

**Product Name:** IRDye<sup>®</sup> 800CW, NHS ester

**Catalog No.:** 8881

**Batch No.:** 1

**CAS Number:** 956579-01-4

**IUPAC Name:** Sodium 2-((*E*)-2-((*E*)-3-(2-((*E*)-1-(6-((2,5-Dioxopyrrolidin-1-yl)oxy)-6-oxohexyl)-3,3-dimethyl-5-sulfonatoindolin-2-ylidene)ethylidene)-2-(4-sulfonatophenoxy)cyclohex-1-en-1-yl)vinyl)-3,3-dimethyl-1-(4-sulfonatobutyl)-3*H*-indol-1-ium-5-sulfonate

## 1. PHYSICAL AND CHEMICAL PROPERTIES

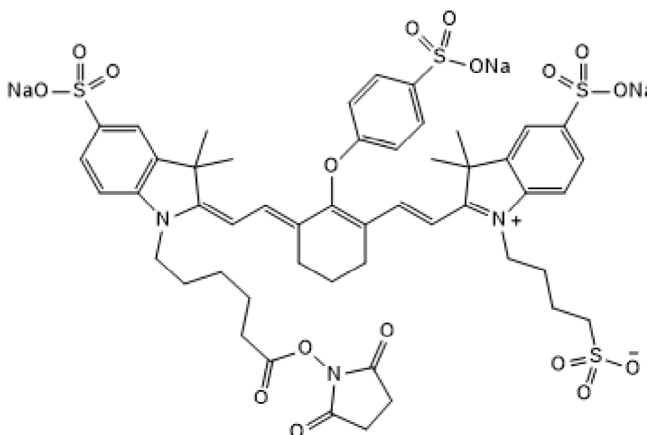
**Batch Molecular Formula:** C<sub>50</sub>H<sub>54</sub>N<sub>3</sub>Na<sub>3</sub>O<sub>17</sub>S<sub>4</sub>

**Batch Molecular Weight:** 1166.2

**Physical Appearance:** Dark green solid

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 88% purity

**Mass Spectrum:** Consistent with structure

**UV Spectrum:** Consistent with structure

**λ<sub>max</sub>:** 775 nm (0.01M PBS pH 7.4)

**λ<sub>ex</sub>:** 777 nm (0.01M PBS pH 7.4)

**λ<sub>em</sub>:** 800 nm (0.01M PBS pH 7.4)

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

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**Description:**

Key information: IRDye<sup>®</sup> 800CW, NHS ester is a near-infrared (NIR) fluorescent dye, supplied with an NHS ester reactive group for the labeling of primary amines. Application: Fluorescence microscopy. Properties and Photophysical Data: Excitation and emission maxima ( $\lambda$ ) are 773 nm and 792 nm, respectively. Please see the

**Physical and Chemical Properties:**

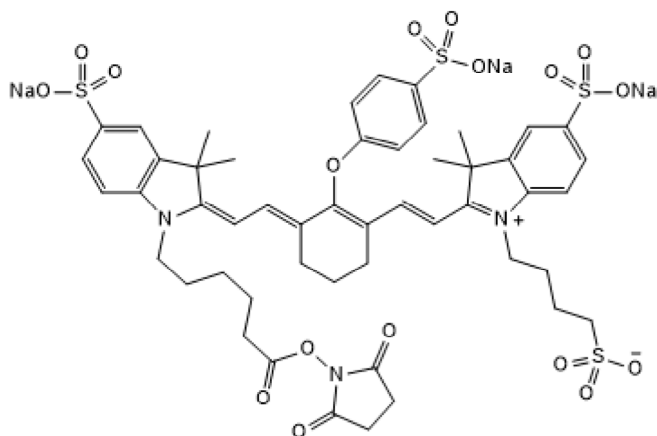
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Batch Molecular Weight: 1166.2

Physical Appearance: Dark green solid

**Minimum Purity:** ≥80%

**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.

**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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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:**

**Sever et al** (2025) Detection properties of indium-111 and IRDye800CW for intraoperative molecular imaging use across tissue phantom models. *J.Biomed.Opt.* **S13705** 30. PMID: 39310036.

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