

SYNTHESIS MADE SYNPLE

Synple Chem – Automated Chemical Synthesis Platform

SYNPLE



The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the U.S. and Canada.

Sigma-Aldrich

Lab & Production Materials

SYNPLE 2

As a leading supplier of reagents and tools for chemical synthesis, we are continuously expanding our portfolio of innovative products to enhance and facilitate your research.

Now, we've partnered with Synple Chem to bring you the ingenious Synple 2: a fully automated organic chemical synthesizer that uses pre-filled reagent cartridges to generate, isolate, and purify your research products for you – at the press of a button – with incredible speed and accuracy.

Say goodbye to hours of manual synthesis.

Key Features



5 x More efficient

- Fully automated organic synthesis
- 5 minutes to set up
- Frees your time to focus on more important experiments



Accurate & convenient

- Optimized reaction, no risk of human error
- Compact size (W 26cm, H 36cm, D 49cm)
- Fast and easy orders through our web shop



70% Cost savings

 Considerably more economical than manual chemical synthesis due to lower personnel and reagent costs



No special training

- Easy to use, requires no detailed chemistry knowledge
- Modular system for a range of reactions at the press of a button



90% Less waste

- Fully optimized reaction sequence
- Uses minimum reagents and solvents, greatly reducing chemical waste





Enhanced safety

- Fully enclosed reaction
- User never exposed to chemicals
- Complies with latest safety standards

Smart, Smarter, Synple

The Synple platform is based on incredibly smart technology, consisting of the Synple 2 chemical synthesizer, and a range of pre-filled reagent cartridges for different reactions.

The Synple 2 synthesizer:

Contains two syringe pumps, and two rotary valves, in addition to a sample holder, cartridge holder, an RFID chip scanner, and a touchscreen. During synthesis, reactions can occur in the cartridge itself, or in the reaction vial.



Synthesis in 4 Simple Steps



1. Set up your reaction

Scan the pre-filled reagent cartridge and insert it into the synthesizer, then add your starting material.



2. Start synthesis

Simply press the START button on the synthesizer.



3. Let Synple work

The synthesizer generates, isolates, and purifies your product in minutes.



4. Collect your product

Synple then performs an automated washing sequence to prepare for your next synthesis.

5-Minute setup:

Scan the cartridge on the synthesizer to automatically load the appropriate reaction method. Although the provided methods are suitable for a broad range of starting materials, you may adjust certain parameters, such as temperature or reaction time.

Automatic synthesis:

The starting material is prepared (e.g., dissolved), and the solution is then circulated between the vial and the first cartridge compartment for a pre-defined time. Next, it is circulated through a further number of compartments, depending on the reagents required for the reaction.

Automatic cleaning:

After your product is generated, the synthesizer performs automated washing so it's contamination-free, and ready for your next synthesis.

Synple cartridges:

are offered for a variety of reactions. Each cartridge contains all the reagents required to generate, isolate, and purify your product, as well as an RFID chip which is encoded with the reaction method.





Synple Cartridges: Choose Your Reaction

We offer Synple cartridges for eight reaction classes, containing more than 40 different reagents – everything you need for fully automated, optimized chemical synthesis.

N-Heterocycle Formation

Reaction:

Conversion of a diverse range of aldehydes into N-heterocycles.

Cartridge contents:

- Immobilized "Snap" reagent
- Catalyst
- Silica
- SCX

Reagent Cartridge	Order No.
Morpholine	SYNPLE-H001
Oxazepane	SYNPLE-H002
2-Methylmorpholine	SYNPLE-H004
Piperazine	SYNPLE-H005
Diazepane	SYNPLE-H006
3-Methylmorpholine	SYNPLE-H007
Morpholine-2-spiro-(2-Pyr)	SYNPLE-H010
Morpholine-2-spiro-(4-Pip)	SYNPLE-H011
9-OMe-Benzoxazepane	SYNPLE-H090
7-Br-9-OMe-Benzoxazepane	SYNPLE-H091



N-Heterocycle Formation

Reductive Amination

Reaction:

Transformation of aldehydes or ketones, and primary or secondary amines into a variety of complex amines.

Cartridge contents:

- Reducing reagent
- Proton source
- Silica
- Scavenger

Reagent CartridgeOrder No.Reductive AminationSYNPLE-R001



Reductive Amination

Protein Degrader Formation

Reaction:

PROTAC[®] synthesis using either VHL or CRBN ligands, and a variety of PEG linker lengths.

Cartridge contents:

- Reducing reagent
- Free-basing agent
- SCX
- Partial degrader building block salt

PROTAC is a registered trademark of Arvinas Operations, Inc., and is used under license.

Reagent Cartridge	Order No.
CRBN-PEG1	SYNPLE-P001
CRBN-PEG2	SYNPLE-P002
CRBN-PEG3	SYNPLE-P003
CRBN-PEG4	SYNPLE-P004
CRBN-PEG5	SYNPLE-P005
VHL-PEG1	SYNPLE-P021
VHL-PEG2	SYNPLE-P022
VHL-PEG3	SYNPLE-P023
VHL-PEG4	SYNPLE-P024
VHL-PEG5	SYNPLE-P025



Protein Degrader Formation

Biotin Tags

Reaction:

Attachment of Biotin tags to aldehydes and ketones through reductive amination, or to amines via acylation.

Cartridge contents:

Amine linker:

- Reducing reagent
- Free-basing agent
- SCX
- Biotinylation agent
- Amide linker:
- Base
- Scavenger
- Biotinylation agent

Reagent Cartridge	Order No.
Biotin tag-PEG2-NH2	SYNPLE-BT002
Biotin tag-PEG3-NH2	SYNPLE-BT003
Biotin tag-PEG4-NH2	SYNPLE-BT004
Biotin tag-PEG2-O-4-P-NH	SYNPLE-BT012
Biotin tag-PEG3-O-4-P-NH	SYNPLE-BT013
Biotin tag-PEG4-O-4-P-NH	SYNPLE-BT014
Biotin tag-PEG2-a-COOTfp	SYNPLE-BT022
Biotin tag-PEG3-a-COOTfp	SYNPLE-BT023
Biotin tag-PEG4-a-COOTfp	SYNPLE-BT024
Biotin tag-PEG2-COOTfp	SYNPLE-BT032
Biotin tag-PEG3-COOTfp	SYNPLE-BT033
Biotin tag-PEG4-COOTfp	SYNPLE-BT034



Biotin Tags

Mitsunobu

Reaction:

Formation of carbon-carbon bonds through dehydrative coupling of a primary or secondary alcohol with a range of pronucleophiles, such as phenols, phthalimides, tosylamides, and tosylhydrazones.

Cartridge contents:

- Triphenylphosphine-resin
- DtBAD
- SCX
- Scavenger

Boc Protection

Reaction:

N-Boc protection of primary and secondary amines, leaving no excess Boc-anhydride.

Cartridge contents:

- Boc-resin
- DMAP
- Free-basing agent
- Base

Reagent Cartridge	Order No.
Mitsunobu	SYNPLE-M001



Mitsunobu

Reagent Cartridge	Order No.
Boc Protection 0.5 mmol	SYNPLE-B001
Boc Protection 1.2 mmol	SYNPLE-B002



Boc Protection



Boc Deprotection

Reaction:

Transformation of Boc-protected primary and secondary amines into free amine salts, without exposing users to volatile and corrosive acids, such as TFA, HCL, or TsOH.

Cartridge contents:

- pTsOH H₂O
- Scavenger

Reagent Cartridge SYNPLE-B011 Boc Deprotection 0.5 mmol





Boc Deprotection

Fluorination

Reaction:

Transformation of primary and secondary alcohols into the corresponding fluorinated product; beneficial for use in pharmaceutical chemistry, especially in late-stage functionalization.

Cartridge contents:

- Fluorination reagent
- Base
- SCX
- Carbonate

Reagent Cartridge Order No. Deoxyfluorination SYNPLE-F100



Fluorination

SYNTHESIS MADE SYNPLE

Ordering is Just as Simple

The Synple 2 automated synthesis platform perfectly complements our existing chemistry portfolio, so you have all the products and tools you need from one reliable source. Take advantage of instant online ordering on our web shop:

www.SigmaAldrich.com/Synple



Sigma-Aldrich_®

Lab & Production Materials

MilliporeSigma 400 Summit Drive Burlington, MA 01803

milliporesigma.com

To place an order or receive technical assistance in the U.S. and Canada, call toll-free 1-800-325-3010 For other countries across Europe and the world, please visit: SigmaAldrich.com/offices For Technical Service, please visit: SigmaAldrich.com/techservice For more information, contact your local representative at 800-234-5362.

© 2021 Merck KGaA, Darmstadt, Germany and/or its affiliates. All Rights Reserved. MilliporeSigma, the vibrant M, Sigma-Aldrich are trademarks of Merck KGaA, Darmstadt, Germany or its affiliates. PROTAC is a registered trademark of Arvinas Operations, Inc., and is used under license. All other trademarks are the property of their respective owners. Detailed information on trademarks is available via publicly accessible resources.

Lit. No. MS_BR8632EN Ver. 1.2 11/2022