

Product Information

KitAlysis™ High-Throughput Copper C-N Cross-Coupling Reaction Screening Kit

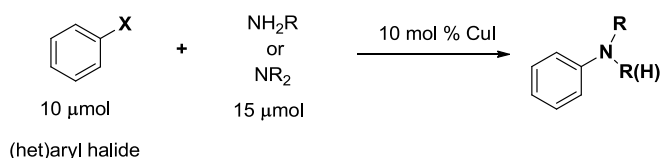
Catalog Number **KITALYSIS-CuCN**

Storage Temperature 20–25 °C

TECHNICAL BULLETIN

Product Description

The KitAlysis™ High-Throughput Copper C-N Cross-Coupling Reaction Screening Kit enables chemists to quickly and efficiently screen reaction conditions for copper C-N cross-coupling 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 Copper C-N Cross-Coupling Reaction Screening Kit contains 2 individual screening sets. Each screening set has components to run 24 unique copper C-N cross-coupling reactions:

- 15–20 μmol of amine (primary, secondary) (user supplied)
- 10 μmol aryl halide substrate (user supplied)
- 4 μmol ligand per vial
- 1 Cu catalyst (Soluble CuI source).
- 4 solvents (DMAc, Toluene, DMSO, and Dioxane) (provided)
- pre-weighed K₃PO₄ base

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

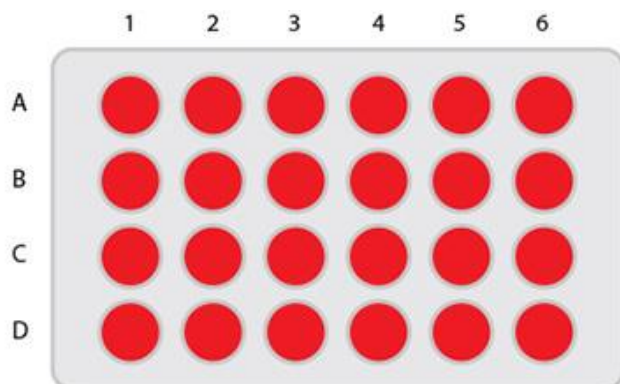
Screening Kit Components

- Two screening sets individually sealed under nitrogen in mylar bags. Each bag includes:
 - 6 × 4 pre-weighed (4 μmol) ligands in glass vials loaded with stir bars and topped with cap mat, see Figures 1 and 2
 - 4 × 4 mL reaction vials with pre-weighed K₃PO₄ base
 - 1 pre-weighed vial of soluble CuI
- Ampule boxes containing degassed, anhydrous liquids:
 - 4 × 2 mL Dioxane
 - 4 × 2 mL DMAc
 - 4 × 2 mL Toluene
 - 4 × 2 mL DMSO
- 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
2,6-Dimethylanilino(oxo)acetic acid	806412	A1, B1, C1, D1
2,6-Dimethoxyanilino(oxo)acetic acid	806455	A2, B2, C2, D2
2,6-Difluoroanilino(oxo)acetic acid	806439	A3, B3, C3, D3
2,3,4,5,6-Pentafluoroanilino(oxo)acetic acid	806447	A4, B4, C4, D4
3,5-Bis(trifluoromethyl)anilino(oxo)acetic acid	806420	A5, B5, C5, D5
2-Fluoro-6-(piperidine-1-sulfonyl)anilino(oxo)acetic acid	805491	A6, B6, C6, D6

Figure 2.
Position of Catalysts



Reagents and Equipment Required, but Not Provided.

- 10 μ mol of (het)aryl halide substrate (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 Copper C-N Cross-Coupling Reaction Screening Kit at room temperature.

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