Hypervalent Iodine Reagent for Photoredox Trifluoromethylation

**Advantages**

- Usable for C-H Trifluoromethylation of (Hetero)arenes with a Photoredox Catalyst
- Applicable under the Neutral Condition
- Pentafluoriodobenzene as a Byproduct Is Easily Recoverable and Recyclable to FPIFA.

**Application**

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\text{FPIFA} \quad \text{[B1616]}
\]

\[
\begin{align*}
\text{CF}_3 \quad & \quad \text{C} \quad & \quad \text{O} \\
& \quad & \quad \text{I} \\
& \quad & \quad \text{C} \quad & \quad \text{O} \\
& \quad & \quad \text{F} & \quad \text{F} \\
& \quad & \quad \text{F} & \quad \text{F}
\end{align*}
\]

\[
\text{Usable for C-H Trifluoromethylation of (Hetero)arenes with a Photoredox Catalyst}
\]

\[
\begin{align*}
\text{CF}_3 & \quad \text{O} & \quad \text{CF}_3 \\
& \quad & \quad \\
& \quad & \quad \text{O} & \quad \text{CF}_3 \\
& \quad & \quad \text{F} & \quad \text{F} \\
& \quad & \quad \text{F} & \quad \text{F}
\end{align*}
\]

**Experimental procedure:**

A Schlenk flask is charged with Ru(bpy)$_3$(PF$_6$)$_2$ (9.0 mg, 0.01 mmol, 2 mol%), FPIFA (650.0 mg, 1.25 mmol, 2.5 equiv.), dimethyl telephthalate (0.5 mmol, 1.0 equiv.). Next, acetonitrile (7.5 mL) is added to the reaction mixture. The mixture is degassed twice by the freeze-pump-thaw procedure, then irradiated under blue LED strips (4.8 W). The reaction mixture is subsequently stirred at 35 °C for 12 h. After the reaction is completed, it is diluted with water (8.0 mL). The aqueous phase is extracted with ether (8.0 mL) three times. The combined organic layers are washed with brine and dried over anhydrous sodium sulfate, and concentrated in vacuo. The residue is purified by silica gel column chromatography (hexane:EtOAc = 15:1) to afford dimethyl (trifluoromethyl)telephthalate in 63% yield (83.9 mg).

For further information please refer to our website at www.TCIchemicals.com.

**Related Product**

**(Bis(trifluoroacetoxy)iodo)pentafluorobenzene (= FPIFA)**

1g / 5g [B1616]

**Tris(2,2'-bipyridine)ruthenium(II) Bis(hexafluorophosphate) (= Ru(bpy)$_3$(PF$_6$)$_2$)**

1g [T3435]