

Product Information

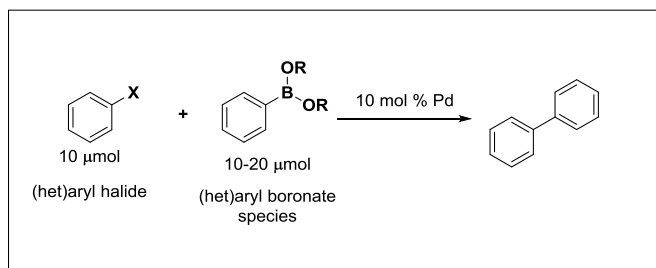
KitAlysis™ Suzuki-Miyaura Cross-Coupling Reaction Screening Kit

Catalog Number **KITALYSIS-SM**
Store at Room Temperature

TECHNICAL BULLETIN

Product Description

The KitAlysis™ Suzuki-Miyaura Cross-Coupling Reaction Screening Kit enables chemists to quickly and efficiently screen conditions for the coupling of aryl halides with organoboronic acids.



Quick identification of optimal conditions allows faster scale-up of the desired synthetic transformation. All required chemicals come pre-weighed for ease of use.

Each Suzuki-Miyaura Cross-Coupling Reaction Screening Kit contains 4 individual screening sets. Each screening set has components to run 24 unique Suzuki-Miyaura reactions:

- 10 μmol (het)aryl halide (user supplied)
- 15–20 μmol (het)aryl boronate (user supplied)
- 1 μmol catalyst per vial (1:1 Pd:Ligand); 6 in this system
- 30 μmol base (1.5 M K₃PO₄)
- 0.1 M solvent concentration (DMAc, Toluene, *n*-butanol, and THF)

Access www.sigmaaldrich.com/kitalysis for detailed step-by-step Protocols and Scale-up Guide. The Protocols include an introductory video, instructions for the Labware, and work-up/internal standard addition procedures.

A downloadable spreadsheet for stock solution recipes for each screening set is available from the step-by-step Protocol.

The spreadsheet provides:

- Calculations for substrate recipes based on the molecular weight of user supplied substrates
- Quick directions for experienced users
- Print button allows you to take experimental recipes to the lab
- Contains all experimental information, which can easily be saved as a pdf file and appended to electronic laboratory notebooks

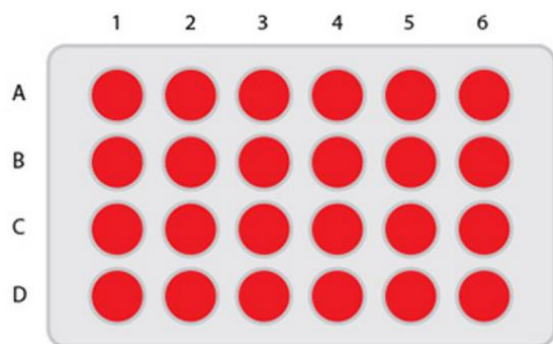
Screening Kit Components

- Four screening sets individually sealed under nitrogen in mylar bags. Each bag includes 24 glass vials loaded with stir bars and pre-weighed catalysts (1 μmol), see Figures 1 and 2
- Ampule boxes containing degassed, anhydrous liquids:
 - 4 × 2 mL Toluene
 - 4 × 2 mL THF
 - 4 × 2 mL *n*-Butanol
 - 4 × 2 mL DMAc
 - 4 × 2 mL aq. 1.5 M K₃PO₄
- Biphenyl Internal Standard (15.4 mg)
- 4 New KitAlysis 24-Well Reaction Block Replacement Films
- 4 substrate stock solution vials with stir bars

Figure 2.
Catalysts

Description	Product No.	Vial
XPhos-Pd-G3	763381	A1, B1, C1, D1
SPhos-Pd-G2	761435	A2, B2, C2, D2
cataCXium A-Pd-G3	753009	A3, B3, C3, D3
APhos-Pd-G3	764183	A4, B4, C4, D4
P(Cy ₃)-Pd-G3	764175	A5, B5, C5, D5
PEPPSI -IPENT	732117	A6, B6, C6, D6

Figure 3.
Positions of Catalysts



Suggested Equipment (Not Provided)

- 96-well plate for automated HPLC analysis (Catalog Number Z688711)
- 96-well plate cap mat for automated HPLC analysis (Catalog Number C1111)
- 10–100 μ L pipette (Catalog Number Z683809)
- 2–200 μ L pipette tip refill (Catalog Number Z640220)
- 100–1,000 μ L pipette (Catalog Number Z683825)
- 50–1,000 μ L pipette tip refill (Catalog Number Z640247)
- 2-inch needles for ease of ampule solvent extraction (Catalog Number Z192570)
- 1 mL syringe for accurate solvent volume extraction from ampule (Catalog Number Z230723)

Specially designed KitAlysis Labware allows screening set up in a hood without the use of a glove box.

- KitAlysis Benchtop Inertion Box (Catalog Number Z742064)
- KitAlysis 24-well Reaction Block and Screwdriver (Catalog Number Z742107)
- KitAlysis 24-well Reaction Block and Inertion Box Starter Set (Catalog Number Z742108)

Instructions for the Labware can be accessed in the Articles section of the website product display page for the kit.

Precautions and Disclaimer

This product is for R&D use only, not for drug, household, or other uses. Please consult the Safety Data Sheet for information regarding hazards and safe handling practices.

Storage/Stability

Store the kit at room temperature.

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