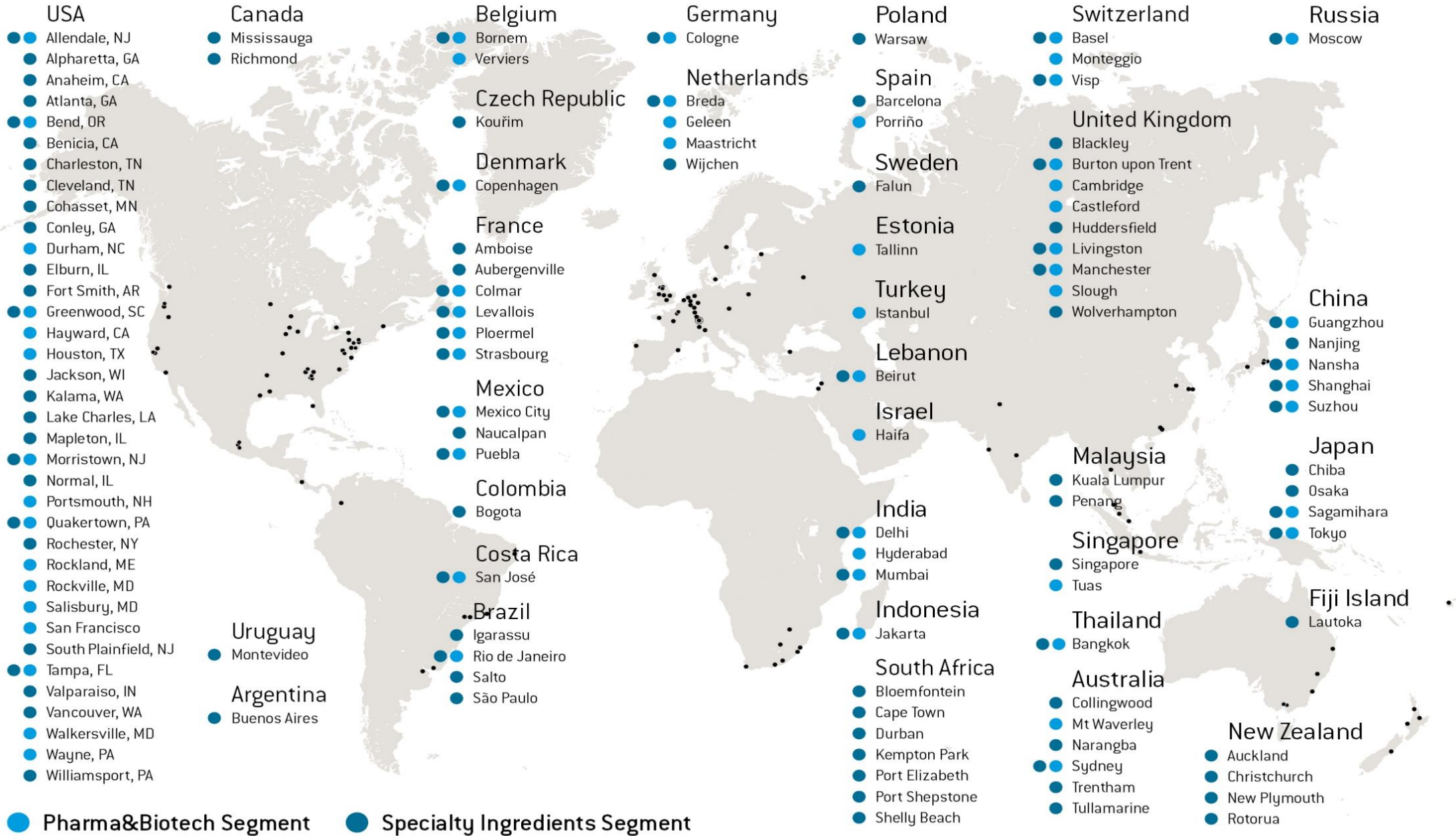
CapeOpen- Meeting

Annual Meeting

Sandra Fillinger | Ludwigshafen | 09.10.2018



Global Footprint



Lonza at a Glance

Delivering synergies with connected technology platforms and fields of expertise

Pharma & Biotech

Specialty Ingredients (LSI)

Patient Healthcare



Consumer Health



Consumer & Resources Protection



PRESCRIPTION



PREVENTION



PROTECTION



PRESERVATION

Lonza's Healthcare Continuum Spans All Our Businesses

Lonza
Closer Than You Think®

Prescription Medicine Actives

Drug-Delivery Technologies

Hydrazine Propellant

Temperature-Resistant Resins

Corrosion Inhibitors

Cell and Gene Therapy

Abrasion Resistant

Anti-Mold Components

Anti-Fouling Coatings

Tools for Researchers

Immunotherapy Actives

Fungal-Decay Protection

Human Tissue Cells

Food Preservatives

Anti-Aging Actives

Disinfectant Wipes

Vitamin B3 Compounds

Antidandruff Agents

Slug Control

Drinking Water Sanitization

Pet Food Supplements

Crop Protection

Pool and Spa Sanitizers

Unfold Lonza – Key Figures

Increasing in size and scope through organic and inorganic growth





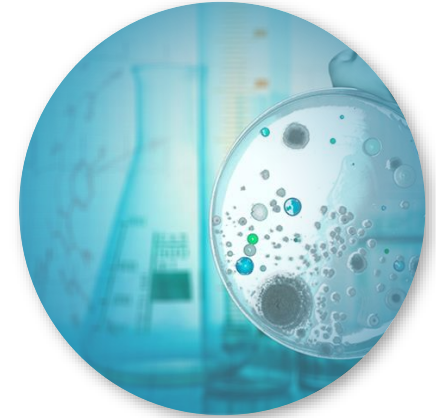
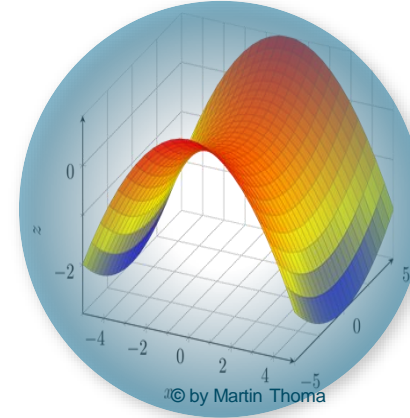
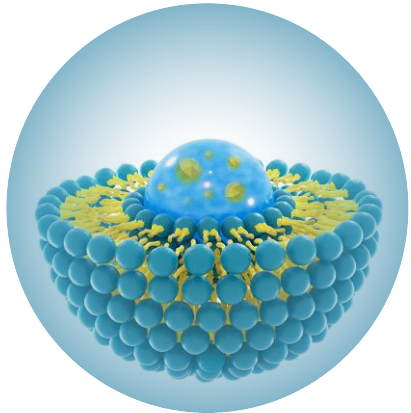
Upstream Technologies (UPS)

Process Technology & Innovation (PTI)

Scale-up & PD Support; New Products (PDN)

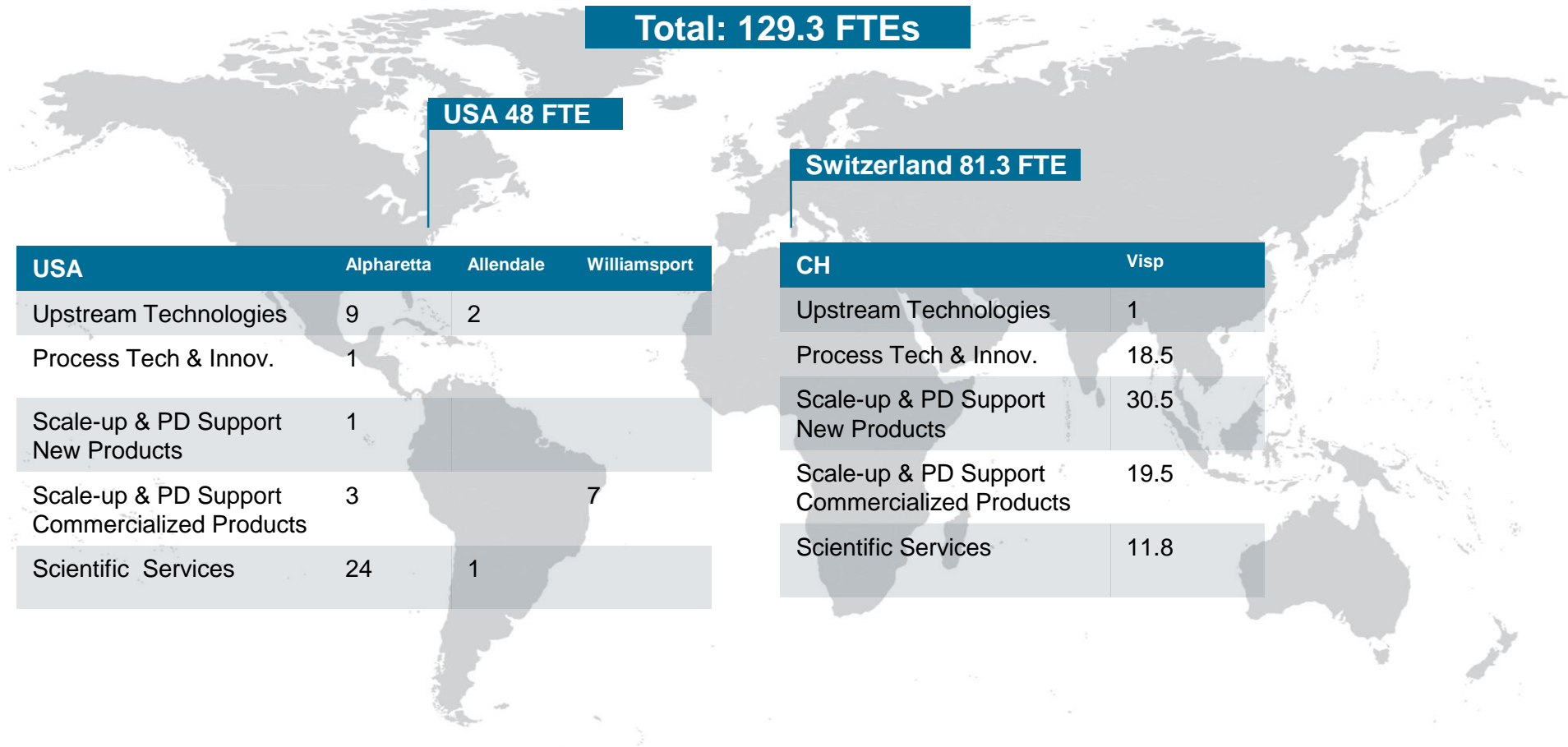
Scale-up & PD Support; Commercialized Products (PDC)

Scientific Services (SCI)



LSI central R&T organization

Locations*

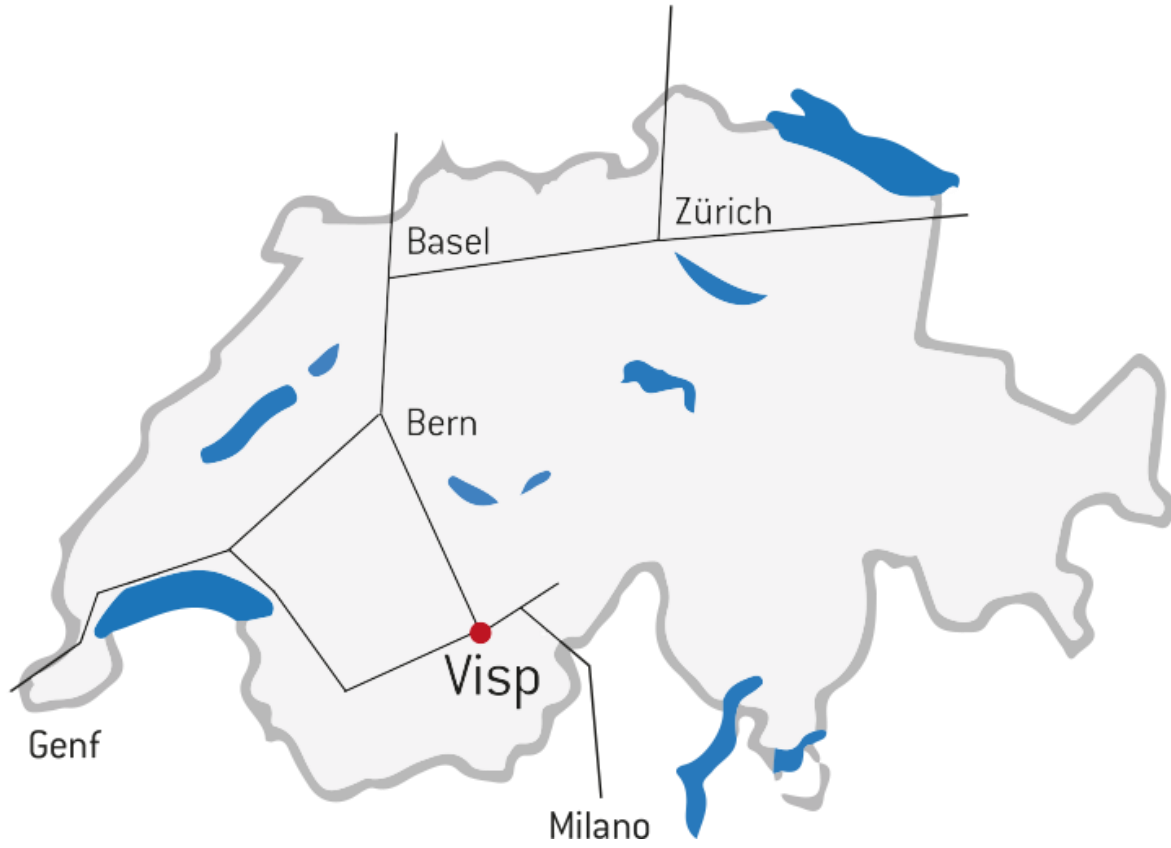


* As of Oct 17, 2017; Only permanent - excl. management team

Corporate

Lonza Visp and R&T – Research and Technology LSI

Sandra Fillinger | Ludwigshafen | 09.10.2018



Visp / Lalden (Switzerland)

Lonza Ltd, Lonza BioPharma Ltd

- Area: 90 ha (twice the size of Vatican city)
- Employees: approx. 2650, thereof 150 apprentices
- Plants:
 - Naphtha cracker
 - Dedicated and multi-purpose plants
 - Fully integrated waste management facilities
 - Microbial biopharmaceuticals cGMP facilities at 20L, 1 000L and 15 000L scale
- Products:
 - Active pharmaceutical ingredients
 - Biopharmaceuticals
 - Antibody drug conjugates (ADC)
 - Chemical intermediates
 - Diketene derivatives
 - High-performance materials
 - Hydrocyanic acid derivatives
 - Meta[®] metaldehyde
 - Niacin / nicotinic acid (vitamin B3)
 - Peptides and oligonucleotides
 - Plant protection agents
 - Pyridine derivatives



The engineer's toolbox at Lonza

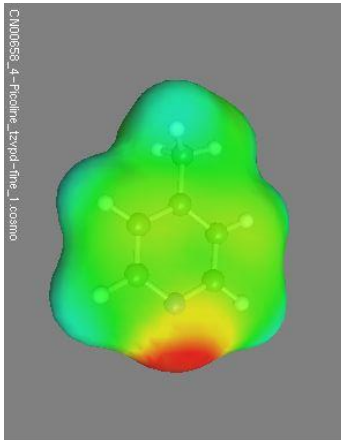
Software and Lab equipment

- Component data (pure component and mixtures)
 - Data bases (DDB, CAPEC, ASPEN DB, ChemCad DB, internal DB, ...)
 - Experimental measurements (internal / external)
 - Predictions (DDBST Tools, CAPEC, molecular dynamic simulations)
- Stationary flowsheet simulation (single unit operations and complete processes) and dynamic simulations
 - ChemCad, ProSim
- Plant-fit for batch processes (multi purpose plants)
 - Super-Pro-Designer
- Fluid dynamics
 - Visi-Mix, Mixit
- Reaction engineering (calorimetry, safety)
 - PRESTO Kinetics, AKTS
- Reaction screening tools
 - Microwave reactors, miniautoclave, combined reaction calorimeter (CRC), temperature controlled UV-VIS
- Lab Automates
 - Recipe controlled reactions, automated distillation, also 24/7
- Distillation
 - Several sizes of packed columns (conti and batch), dividing wall column, wiped-film evaporators, short path evaporator
- Extraction
 - Continuous extraction columns, 1-stage extraction centrifuge, Mixer-settler, ...
- Crystallization

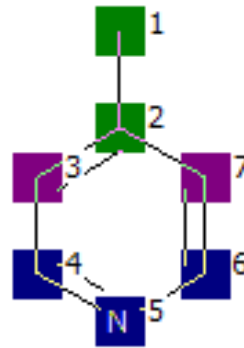
Modeling and simulation

Physical properties

- Thermodynamic properties of pure components and mixtures from databases
- If no data available, application of predictive models (e.g. COSMO-RS or UNIFAC)
- Experimental measurements of VLE, LLE, SLE, VLLE, ... only in cases when very high accuracy is mandatory or when predictive results are poor
- Internal guideline for modeling procedure in place



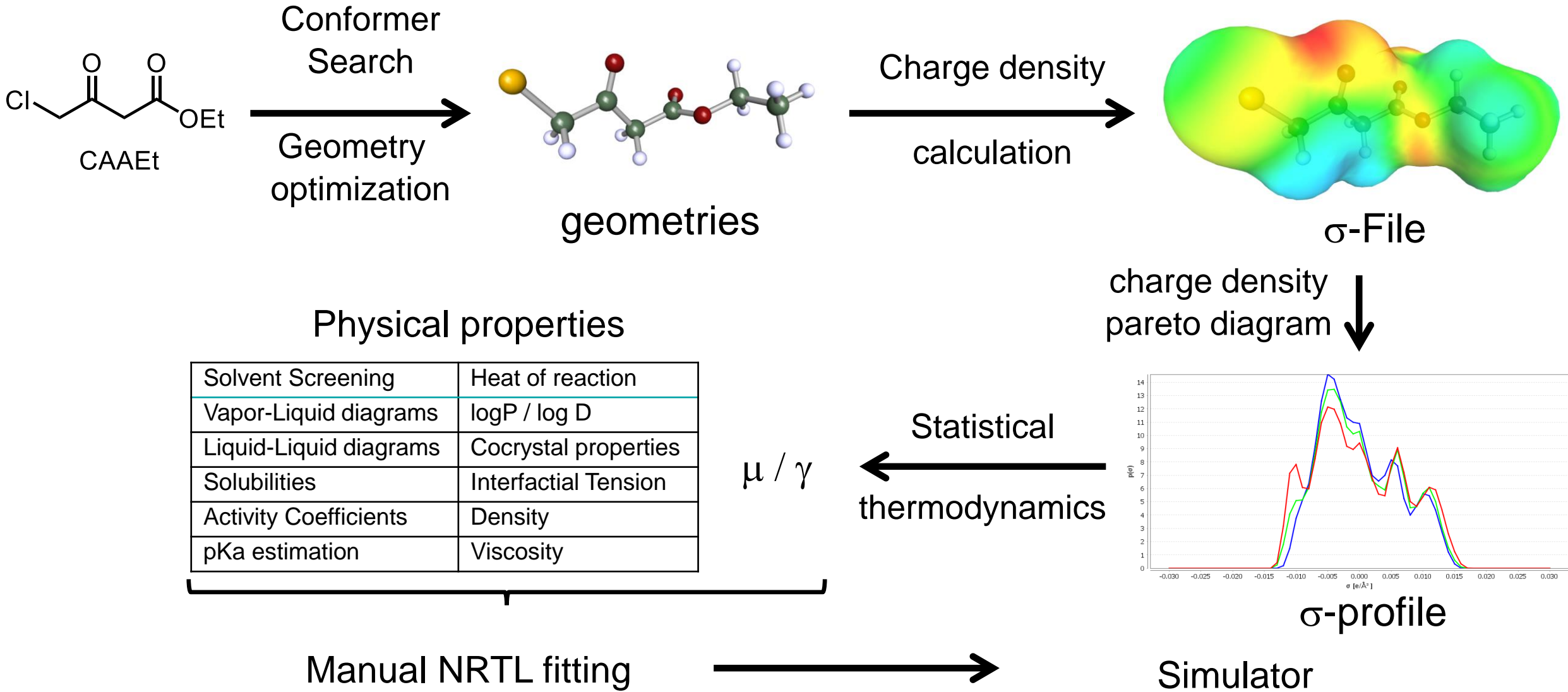
COSMO –Surface
(load distribution) of
4-Picoline



UNIFAC-
Incrementation of
4-Picoline

Typical workflow

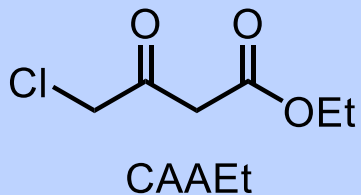
From a structure to a simulation



Typical workflow

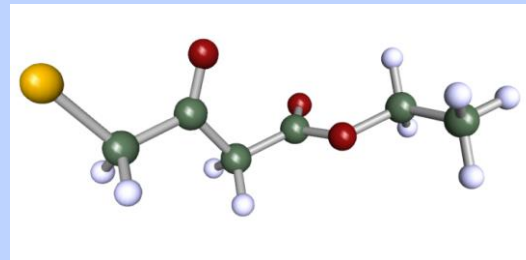
From a structure to a simulation

Molecular Modeling



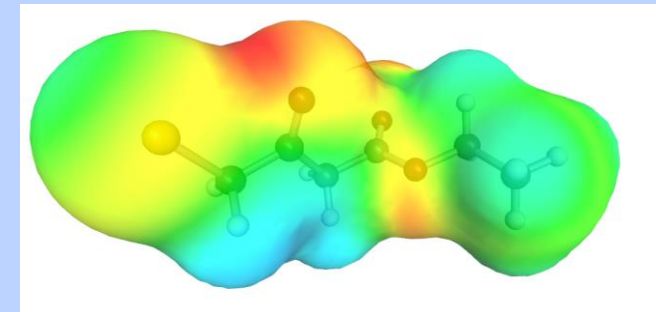
Conformer Search

Geometry optimization



geometries

Charge density calculation



σ -File

COSMOtherm

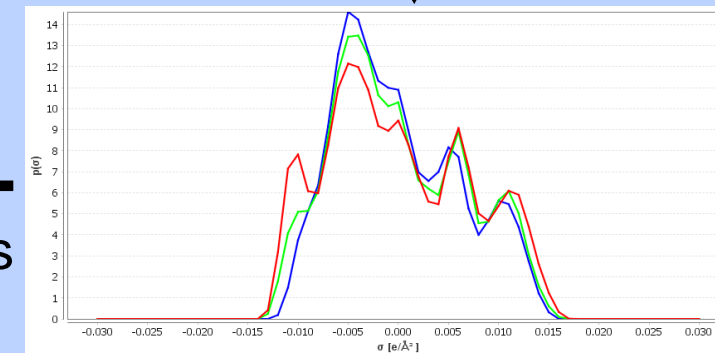
Physical properties

Solvent Screening	Heat of reaction
Vapor-Liquid diagrams	logP / log D
Liquid-Liquid diagrams	Cocrystal properties
Solubilities	Interfacial Tension
Activity Coefficients	Density
pKa estimation	Viscosity

μ / γ

Statistical thermodynamics

charge density
pareto diagram



σ -profile

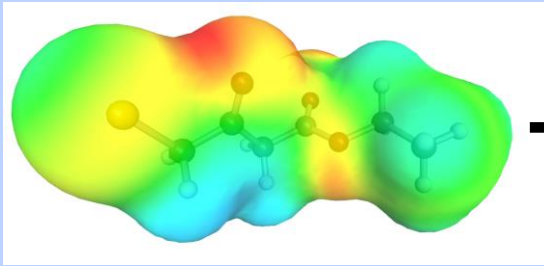
Manual NRTL fitting

Simulator

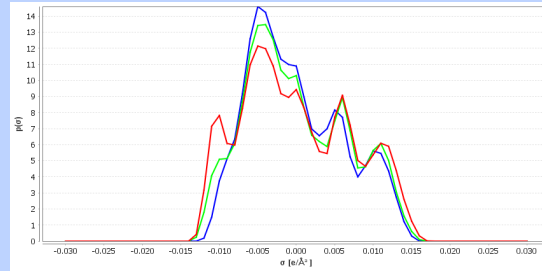
Future Workflow

Role of CAPE OPEN?

COSMOtherm



σ -File



σ -profile



$$\mu(i, c, T, p)$$

$$\gamma(i, c, T, p)$$

Manual NRTL fitting ?

CAPE OPEN ?



Simulator

Lonza needs & requests:

- Interoperability between property prediction & simulation tools
- Interconnection to databases (DDB, tool and user-specific databases)
- Model exchange for user-specific models
- CAPE OPEN – underlying conditions

Corporate

Thank you very much for your attention
Questions welcome

contact:

Sandra Fillinger & Andreas Klein

sandra.fillinger@lonza.com,

andreas.klein@lonza.com

Tel +41 27 948 7193

<http://www.lonza.com>