

Sold in collaboration with HepatoChem

96-7560 EvoluChem™ Photocatalytic Alkylation Kit

1 kit

Product overview:

The trifluoroborate alkylation reaction (Minisci reaction)¹ is a powerful late stage functionalization tool. Our kit allows convenient, one-step production of eight different analogues of a lead compound in mg quantities. Each reaction vial contains 75 μmol of trifluoroborate alkylation reagent (pre-weighed) and a stirring bar to react with 50 μmol of substrate. C-H functionalization will primarily occur on electron-deficient heteroarenes at one or several positions.

Benefits

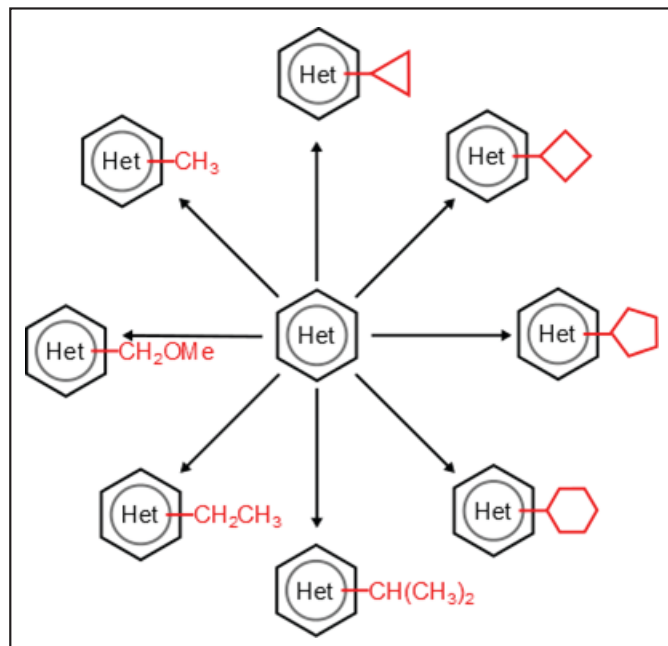
- Facilitates screen of photochemical reaction conditions
- Enables up to 32 reaction conditions simultaneously
- Save substrate using low scale reaction conditions
- Save time on optimization

Material required, but not supplied

- Customer supplied substrate
- Customer supplied reaction solvent(s)
- Trifluoroacetic acid
- EvoluChem™ PhotoRedOx Box
- EvoluChem™ Light Source 18W-450 nm
- EvoluChem™ Vial Holder (98-7650)
- Nitrogen or Argon line for sparging solvents with two needles
- DMSO
- Stirring plate
- 500 μL - 1.0 ml syringe

Recommendations

- Safety personal protection such as gloves, safety glasses and lab coat should be worn at all times.
- Always use a clean and dry syringe to add and transfer solution.



Storage and Stability

- Store at 2-8°C in dark.
- Stable for 12 months.

Kit Contents

Description	Label	Quantity	Amount
Potassium cyclopropyltrifluoroborate / Potassium persulfate	cyclopropyl-BF ₃ K/ K ₂ S ₂ O ₈	2 x vials	75 μmol / 100 μmol
Potassium cyclobutyltrifluoroborate / Potassium persulfate	cyclobutyl-BF ₃ K/ K ₂ S ₂ O ₈	2 x vials	75 μmol / 100 μmol
Potassium cyclopentyltrifluoroborate / Potassium persulfate	cyclopentyl-BF ₃ K/ K ₂ S ₂ O ₈	2 x vials	75 μmol / 100 μmol
Potassium cyclohexyltrifluoroborate / Potassium persulfate	cyclohexyl-BF ₃ K/ K ₂ S ₂ O ₈	2 x vials	75 μmol / 100 μmol
Potassium ethyltrifluoroborate / Potassium persulfate	ethyl-BF ₃ K/ K ₂ S ₂ O ₈	2 x vials	75 μmol / 100 μmol
Potassium isopropyltrifluoroborate / Potassium persulfate	isopropyl-BF ₃ K/ K ₂ S ₂ O ₈	2 x vials	75 μmol / 100 μmol
Potassium methoxymethyltrifluoroborate / Potassium persulfate	MOM-BF ₃ K/ K ₂ S ₂ O ₈	2 x vials	75 μmol / 100 μmol
<i>tert</i> -butyl peracetate	TBA	2 x vials	250 μmol
Ir[dF(CF ₃)ppy] ₂ (dtbbpy)[PF ₆] (Strem# 77-0425) /	Ir-cat-1	2 x vials	8 μmol

Visit www.strem.com for new product information and a searchable catalog.

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Reagent Information			
Strem Item#	Vial	CAS	MW
77-0425	Ir[dF(CF ₃)ppy] ₂ (dtbbpy)][PF ₆]	870987-63-6	1121.91
---	Potassium cyclopropyltrifluoroborate	1065010-87-8	147.98
---	Potassium cyclobutyltrifluoroborate	1065010-88-9	162.00
---	Potassium cyclopentyltrifluoroborate	1040745-70-7	176.03
---	Potassium ethyltrifluoroborate	44248-07-9	135.97
---	Potassium isopropyltrifluoroborate	1041642-13-0	149.99
---	Potassium methoxymethyltrifluoroborate	910251-11-5	151.97
---	<i>tert</i> -butyl peracetate solution TBPA (50% mineral spirits)	107-71-1	132.16
---	Potassium persulfate	7727-21-1	270.32

Typical Protocol

- The typical protocol is performed at 0.1 mol/l of substrate prepared as solution in DMSO or H₂O/ACN with 5 equiv. of trifluoroacetic acid. Each sealed reaction vial contains either 75 μmol of BF₃K reagent with 100 μmol of K₂S₂O₈ or 250 μmol of *tert*-butyl peracetate.
- Typically, the reaction is performed with 6200K white LED or blue LED (450 nm).
- The alkylation production kit contains 2 sets of vials allowing the screening of two different substrates or 1 substrate in two solvents.
- Sparging reaction solvents with nitrogen or argon while transferring reagents is important to achieve highest conversions of product. See protocol diagram for instructions.

Protocol at 500 μl volume reaction condition

1. In the vial provided containing the Ir catalyst, prepare 4.0 ml of substrate solution at 0.1 mol/L of substrate (400 μmol substrate needed) in either DMSO or H₂O/ACN with 153 μL of trifluoroacetic acid (5 equiv.). Mix thoroughly.
2. Degas the substrate/catalyst solution with subsurface sparging via N₂ or Ar line with exit needle for 5 minutes.
3. Using a clean and dry syringe, add 500 μL of the substrate solution to each reaction vial (8 reactions).
4. Place samples in vial holder **98-7650**.
5. Turn on lamp (6200K white LED or blue LED 450 nm) and stir vials for 2 to 4 hours (or longer if necessary and there is substrate remaining). Be sure to plug in fan to maintain RT.
6. Upon completion of reaction, prepare analytical sample for each reaction condition with 5 μl sample diluted into 200 μl in either DMSO or water/acetonitrile 50/50.
7. Analyze resulting analytical samples by LC/MS.

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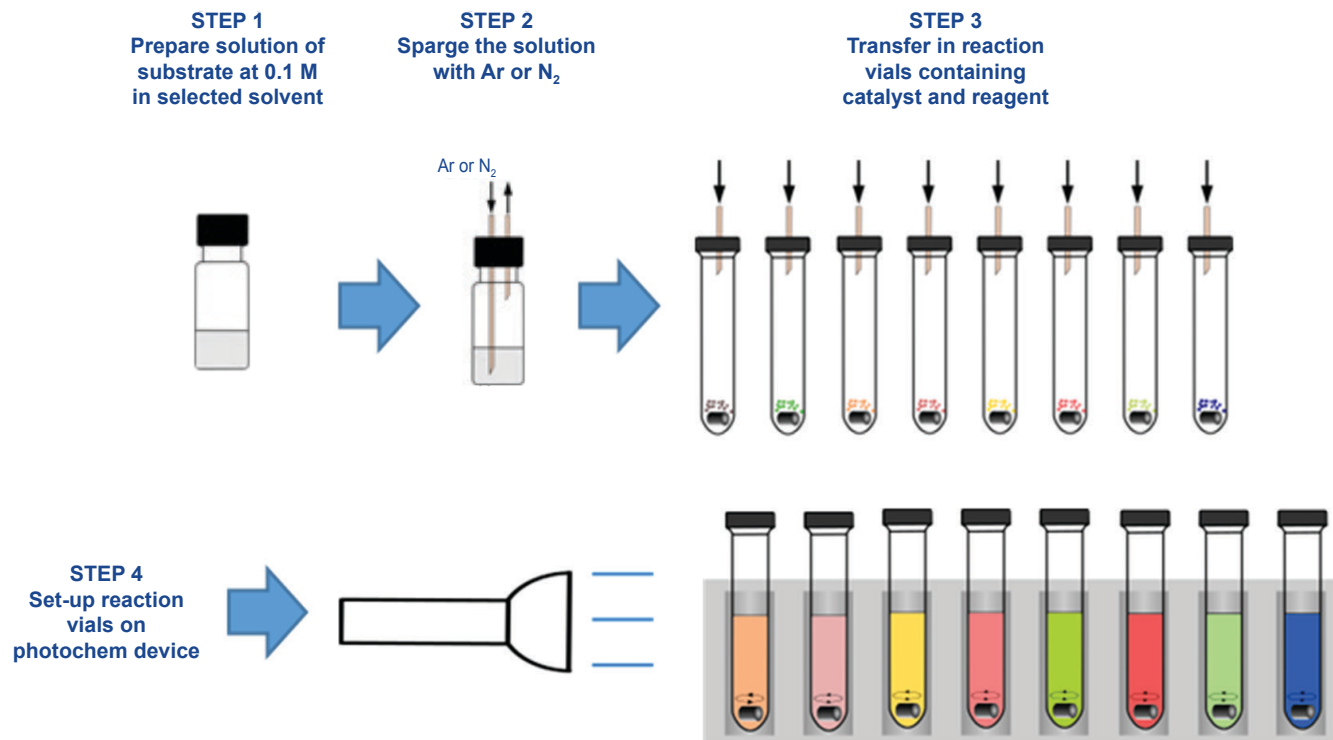
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Protocol Diagram



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