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Product Information

KitAlysis™ High-Throughput 24-Catalyst Photoredox Reaction Screening Kit

Catalog Number **KITALYSIS-PHO**Storage Temperature 20–25 °C

TECHNICAL BULLETIN

Product Description

The KitAlysis™ High-Throughput 24-Catalyst Photoredox Reaction Screening Kit enables chemists to quickly and efficiently screen reaction conditions for many photocatalyzed transformations.

Note: While the above scheme depicts a generic decarboxylative coupling reaction, KitAlysis High-Throughput 24-Catalyst Photoredox Reaction Screening Kit can be used for any photocatalytic 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 KitAlysis High-Throughput 24-Catalyst Photoredox Reaction Screening Kit contains 2-individual screening sets. Each screening set has components to run 24 unique photocatalysis reactions:

- 24 × 1 photocatalysts (provided)
- 10 μmol substrate(s), reagent(s), co-catalyst(s) (user supplied)
- 4 solvents (DCM, DCE, DMF, and MeCN) (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 lab ware, 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

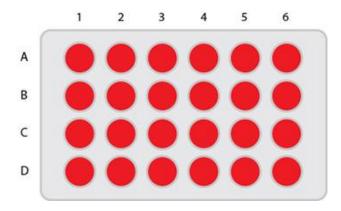
Screening Kit Components

- Two screening sets individually sealed under nitrogen in mylar bags. Each bag includes:
 - 24 pre-weighed (1 μmol) photocatalysts in glass vials loaded with stir bars and topped with cap mat, see Figures 1 and 2
 - 2 × 4 mL reaction vials for preparing substrate stock solutions
- Ampule boxes containing degassed, anhydrous liquids:
 - o 4 × 2 mL DCM
 - o 4 × 2 mL DCE
 - \circ 4 × 2 mL DMF
 - o 4 × 2 mL MeCN
- 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
$[Ru(bpz)_3][PF_6]_2$	747777	A1
[Ir(dtbbpy)(ppy) ₂]PF ₆	747769	A2
Bismuth(III) oxide	637017	А3
Acridine Orange HCl hydrate	318337	A4
Proflavine hemisulfate salt hydrate	P2508	A5
9,10-Anthracenedicarbonitrile	459852	A6
[Ru(bpm) ₃][Cl] ₂	747785	B1
(Ir[dF(CF ₃)ppy] ₂ (dtbpy))PF ₆	747793	B2
Bismuth(III) sulfide	333190	B3
9-Mesityl-10-phenylacridinium tetrafluoroborate	793221	B4
9-Mesityl-3,6-di- <i>tert</i> -butyl- 10-phenylacridinium tetrafluoroborate	900421	B5
Fluorescein	46955	B6
Ru(bpy) ₃ Cl ₂ ·6H ₂ O	224758	C1
[Ir{dFCF ₃ ppy} ₂ (bpy)]PF ₆	804215	C2
Tetrachloro-1,4-benzoquinone	232017	C3
9-Mesityl-2,7-dimethyl- 10-phenylacridinium tetrafluoroborate	793876	C4
9-Mesityl-1,3,6,8-tetramethoxy- 10-phenylacridin-10-ium tetrafluoroborate	900693	C5
2,4,6-Triphenylpyrylium tetrafluoroborate	272345	C6
Ru(phen) ₃ Cl ₂ ·xH ₂ O	343714	D1
Ir(ppy) ₃	688096	D2
2,3-Dichloro-5,6-dicyano- p-benzoquinone	D60400	D3
9-Mesityl-10-methylacridinium tetrafluoroborate	794171	D4
10-(3,5-Dimethoxyphenyl)- 9-mesityl-1,3,6,8- tetramethoxyacridin-10-ium tetrafluoroborate	900694	D5
2,4,6-Tris(4-methoxyphenyl) pyrylium tetrafluoroborate	900692	D6

Figure 2. Position of Catalysts



Reagents and Equipment Required, but Not Provided.

- 10 μmol substrate(s), reagent(s), co-catalyst(s)
- Photo KitAlysis Starter Kit (Z742612)
- Nitrogen (or argon): from hood line or tank
- Pipette (0–100 μL) and tips
- 4 (1 mL) syringes with long needles
- 2 stir plates
- 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)

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 KitAlysis High-Throughput 24-Catalyst Photoredox Reaction Screening Kit at room temperature.

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