



Certificate of Analysis

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Product Name: TokeOni Catalog No.: 6555 Batch No.: 2

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: C₁₆H₁₈N₂O2S.HCI.16H₂O

Batch Molecular Weight: 627.01

Brown solid **Physical Appearance:**

Solubility: water to 5 mg/ml with gentle warming

DMSO to 10 mg/ml

Storage: Store at -20°C

Batch Molecular Structure:

HCI

2. ANALYTICAL DATA

HPLC: Shows 95.4% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

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Product Information

Print Date: Oct 15th 2019

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

Description:

Near-infrared red (NIR)-emission luciferin analog. Peak luminescence at 677 nM. ~40-fold brighter than luciferase. 100-1000 times brighter in vivo than conventional systems. Allows non-invasive visualization of single cells deep inside freely moving animals. Orally bioavailable and brain penetrant. The batch molecular weight of the product may vary significantly due to hydration level. Please refer to the Certificate of Analysis for the current batch.

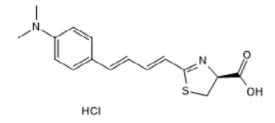
Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₈N₂O2S.HCl.16H₂O

Batch Molecular Weight: 627.01 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.

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.