Certificate of Analysis

Product Name: **TokeOni** **Catalog No.: 6555** **Batch No.: 3**

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{18}N_2O_2S.xHCl$

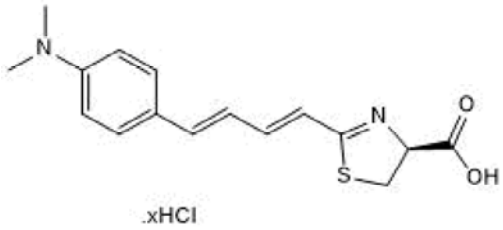
Batch Molecular Weight: 302.39

Physical Appearance: Purple 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 96.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Net content (free base):: 72%

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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:

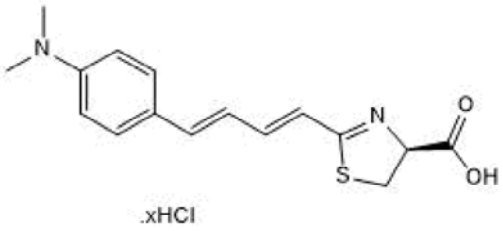
Batch Molecular Formula: $C_{16}H_{18}N_2O_2S.xHCl$

Batch Molecular Weight: 302.39

Physical Appearance: Purple 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.

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