

Certificate of Analysis

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Product Name: TokeOni

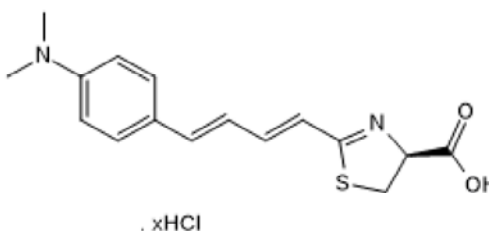
Catalog No.: 6555

Batch No.: 4

IUPAC Name: (4S)-2-[(1E,3E)-4-[4-(Dimethylamino)phenyl]-1,3-butadien-1-yl]-4,5-dihydro-4-thiazolecarboxylic acid hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₁₆ H ₁₈ N ₂ O ₂ S.xHCl
Physical Appearance:	Brown solid
Solubility:	water to 5 mg/ml with gentle warming DMSO to 10 mg/ml
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 98.8% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Net content (free base)::	69%

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

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Description:

TokeOni is a near-infrared red (NIR)-emission luciferin analog. Peak luminescence at 677 nM. ~40-fold brighter than the luciferin-luciferase system in vitro, and 100-1000 times brighter in vivo. Allows non-invasive visualization of single cells deep inside freely moving animals. Ideal for deep tissue applications. Water soluble (<40 mM), orally bioavailable and brain penetrant. This product is supplied as a hydrochloride salt, the stoichiometry of which is batch dependant. Please refer to the Certificate of Analysis to obtain the batch specific Net Product Content.

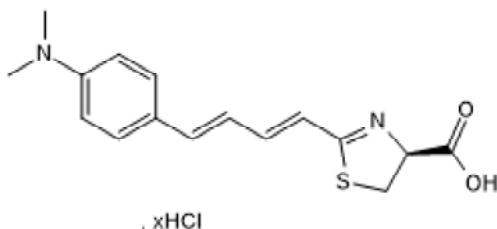
Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₈N₂O₂S.xHCl

Physical Appearance: Brown solid

Minimum Purity: ≥90%

Batch Molecular Structure:



Storage: Store at -20°C. This product is packaged under an inert atmosphere.

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:

water to 5 mg/ml with gentle warming

DMSO to 10 mg/ml

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.

Other Information:

Molecular Weight: 302.39 (Free base)

References:

Iwano et al (2018) Single-cell bioluminescence imaging of deep tissue in freely moving animals. *Science* **359** 935. PMID: 29472486.

Nasu et al (2018) Unnaturally aglow with a bright inner light. *Science* **359** 868. PMID: 29472468.

Kuchimaru et al (2016) A luciferin analogue generating near-infrared bioluminescence achieves highly sensitive deep-tissue imaging. *Nat. Commun.* **7** 11856. PMID: 27297211.

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