

Product Information

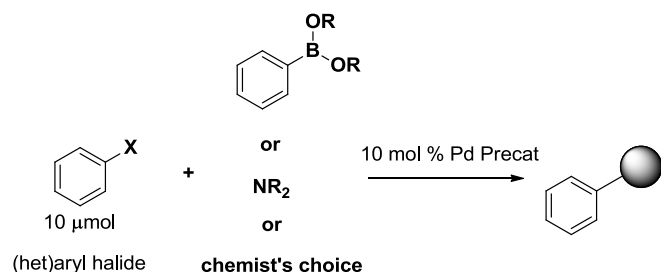
KitAlysis™ High-Throughput 24 Pd Precatalyst Reaction Screening Kit

Catalog Number **KITALYSIS-24Pd**
Store at Room Temperature

TECHNICAL BULLETIN

Product Description

The KitAlysis™ High-Throughput 24 Pd Precatalyst Reaction Screening Kit enables chemists to quickly and efficiently find good reaction conditions for a wide range of cross-coupling reactions. The kit is meant to widen the chemical space offered in more tailored kits (e.g., Suzuki, Buchwald-Hartwig) allowing chemists to customize a reaction of their choice.



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 24 Pd Precatalyst Reaction Screening Kit contains 2 individual screening sets. Each screening set has components to run 24 unique cross-coupling reactions:

- 10–20 μmol of (het)aryl boronate species, amine, or user selected coupling partner (user provided)
- 10 μmol of (het)aryl halide substrate (user provided)
- 1 μmol of catalyst per vial; 24 in this system.
- 10 mol % Pd/ligand complex per reaction (provided)
- 0.1 M solvent concentration (recommended, user provided)
- 30 μmol of base (recommended, user 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

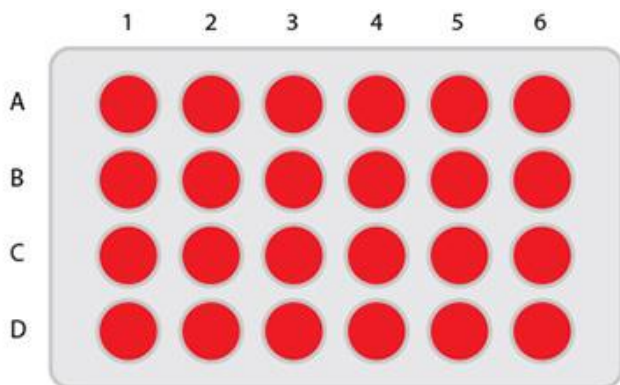
Screening Kit Components

- Two screening sets individually sealed under nitrogen in mylar bags. Each bag includes 24 glass microvials loaded with stir bars and pre-weighed catalysts (1 μmol), see Figures 1 and 2.
- Two New KitAlysis 24-Well Reaction Block Replacement Films
- 3 New stir bars for substrate stock solution vials
- Biphenyl Internal Standard (30 mg)

Figure 1.
Catalysts

Description	Catalog Number	Vial
AdBrettPhos Pd G3	776106	A01
APhos Pd G3	764183	A02
rac-BINAP-Pd-G3	804967	A03
BrettPhos Pd G4	804355	A04
cataCXium® A Pd G3	761435	A05
CPhos Pd G3	763004	A06
CyJohnPhos Pd G3	900621	B01
DavePhos Pd G3	804959	B02
DPPF Pd G3	804983	B03
JackiePhos Pd G3	762830	B04
Josiphos SL-J009-1 Pd G3	747130	B05
meCgPPh Pd G3	762822	B06
Me4tBuXPhos Pd G3	900620	C01
MorDalphos Pd G3	792357	C02
P(Cy ₃) Pd G3	764175	C03
P(t-Bu) ₃ Pd G2	756482	C04
Pd-PEPPSI™-IPent catalyst	732117	C05
RuPhos Pd G4	804290	C06
SPhos Pd G4	804282	D01
tBuBrettPhos Pd G3	745979	D02
tBuXPhos Pd G3	762229	D03
XantPhos Pd G3	763039	D04
XPhos Pd G4	804274	D05
PdCl ₂ (PPh ₃) ₂	412740	D06

Figure 2.
Position of Catalysts



Reagents and Equipment Required, but Not Provided.

- 10-20 μmol of (het)aryl boronate species, amine, or user selected coupling partner (user provided)
- 10 μmol of (het)aryl halide substrate (user provided)
- Nitrogen (or argon): from hood line or tank
- Pipette (0–100 μL) 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 24 Pd Precatalyst Reaction Screening Kit at room temperature.

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