MilliporeSigma

Accelerating Drug Discovery from PREDICTION TO PRECLINICAL

MilliporeSigma is the U.S. and Canada Life Science business of Merck KGaA, Darmstadt, Germany.

Sigma-Aldrich®

Lab & Production Materials

Advancements to life science research demand access to cutting-edge technologies and premium lab materials.

We understand the unique challenges you face in ensuring consistency, reliability, and timely access to high-quality products. While navigating small molecule drug discovery – from prediction to preclinical – our expansive portfolio of chemistry materials and digital solutions supports biochemistry, chemical synthesis, materials science, and more, bringing groundbreaking discoveries within reach.

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Supelco® Analytical Products

Drug Delivery

- Drug Delivery Devices and Formulation Kits
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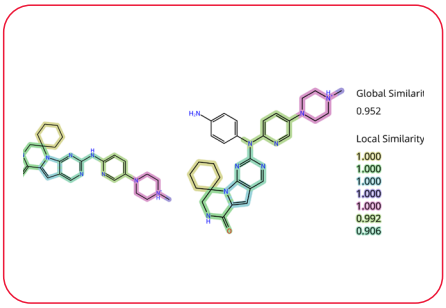
- Biological Buffers

Explore workflow-specific offerings for your focus area: **SigmaAldrich.com/drug-discovery-chemistry**

**We are the exclusive global supplier of Avanti Research™ products outside of the U.S.*

Streamline early-stage drug discovery with AIDDISON™ and SYNTHIA™ software — two powerful tools designed to help you design, optimize, and synthesize molecules with greater speed and accuracy.

smarter chemistry

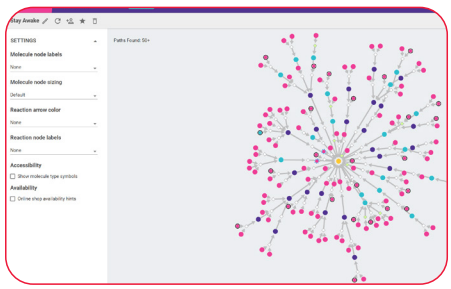


design smarter

with AIDDISON™ Software

- **Explore vast chemical space:**
  Generate novel drug candidates using AI/ML models trained on decades of experimental data.
- **Prioritize promising leads:**
  Identify potential hits with rapid *in silico* screening and flexible *de novo* design tools.
- **Optimize for success:**
  Refine your candidates with structure-based alignment and robust ADMET predictions.

Learn more



synthesize faster

with SYNTHIA™ Retrosynthesis Software

- **Simplify route design**
  Quickly and efficiently scan hundreds of pathways to help you identify the best option according to your needs.
- **Save time and reduce costs**
  Explore the most cost-effective routes to your target molecules with state of the art visualization and filtering options.
- **Generate new ideas and intellectual property**
  Explore unique and innovative syntheses that may be unknown for building your desired molecule.

Learn more

source easier

with essential starting materials

Both AIDDISON™ and SYNTHIA™ software integrate seamlessly with **Aldrich Market Select (AMS)** and the Sigma-Aldrich® catalog, connecting you to the materials and reagents you need.

Learn more

Small Molecule screening

Efficient drug library screening and compound design are essential to seamlessly progress from hit identification to lead selection and optimization for successful drug design.

Aldrich Market Select (AMS) offers an efficient online platform for sourcing synthetic building blocks and small-molecule compound libraries.

Upload a structure or product list, filter by properties, request a quote, consult with specialists, and order – all in one place. With access to over 14 million chemical products, AMS makes it easy to build your personalized library.

Imagine accelerating your drug discovery process with a single, comprehensive service

Learn more

Select. Screen. Synthesize.

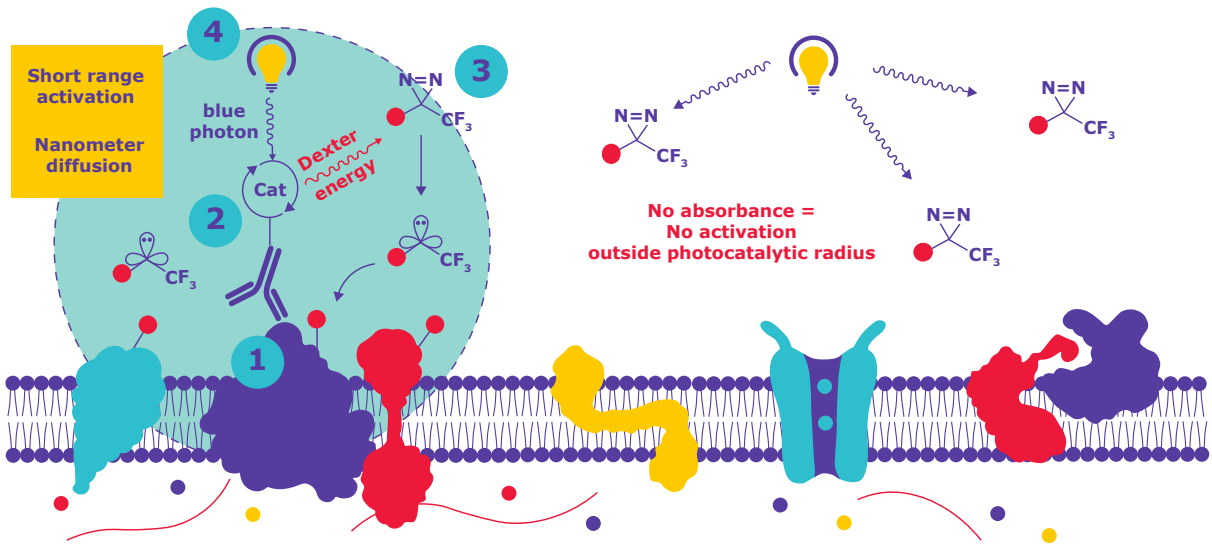
protein proximity labeling

Enhance your Drug Target Identification

In partnership with the MacMillan lab, we offer the µMap kits designed for photoinduced proximity labeling applications. The **Atlas Kit** identifies proteins interacting with a target protein and maps protein microenvironments on cell surfaces.

The **Hyas** and **Dione Kits** label proteins interacting with a small molecule or drug of interest. The Hyas kit features an iridium photocatalyst with a terminal carboxylic acid, while the Dione kit contains a photocatalyst with a terminal amine.

Adapted from MacMillan et. Al. Science, *367, 1091-1097 (2020)*



1. **Selectively bind to your Protein of Interest** – can be done with an antibody (Atlas Kit) or small molecule (Hyas/Dione)
2. **Tether an 'antenna' to the protein** - An optimized (IP protected) photocatalyst is conjugated to the antibody or small molecule
3. **Sprinkle in your locator tags** - a diazirine with a fluorescent probe or handle attached, it remains inert until light activated
4. **Hit the lights!** Using a photoreactor, the low-frequency blue light leaves everything untouched except the diazirines in *close proximity* to the photocatalyst tethered to your protein

Advantages of Micromapping Technology

- Precise labeling within 4 nm radius of the target protein
- Significantly lower false positive rates compared to traditional methods
- Catalytic activation of the labeling agent allows multiple opportunities for protein labeling
- Enables study of endogenous proteins without genetic engineering modifications
- Reduced toxicity from activation method

Pinpoint your drug target

Explore products

DNA-encoded libraries (DELs)

DNA-encoded libraries (DELs) enable the screening of vast compound libraries in a single tube, reducing infrastructure needs and resource costs. Our partnership with **DyNAbind®** offers off-the-shelf DEL kits for efficient, cost-effective drug discovery.

DYNA001
Fragment-based drug discovery (FBDD) excels in identifying new drug candidates for challenging targets, such as protein-protein interactions (PPIs) and molecular glues, which lack traditional binding pockets. By pinpointing fragment-binding sites on macromolecules, FBDD reveals druggable areas, assesses target druggability, and establishes starting points for new chemical entities. Fragment-based hits also offer higher ligand efficiency compared to small molecules.

DYNA002
Small molecule screening technology enables the rapid identification of potent, selective hits for difficult targets by screening millions of compounds simultaneously. Its broad chemical diversity enhances the discovery of novel bioactive molecules and allows for thorough assessment of target druggability, creating a strong foundation for lead optimization. Available in 2-or 5-vial kits, each vial is optimized for testing single conditions.

DEL DATA offers a comprehensive view of hit compounds' chemical structures and binding affinities, derived from DYNA002 screening. This data can be leveraged in AI and virtual screening applications, such as with the **AIDDISON™ platform**, to predict drug interactions and determining structure-activity relationships prior to custom synthesis.

Expand chemical space

Learn more

DyNAbind® is a registered trademark of DyNAbind GmbH

Targeted protein degradation

With approaches like hetero-bifunctional degraders (PROTACs) and molecular glues, previously ‘undruggable’ proteins are now accessible for therapeutic use.

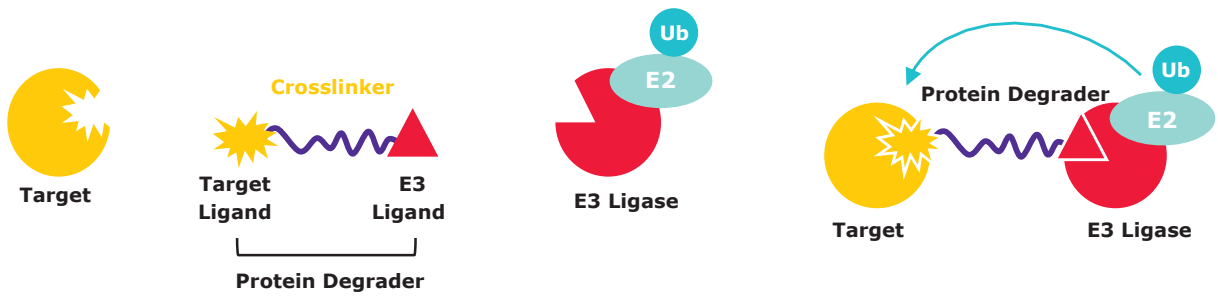
Our curated range of Degrader Building Blocks supports PROTAC® design, including E3 ligase ligands and linkers with functional handles for easy conjugation.

PROTAC® development typically involves creating and testing panels of candidate degraders, adjusting E3 ligase ligands, exit vectors, and linkers. Our collection includes functionalized ligands targeting VHL, CRBN, and IAP, attached to PEG or alkyl linkers with amine, acid, alkyne, azide, or alcohol functionalities for advanced modifications, enabling efficient construction of candidate degrader libraries.

Accelerate novel therapeutic discovery with our protein degrader building blocks

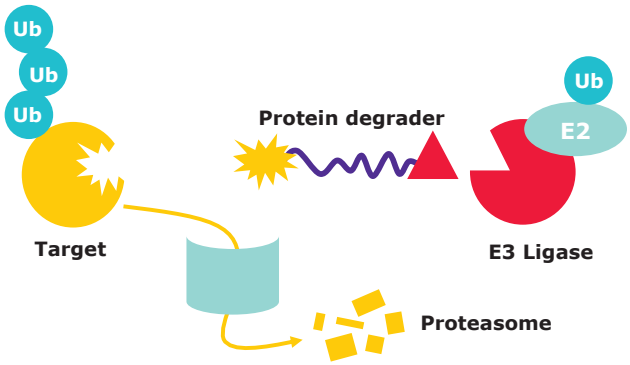
Explore products

Targeted protein degradation via proteolysis chimeras (PROTACs)



1 **Degrader design** Constructed to bind both target and E3 ligase

2 **Ternary complex** The protein degrader recruits target to E3 ligase



3 **Polyubiquitination** Ubiquitin (Ub) added to Lys residues on target

4 **Target degradation** Ub-marked target is degraded by the proteasome

High-Throughput Experimentation

Catalyst screening platforms empower chemists to make faster, more informed decisions to optimize their workflows, and ultimately achieve better, more reproducible results with fewer resources.

Catalexis is a data-driven catalyst screening platform that optimizes palladium-catalyzed reactions such as Buchwald-Hartwig Amination and Suzuki-Miyaura Coupling reactions.

Learn more

This hybrid solution offers chemists everything needed for successful catalyst optimization:

- A curated set of 23 phosphine ligands, a palladium source, and access to the digital portal
- Post-reaction data can be uploaded in the Catalexis portal for advanced algorithmic analysis, ranking the optimal phosphine ligands for your specific reaction.

Catalexis not only streamlines material selection but also facilitates efficient scale-up strategies. Explore how Catalexis can integrate into your workflow, making catalysis research faster, more reliable, and scalable.

KitAlysis™ High-Throughput Screening Platform

KitAlysis™ Screening Kits run 24 unique reactions with ~100 mg of user-provided substrate and are available pre-plated for seven different reaction types, including:

- Buchwald-Hartwig amination reaction
- Copper C-N cross-coupling reaction
- Miyaura Borylation
- Suzuki-Miyaura cross-coupling reaction
- Palladium cross-coupling reactions
- Medium (5, 6, 7) ring-closing metathesis (RCM)

While utilizing the **KitAlysis™ Benchtop Inertion Box,** these reactions can be conducted in an inert atmosphere without the use of a glovebox.

Use in combination with the **KitAlysis™ 24-well Reaction Block and Screwdriver Set**.

Identify optimal catalytic reaction conditions *Explore products*

synthesis-enabling technologies

Automated Chemical Synthesis

The **SYNPLE Chem platform** automates and simplifies complex chemical synthesis, ensuring reproducible, efficient, and scalable production of novel compounds, leaving you more time for research.

The platform consists of the SYNPLE 2 automated synthesizer and over 50 pre-filled reagent cartridges for 10 reaction classes containing RFID chips with optimized reaction protocols.

Reaction classes available for the include Suzuki coupling, targeted protein degrader synthesis, Mitsunobu coupling, reductive amination, biotin tagging, and multiple types of protections and deprotections.

Redox Chemistry

The **PennPhD Photoreactor M2** is an advanced device with variable light sources (365nm, 395 nm, 420 nm, 450 nm) and user-controlled temperature (30-50°) and light-intensity (max. 3.4 W) parameters.

The **SynLED Parallel Photoreactor 2.0** and **UV** are entry-level devices that run 16 reactions in parallel at 450 or 365 nm fixed wavelength, fixed temperature (30 °C), and light-intensity (1W per LED).

With the **SynLectro™ Electrolysis** platform, there is no need to self-design electrochemistry. This standardized labware consists of 50 ml or 200 ml Starter Kits, glass cells and stoppers, electrodes and electrode holders for easy setup.

The compact **Faraday Lab Electrosynthesis Workstation** is a universally compatible power supply for constant current, constant voltage, and cyclic voltammetry experiments, with adjustable parameters, real-time monitoring, and USB interface for data storage and export.

Let automated technology do the work

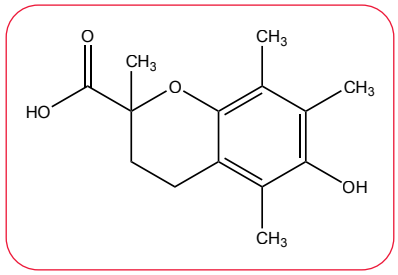
Explore products

Building compounds for breakthroughs

Synthesizing molecules with precise structures is complex. Achieving high purity and yield can be challenging, especially when dealing with unstable intermediates or side reaction that complicate the purification process.

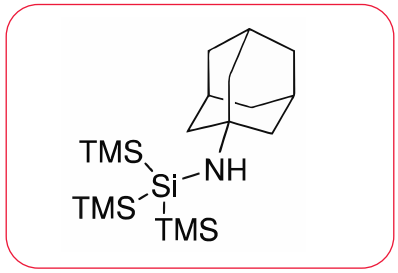
Building Blocks
Our chemical building blocks are highly pure, stable, and available in diverse structural variations to enable precise and efficient synthesis of complex molecules. Explore fluorinated, halogenated, heterocyclic, and organic building blocks.

Browse products



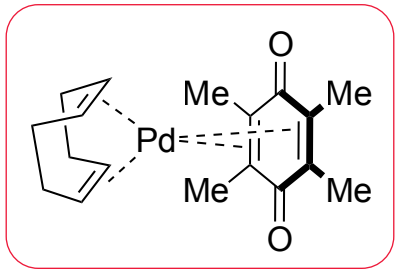
Synthesis Reagents
We collaborate with the leading researchers in academia and industry to bring you state-of-the-art reagents every year. Our vast product offering includes coupling, halogenation, Grignard, oxidation, protection, deprotection, reduction, organoaluminium, and organosilicon reagents.

Browse products



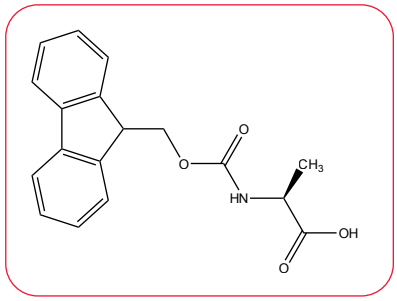
Catalysts
We offer a wide variety of heterogeneous metal catalysts, homogeneous metal catalysts, photocatalysts, and organocatalysts, along with an extensive collection of ligands suitable for your chemical reactions. Our extensive range of catalysts and ligands enable you to use the optimal catalyst, whether you are doing an asymmetric hydrogenation, a Buchwald–Hartwig amination, ring-closing olefin metathesis, or C-C cross coupling using nickel catalyzed photoredox catalysis.

Browse products



Novabiochem® reagents
Choose high-quality Novabiochem® reagents and resins for peptide synthesis and other complex chemical processes. These products stand out for their high purity and consistency, which are critical for achieving accurate and reproducible results in demanding synthetic methodologies. We offer a broad range specifically designed to be compatible with both manual and automated synthesis systems to achieve high yields with minimal impurities.

Browse products



In addition to our catalog business, many catalysts are also available in bulk quantities.

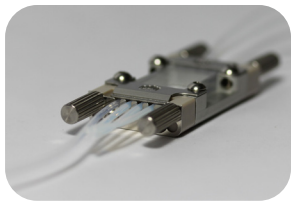
Order in bulk now

Drug Delivery Nanoformulation

Nanoformulation tools precisely manage nanoparticle size, stability, and encapsulation efficiency, addressing key challenges in formulation.

The **NanoFabTx™** drug delivery platform offers ready-to-use kits for reproducible and consistent nanocarrier production with various synthesis methods and are compatible with existing laboratory equipment.

Our curated and tested **NanoFabTx™** formulation reagent kits and lipid mixes facilitate rapid nanocarrier screening and optimization of various polymer and lipid formulations to achieve desired size, encapsulation efficiency, targetability, and *in vitro* delivery.



The pre-assembled **NanoFabTx™** microfluidic device kits synthesize polymeric microparticle, nanoparticles, lipid nanoparticles, or liposomes with better control and tunability than traditional methods such as nanoprecipitation or extrusion.

The **NanoFabTx™** NanoFlash CIJ flash-nanoprecipitation device for nanoparticle synthesis brings the technology used in vaccine manufacturing to the bench. Create precise nanoparticles with flexible and customizable setup that doesn't require complex pump systems.

3. SELECT FORMULATION

By: drug type, particle size, delivery vehicle, carrier material

NanoFabTx™ formulation screening kits or lipid mixes

2. SELECT PREPARATION METHOD

By: conventional methods, microfluidics, flash nanoprecipitation

NanoFabTx™ micro & nano device kits, NanoFabTx™ NanoFlash CIJ

1. SYNTHESIZE

Using step-by-step protocols

Available for each NanofabTx™ formulation kit and lipid mix

Use our NanofabTx™ device kits for uniform synthesis of nano- to micro-sized drug-loaded particles for drug delivery

Explore products

We also offer a wide range of gold, silver, iron oxide, silica and carbon nanoparticles for targeted drug delivery applications.

Explore products

Interested in creating your own formulation?

Learn more

Avanti Research™ are high-quality lipids essential for forming stable liposome bilayers and other delivery vesicles, ensuring the consistency and efficacy of drug delivery systems.

The Avanti® Mini Extruder is a crucial tool in this process, allowing for the precise control of liposome size through extrusion, which is vital for achieving uniform particle size distribution.

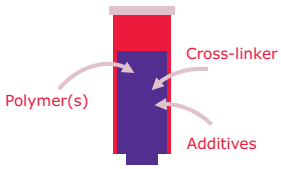
Avanti Research
A CRODA BRAND

**We are the exclusive global supplier of Avanti Research™ products outside of the U.S.*

In-vitro Testing & Screening with 3D Bioprinting

3D bioprinting precisely positions polymers, extracellular matrix components and living cells to create physiologically relevant 3D cell models in 3 easy steps.

1. Formulate

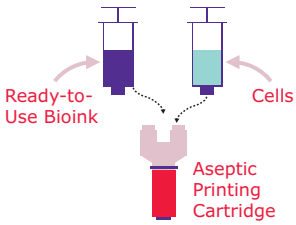


Interested in formulating your own bioink? We offer a complete range of biocompatible fit-for-purpose functionalized natural polymers, water-soluble photoinitiators, and additives as **bioink precursors.**

A variety of bioink precursors are available for various crosslinking chemistries including:

- *Alginate methacrylate*
- *Hyaluronic acid methacrylate*
- *Gelatin methacrylate*
- *Collagen*

2. Fabricate



Formulating custom bioinks with the right mechanical properties, biocompatibility, and printability is complex, requiring time-consuming trial and error.

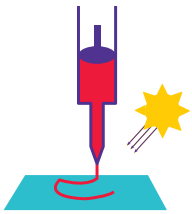
Our **ready-to-use TissueFab® bioinks** are pre-formulated to meet specific requirements and consistent quality, reducing the need for extensive preparation and optimization.

Simply add your cells and start printing with our TissueFab® bioinks.

Available in:

- *TissueFab® general purpose bioinks*
- *TissueFab® tissue specific bioinks*
- *TissueFab® ECM-mimetic bioink kits*

3. Bioprint & Cure



Our TissueFab® bioinks are available in a wide range of crosslinkng chemistries including photopolymerization, thermal, or chemical. To ensure you get the best print every time, each TissueFab® bioink comes with step-by-step protocols and application data.

We also offer extrusion-based bioprinting consumables.

- *Bioprinting cartridges*
- *Printing tips*

Explore products

Accurate Analytical Chemistry

Our solutions provide precision, reliability, and consistency in identifying, quantifying, and characterizing drug candidates to ensure their efficacy and safety. We support every step of your process, from initial discovery through final validation.

Product Highlights

TLC Explorer

The TLC Explorer is a device designed to enhance thin-layer chromatography (TLC) analysis. It provides high-resolution digital imaging of TLC, HPTLC, and PLC plates in less than 2 minutes and densitometric measurement capabilities for precise quantitative analysis and consistent data interpretation.

Learn more

ChemisTwin™ Portal

Our digital reference material platform, ChemisTwin™ portal, automates IR and NMR analysis. Just upload your experimental data into this cloud platform and access certified reference material data on-demand for automated and standardized IR and NMR spectra interpretation.

Learn more

Volumetric Solutions & Standards

Designed specifically for pharmaceutical quality control laboratories, our range of Titripur® volumetric solutions and Certipur® volumetric standards complies with the Reagents Chapter of both the European and United States Pharmacopeias. These solutions and standards are essential for the precise analysis of raw materials, active pharmaceutical ingredients (APIs), and finished pharmaceuticals.

Our volumetric solutions and standards are renowned for their exceptional precision and consistent quality. Manufactured under stringent quality control measures, they ensure accurate and comparable results. All Titripur® volumetric solutions are measured in a DIN EN ISO / IEC 17025 accredited laboratory, while our Certipur® volumetric standards are certified reference materials in accordance with ISO 17034 accreditation.

Learn more

Explore our range of analytical chemistry products designed to meet the precision, reliability, and efficiency that chemists demand in their pursuit of accurate and reproducible results.

Explore products

Analytical Chromatography

Discover our premium products for accurate results in HPLC, gas chromatography (GC), and more.

High-Purity Solvents

Use our highest grade of solvents to minimize the risk of impurities.

Analytical Reagents

Count on our high-quality reagents for analytical characterization.

Reference Materials

Use for calibrating and validating analytical methods to ensure high purity and accuracy.

Supelco®
Analytical Products

greener chemistry

Our portfolio of greener laboratory chemicals supports sustainable lab work by offering less hazardous chemicals, biodegradable reagents and greener alternatives to improve lab safety, reduce waste, lower costs and environmental impact.

Greener Organic Synthesis

Green chemistry methods like electrochemistry and micellar catalysis enhance reaction efficiency while minimizing harmful waste. Our iron-based catalysts and biodegradable reagents support greener synthesis of compounds and materials. Retrosynthetic planning with SYNTHIA™ ensures atom economy, reducing waste, time, and costs.

- Non-Precious Metal Catalysts
- Designer Biosurfactants for Micellar Catalysis
- SYNTHIA™ Retrosynthesis Software
- SynLectro™ Electrolysis Platform
- Polymerization Tools
- Bio-based Polymers
- Silica Gel Orange

Greener Surfactants & Detergents

Our ECO Tween™ and ECO Brij™ biosurfactants made from bio-based ethylene oxide (EO) offer the same high performance as traditional petroleum-based products, but with the added benefit of being fully renewable. Similarly, our Extran® detergents crafted from biodegradable, non-toxic ingredients provide thorough, residue-free cleaning of lab utensils

- Bio-based and biodegradable surfactants
- EXTRAN® detergents

Biorenewable Solvents

Our greener solvent portfolio features plant-based alternatives like bio-ethanol, ethyl lactate, bio-based glycerol, and Methyl THF, derived from renewable sources like grain, sugar cane, and corncobs. Our Cyrene™ solvent and Cyrene™ Blends offer safer options compared to NMP, DMF, and other harmful solvents.

- Bio-Based or Synthetic-Based Safer Solvents
- Cyrene™ & Cyrene™ Blends
- Greener Chromatography Solvents
- Polyethylene Glycol (PEGs)

Use the DOZN™ Tool to assess the relative greenness of synthetic routes and chemical processes, helping you integrate more sustainable practices in the lab.

Practice sustainable science with waste reduction, greener lab chemicals and synthesis methods

Explore products

Sigma-Aldrich®

Lab & Production Materials

MilliporeSigma
400 Summit Drive
Burlington, MA 01803

SigmaAldrich.com

Related Product Resources

Drug Discovery Chemistry Product Offerings

Drug Discovery Chemistry Newsletter

Drug Discovery Chemistry Webinar Hub

Lab Safety Products

Bulk & Custom Services

Software & Digital Platforms

Aldrichimica Acta Publications

Material Matters Publications

Professor Product Portal

Calculators & Apps

To place an order or receive technical assistance:
SigmaAldrich.com/support

For local contact information:
SigmaAldrich.com/offices

We have built a unique collection of life science brands with unrivalled experience in supporting your scientific advancements.

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