6000 Teutonia Avenue, Milwaukee, WI 53209 USA Tel: (800) 231-8327 (414) 438-3850 Fax: (414) 438-4234 email: techservice@sial.com sigma-aldrich.com

### **Product Information**

#### KitAlysis™ High-Throughput Base Screening Kit

Catalog Number **KITALYSISBASE** Storage Temperature 20–25 °C

### **TECHNICAL BULLETIN**

#### **Product Description**

The KitAlysis™ High-Throughput Base Screening Kit enables chemists to quickly and efficiently screen bases for cross-coupling reactions as well as a variety of other base promoted synthetic transformations.

Note: While the above scheme depicts a generic cross-coupling reaction, *KitAlysis* High-Throughput Base Screening Kit can be used for many other coupling reactions as well as other base promoted synthetic transformations.

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 Base Screening Kit contains 2 individual screening sets. Each screening set has components to run 22 unique reactions, with 2 customizable positions for chemist's choice of base:

- pre-weighed base or base solution (provided)
- 10–20 μmol coupling partner (user supplied)
- 10 μmol aryl halide substrate (user supplied)
- catalyst and ligand (user supplied).
- 4 solvents (DMF, MeOH, THF, and Toluene) (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-bystep 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

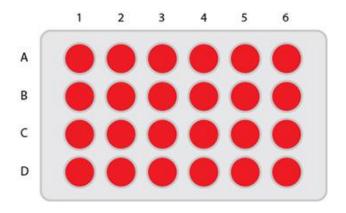
#### **Screening Kit Components**

- Two screening sets individually sealed under nitrogen in mylar bags. Each bag includes:
  - $7 \times 2$  pre-weighed (30  $\mu$ mol) bases in glass vials loaded with stir bars and topped with cap mat, see Figures 1 and 2
  - 4 × 4 mL reaction vials
- Ampule boxes containing degassed, anhydrous liquids:
  - 2 × 2 mL DBU
  - $\circ$  2 × 2 mL Et<sub>3</sub>N
  - $\circ$  2 × 2 mL LiHMDS (1.0 M in THF)
  - $\circ$  2 × 2 mL NaO<sup>t</sup>Bu (2.0 M in THF)
  - $\circ$  4 × 2 mL DMF
  - o 4 × 2 mL MeOH
  - $\circ$  4 × 2 mL THF
  - o 4 x 2 mL Toluene
- Two new KitAlysis 24-Well Reaction Block Replacement Films
- 8 new stir bars for substrate stock solution vials

## Figure 1. Bases

Description	Catalog Number	Vial
K <sub>3</sub> PO <sub>4</sub>	RDD019	A1, C1
K <sub>2</sub> CO <sub>3</sub>	900501	A2, C2
KOAc	791733	A3, C3
KHCO <sub>3</sub>	237205	A4, C4
KOH	757551	A5, C5
NaOH	795429	A6, C6
Cs <sub>2</sub> CO <sub>3</sub>	441902	B1, D1
LiHMDS 1.0 M in THF	225770	B2, D2
NaO <sup>t</sup> Bu 2.0 M in THF	702706	B3, D3
DBU	139009	B4, D4
Et <sub>3</sub> N	900632	B5, D5
Chemist's Choice	n/a	B6, D6

Figure 2.
Position of Bases



# Reagents and Equipment Required, but Not Provided.

- Desired reaction substrates (10 μmol scale) and catalysts (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 Base Screening Kit at room temperature.

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

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