

NUVISAN

Agrochemical Solutions

Today's Agenda



About
NUVISAN



Drug Discovery



Agrochemical
Solutions

NUVISAN The Science CRO

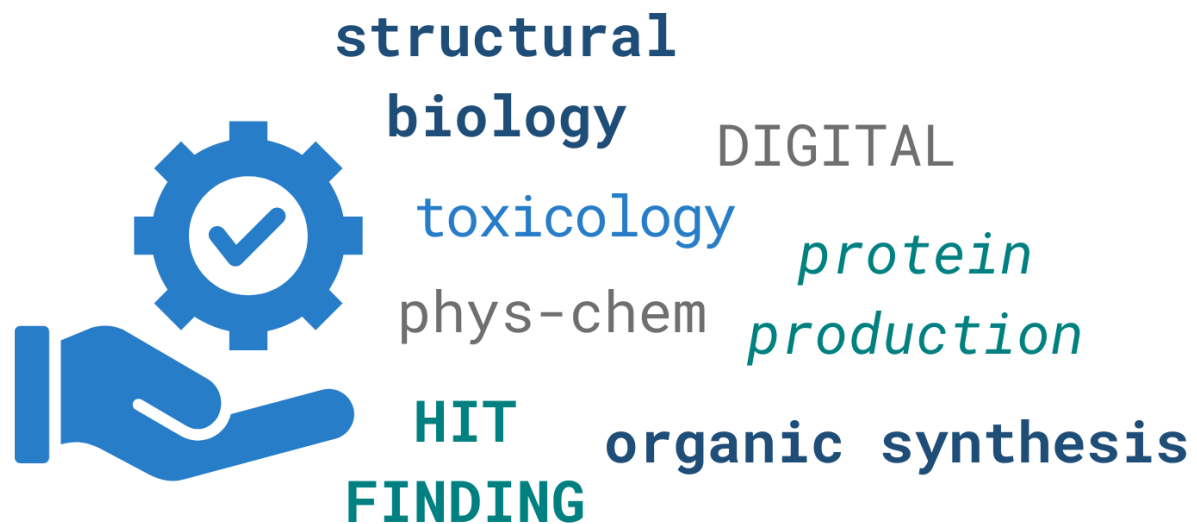
Crop Science R&D Meets Scientific
Excellence



➤ Growing Demands on Outsourcing Settings

Integrated Solutions & One-stop Shop

Encompassing a wide range of services including



Single Master Agreement

keeping minimum contractual burden

Flexibility of Research

of outsourcing capabilities

1 Project Manager

for multidisciplinary operations



Focus on Science & Bioactive Compounds

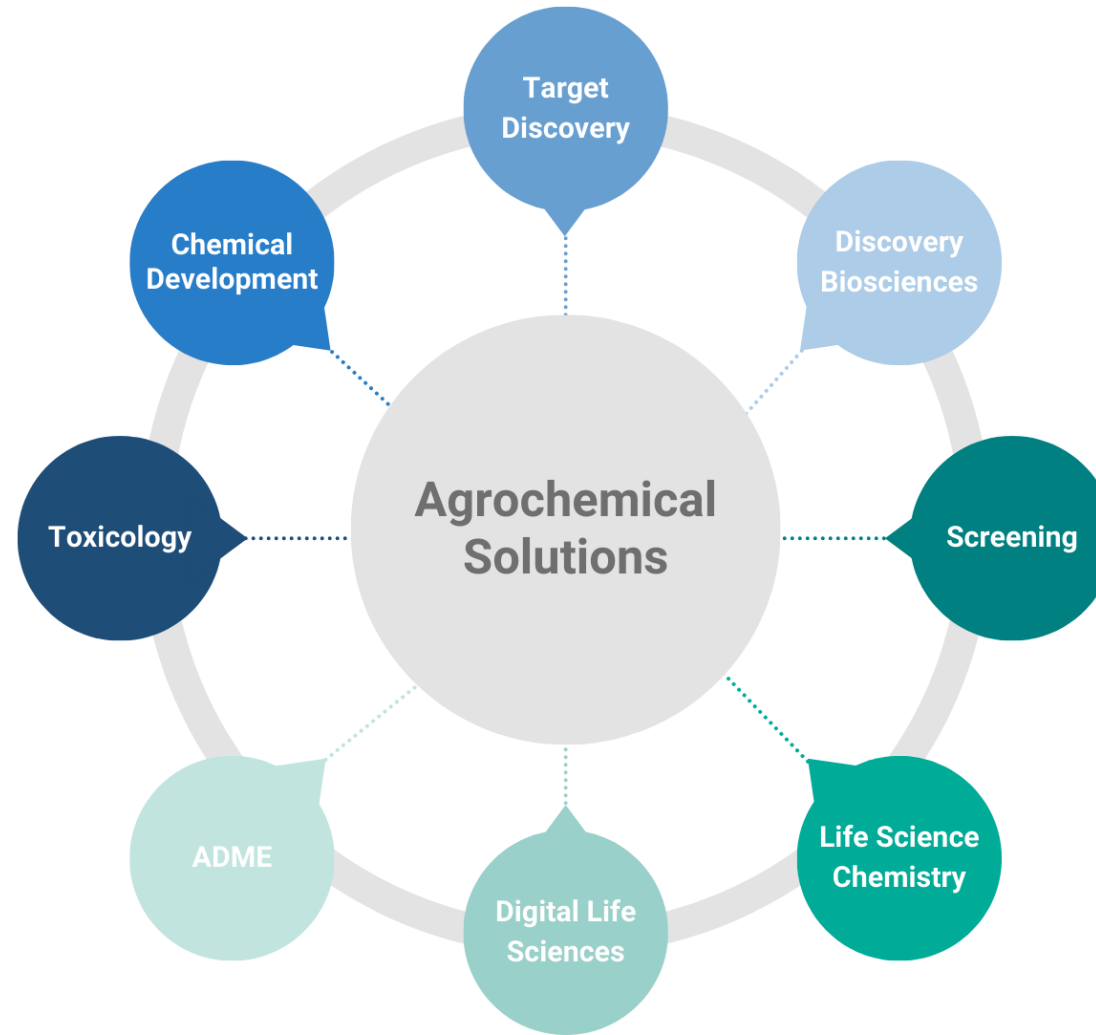
- Skilled synergy: Integrating Pharma and Agrochemical sectors for precision pesticide R&D project support.
- “Science first” & customer-centric focus paired with creative, flexible & solution-driven mindset to meet your individual needs
- Empowering Agrochemical Innovation: From discovering new chemical matter to designing and generating compound libraries, characterizing compounds, and assessing safety profiles



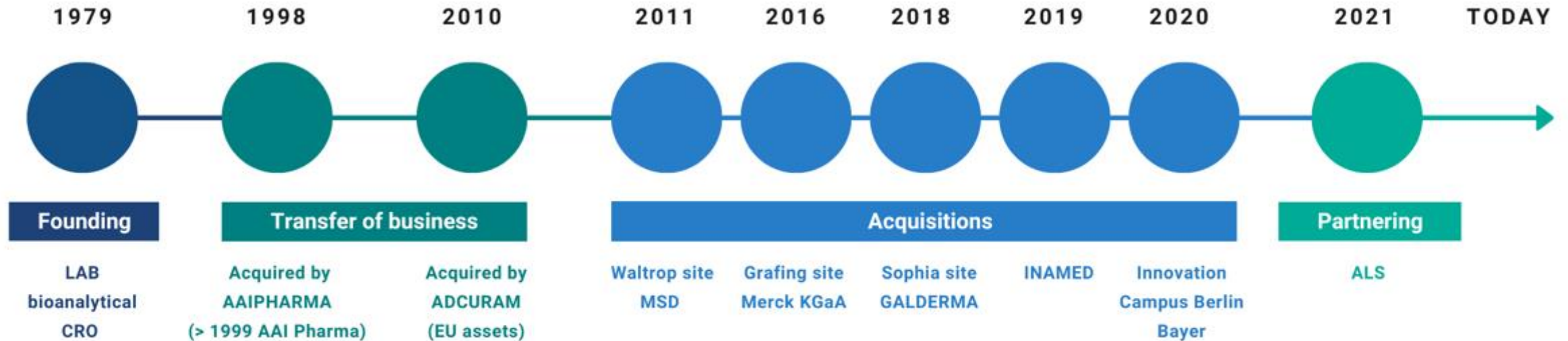
Balanced Client Portfolio

- Clients & partners from Crop Science and Pharma industry, biotech / startup companies, venture capitals & non-profit organizations
- With a focus on transparent discussion, review & revision of project strategies, our industry-experienced scientists
 - Increase your project value
 - Optimize your portfolio with enabling solutions

Agrochemical Solutions



Our History

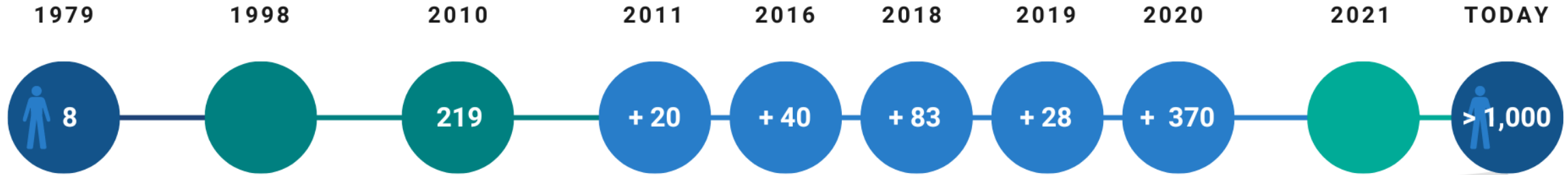


2014

Management buy-out
Name changed to

NUVISAN

Our People



~ 31% scientists (69 % *Ph.D.*)
~ 40 % lab professionals
~ 29 % non-scientific staff



➤ Our Sites in Europe & Beyond



Berlin (GER)



Neu-Ulm (GER)



Waltrop (GER)



Grafing (GER)



Sophia (FRA)

Active Ingredient Discovery & Development

Agrochemical Solutions



Our Leadership Team



Charlotte Kopitz
Discovery Pharmacology



Boiteau Jean-Guy
Chemical Development
& Manufacturing



Franz von Nussbaum
Life Science Chemistry
& Digital Life Sciences



Olaf Prien
ADME
& Toxicology



Holger Steuber
Discovery Biosciences
& Screening

Target Discovery



Target
Validation



In Vitro
Biology



Functional
Genomics

Target Discovery

Target Validation

- Bioinformatics *in silico* target analysis

In Vitro Biology

- Cellular assays with human & rodent cell lines incl. flow cytometry
- IHC & *in situ* hybridization, microscopy units

Functional Genomics

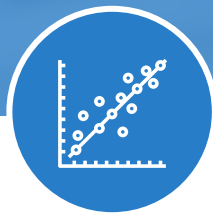
- Next-generation & single-cell sequencing
- Expression analysis
- Bioinformatics services



Discovery Biosciences



**Protein
Sciences**



Assays



**High-Content
Analysis**



Biophysics



**Mass
Spectrometry**



**Structural
Biology**

Discovery Biosciences

Protein Sciences



- Customized molecular biology service
- Multi-parallel expression optimization (*E.coli*, insect & mammalian cells)
- High quality protein production for assays, structural biology & biophysics
- Protein QC (MS, fSEC, aSEC, nDSF, DLS)
- Membrane protein platform

Biophysics



- Versatile platform: SPR, TSA, nDSF, NMR, ITC, DLS, MST
- Hit characterization, kinetic profiling & SAR support
- Mode-of-action & target engagement
- Biophysical fragment screening (SPR, TSA, NMR, ASMS)

Assays



- Assay development incl. tool generation (stable cell lines)
- Biochemical, cellular & high content assays
- Binding & enzyme activity assays
- Adaptation to ultra high-throughput

Mass Spectrometry



- High-throughput (HT) MS (RapidFire MS & MALDI-MS)
- Intact mass measurement
- Native mass spectrometry
- Targeted metabolomics
- Proteomics & peptide mapping

High-Content Analysis



- Phenotypic & multiplexed HTS
- SMOL & CRISPR libraries
- Eukaryotic cells (animal, fungi), bacteria & 2D and 3D cell systems
- Single time points & live-cell kinetics

Structural Biology

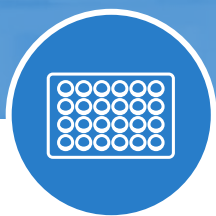


- X-ray determination & analysis
- High-throughput platform for multi-target crystallization
- Cryo-EM, NMR
- HT Crystallography (HTX) for fragment screening
- Small molecule structure determination

Screening



Libraries



**High-Throughput
Screening**



**Fragment
Screening**



**Virtual
Screening**

Screening

Libraries

- Accelerate Screening Process
- Discover Valuable Hist and Leads
- NUVISAN Explorer Library: 340k Commercial Compounds
- Lead-like Compounds
- Streamlining Optimization for Targeted Drug Discovery

Fragment Screening

- Biophysical screening (SPR, TSA, NMR, ASMS) of customized library (~ 2k Ro3 fragments)
- X-ray screening of customized library (~ 900 fragments @500 mM DMSO)
- 1° screen / hit confirmation → hit validation → fragment-to-lead

High-Throughput Screening

- Biochemical, biophysical, cellular with up to 300,000 tests / day
- Mass spectrometry HTS (MALDI-HTOF, RapidFire)
- Best-in-class high content analysis (HCA) screening platform
- > 8 yrs of high content imaging/screening experience of plant-pathogenic fungi in high-throughput (384-/1536-well format)
- > 20 yrs of Pharma HTS experience (> 10 clinical cpds)
- State-of-the-art screening data management

Virtual Screening

- NUVISAN Explorer library (340k Commercial Compounds)
- External libraries (100k - > 1b)
- *In silico* virtual screening
- Target / ligand data mining
- Hit expansion

Life Science Chemistry



**Design
& Synthesis**



**Analytics
& Purification**



**Scale-up
& Special
Technologies**



**Microbiological
Chemistry**



**Compound
Logistics**



PhysChem

Life Science Chemistry

Design & Synthesis

- Decades of optimization experience from hit assessment to clinical compound
- ID of new leads for challenging targets
- Multi-parameter optimization of molecules (Hit-to-lead, Lead-to-field candidate)
- SMOLs, probes & new modalities (incl. PROTAC[®]s)

Microbiological Chemistry

- Biotransformation & protein / plasmid production
- Integration in NUVISAN metabolite discovery platform
- Metabolite identification, screening, synthesis & characterization

Purification & Analytics

- Separation technology platform (from < 1 mg up to 1 kg)
- Chiral separation incl. SFC
- NMR, MS & OPT expertise for structure services
- Ligand-protein interaction analysis via NMR & MS

Compound Logistics

- Collection, storage, plating & shipping of compounds
- Building block collection for fast synthetic diversity

Scale Up & Special Technologies

- Large-scale synthesis of API or intermediates incl. route optimization
- High pressure reactions, photochemistry, hydrogenation, carbonylation
- Plate-based chemistry
- PROTAC libraries via split-and-pool synthesis

PhysChem

- Solubility
- Lipophilicity
- Stability
- Crystallinity (XRPD) & pKa
- Photostability

Digital Life Sciences



**Molecular
Modeling**



**Cheminformatics
& Machine Learning**



**Omics Data Analysis
& Bioinformatics**

Digital Life Sciences

Cheminformatics & Machine Learning



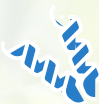
- Fingerprint, substructure & similarity search
- ML models for ADME end points
- QSAR predictions
- Clustering & SAR
- Chemical space analysis
- R-group decomposition & visualization, activity cliffs

Omics Data Analysis & Bioinformatics



- Interpretation of transcriptomics, genomics, epigenomics (single-cell & bulk next-generation sequencing) / spatial profiling / pooled, arrayed & single-cell CRISPR screens
- Microscopy image analysis at single-cell resolution
- *In silico* target & indication space evaluation
- Literature & database mining

Molecular Modeling



- Virtual screening
- Structure-based design
- Ligand shape-based screen
- Scaffold hopping
- Molecular docking
- Molecular dynamics & free energy calculation

DMPK

Discovery & Development



In Vitro PK



In Vivo DMPK



Biotransformation
& MET ID



Consultancy
Services



Isotope
Chemistry

DMPK (Discovery & Development)

In Vitro ADME



- *In vitro* ADMET assay panel for research (HT)
- *In vitro* HT assays with custom protocols
- Investigation of absorption, distribution, metabolism, excretion (ADME) with radio- / non-labeled material

Biotransformation & MetID



- *In vitro* & *in vivo* metabolite profiling, quantification & structure elucidation in various matrices
- Mass spectrometry imaging

In Vivo DMPK



- PK in rodents, minipigs - single compound & cassette dosing, different admin routes
- Microsurgical rodent models e.g. ???
- Absorption, metabolism & excretion

Consultancy Services



- DMPK consultancy through all R&D phases
- Project management, DMPK representation

Isotope Chemistry



- GMP Radioactive Synthesis
- Stable Isotope Synthesis
- Radioanalytical and Purification Solutions
- Radioactive Compound Storage Solutions



Best Practice in Animal Welfare

- We believe that humane care & use of animals is a key element of high-quality science
- Our high standards are confirmed by continuous positive feedback from client audits, authorities & full AAALAC accreditation at all sites working with animals
- In addition to complying with legal requirements, we strive to continuously improve our practices & husbandry conditions in the interest of animal welfare

Toxicology



In Vitro
Toxicology



In Vivo
Toxicology



Toxicologic
Pathology



Clinical
Pathology



Formulation

Toxicology

In Vitro Toxicology

- Genotoxicity: Bacterial Reverse Mutation & Mammalian Cell / Erythrocyte Micronucleus Test, Mammalian Erythrocyte, Pig-a Gene Mutation & *In Vivo* Mammalian Alkaline Comet Assay
- Skin toxicity: Skin irritation, corrosion & sensitization assays
- NRU 3T3 phototoxicity test

Toxicologic Pathology

- Gross examination, histotechnique & histopathology assessment
- Molecular services incl. development of customized staining / biomarker assays
- Digital pathology platform
- Organ databank
- Peer review for external studies

In Vivo Toxicology

- Dose range finder & toxicokinetics
- Subacute, subchronic and chronic toxicity studies
- *In vivo* genotoxicity
- Customized mechanistic toxicity
- Investigations: clinical observations, ophthalmology, sensory reactivity, functional observations & motor activity

Clinical Pathology

- Analysis of clinical chemistry, hemostasis, hematology & urine parameters
- Specific clinical biomarkers services, (e.g. insulin, thyroid hormones) from discovery & validation to robust assay development

Formulation

- Formulation stability, homogeneity & test substance concentration
- Development & validation of analytical methods

Chemical Development



**Process Research
& Development**



**GMP Batch
Manufacturing**



**Solid Phase
Investigations**



**Impurities ID
& Assessment**

Chemical Development

Process Research & Development



- Fast, efficient route evaluation, selection & scale-up
- Co-localized process development & Kg batch manufacturing
- Production of 1 - 10 kg batches incl. impurity control

Impurities ID & Assessment



- Isolation, identification, synthesis & assessment of unknown impurities Analysis of degradation pathways
- Identification of potential ingredient interactions for dossier examination by regulatory agencies

Solid Phase Investigations



- Selection & control of solid state
- Identification of new solid forms of small organic molecules (e.g. polymorphs, salts, co-crystals, or amorphous forms)
- Polymorph & salt screening, solubility curves, filtration assessments

- GLP environment
- Batches up to 10 kg
- HPAPI up to OEL 0.1 $\mu\text{g}/\text{m}^3$
- Prep-HPLC / SFC, high-res MS, 400 MHz NMR
- State-of-the-art laboratory

Contact Us



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