

Product Name: Caffeine Orange

Catalog No.: 7181

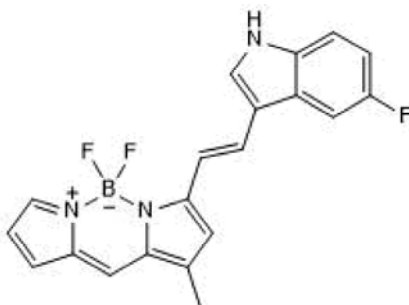
Batch No.: 1

CAS Number: 1632296-13-9

IUPAC Name: (E)-5,5-Difluoro-3-(2-(5-fluoro-1*H*-indol-3-yl)vinyl)-1-methyl-5*H*-5λ⁴,6λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₀ H ₁₅ BF ₃ N ₃
Batch Molecular Weight:	365.17
Physical Appearance:	Black solid
Solubility:	DMSO to 10 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 99.5% purity at 573 nm
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
UV Spectrum:	Consistent with structure
λ_{max}:	585 nm (DMSO)
λ_{ex}:	580 nm (DMSO)
λ_{em}:	618 nm (DMSO)

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Caffeine Orange is a selective, BODIPY-based fluorescent caffeine chemosensor, which exhibits up to 250-fold enhancement in its fluorescence upon caffeine activation ($K_D = 16.81$ mM and detection limit of 50 μM). Caffeine Orange works both in aqueous and in dry state, and its red emission intensity increases with increasing caffeine concentrations. Excitation maximum ~580 nm; emission maximum ~629 nm.

Physical and Chemical Properties:

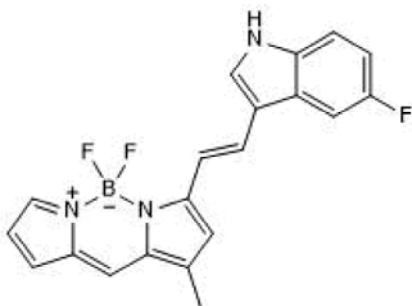
Batch Molecular Formula: C₂₀H₁₅BF₃N₃

Batch Molecular Weight: 365.17

Physical Appearance: Black solid

Minimum Purity: ≥95%

Batch Molecular Structure:



References:

Xu *et al* (2013) Make caffeine visible: a fluorescent caffeine "traffic light" detector *Sci.Rep.* **3** 2255. PMID: 23877095.

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 10 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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