

Product Information

KitAlysis™ High-Throughput Miyaura Borylation Reaction Screening Kit

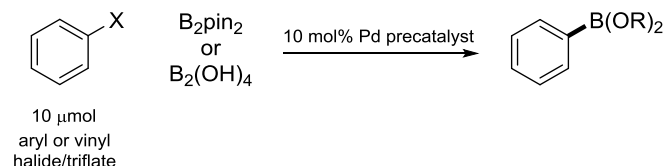
Catalog Number **KITALYSIS-BOR**

Storage Temperature 20–25 °C

TECHNICAL BULLETIN

Product Description

The KitAlysis™ High-Throughput Miyaura Borylation Reaction Screening Kit enables chemists to quickly and efficiently screen reaction conditions for Pd catalyzed Miyaura borylation reactions.



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 Miyaura Borylation Reaction Screening Kit contains 2 individual screening sets. Each screening set has components to run 24 unique Miyaura borylation reactions:

- 6 \times 4 Pd precatalysts (provided)
- 10 μ mol aryl or vinyl halide/triflate substrate (user supplied)
- 10–30 μ mol diboron (provided)
- pre-weighed KOAc (provided)
- 8 solvents (toluene, ethylene glycol, THF, DMA, 1-butanol, MeOH, MeCN, and DIPEA) (provided)

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 that 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

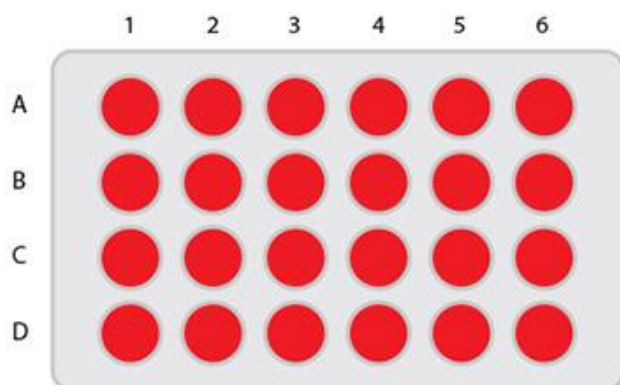
Screening Kit Components

- Two screening sets individually sealed under nitrogen in mylar bags. Each bag includes:
 - 6 \times 4 pre-weighed (1 μ mol) catalysts in glass vials loaded with stir bars and topped with cap mat, see Figures 1 and 2
 - 4 \times 4 mL reaction vials with pre-weighed KOAc base
- Two diborons: B₂pin₂ (500 mg) and B₂(OH)₄ (250 mg)
- Ampule boxes containing degassed, anhydrous liquids:
 - 4 \times 2 mL toluene
 - 2 \times 2 mL ethylene glycol
 - 4 \times 2 mL DMA
 - 4 \times 2 mL THF
 - 4 \times 2 mL 1-butanol
 - 4 \times 2 mL MeOH
 - 4 \times 2 mL MeCN
 - 2 \times 2 mL DIPEA
- Two new KitAlysis 24-Well Reaction Block Replacement Films
- 8 new stir bars for substrate stock solution vials
- Biphenyl Internal Standard (30 mg)

Figure 1.
Catalysts

Description	Catalog Number	Vial
SPhos Pd G4	804282	A1, B1, C1, D1
XPhos Pd G4	804274	A2, B2, C2, D2
CataCXium Pd G4	900349	A3, B3, C3, D3
RuPhos Pd G4	804290	A4, B4, C4, D4
PCy ₃ Pd G4	764175	A5, B5, C5, D5
DTBPF Pd G3	804975	A6, B6, C6, D6

Figure 2.
Position of Catalysts



Reagents and Equipment Required, but Not Provided.

- 10 μ mol aryl or vinyl halide/triflate (user provided)
- Nitrogen (or argon): from hood line or tank
- Pipette (0–100 μ L) and tips
- 4 (1 mL) syringes with long needles
- 1 hot plate with stir capabilities
- 1 stir plate (or hot plate to be used without heat)
- HPLC vials, 96-well HPLC auto sampler block, or TLC plates.

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 High-Throughput Miyaura Borylation Reaction Screening Kit at room temperature.

KitAlysis is a trademark of Sigma-Aldrich Co. LLC.

CK,MAM 10/18-1