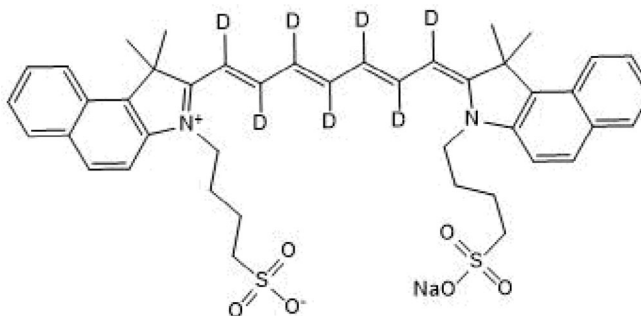


Product Name:	ICG-d7	Catalog No.:	7749	Batch No.:	1
CAS Number:	2861905-57-7				
IUPAC Name:	Sodium 4-(2-((1 <i>E</i> ,3 <i>E</i> ,5 <i>E</i> ,7 <i>Z</i>)-7-(1,1-Dimethyl-3-(4-sulfonatobutyl)-1,3-dihydro-2 <i>H</i> -benzo[<i>e</i>]indol-2-ylidene)hepta-1,3,5-trien-1-yl)-1,2,3,4,5,6,7- <i>d</i> ₇)-1,1-dimethyl-1 <i>H</i> -benzo[<i>e</i>]indol-3-ium-3-yl)butane-1-sulfonate				

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₃H₄₀D₇N₂O₆S₂Na
Batch Molecular Weight: 782.01
Physical Appearance: Red metallic solid
Solubility: water to 10 mM
DMSO to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.0% purity at 780nm
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
UV Spectrum: Consistent with structure
λ_{max}: 790 nm (DMSO)
λ_{em}: 816 nm (DMSO)
Atom %D: 97.4%

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

Product Name: ICG-d7

Catalog No.: 7749

1

CAS Number: 2861905-57-7

IUPAC Name: Sodium 4-(2-((1*E*,3*E*,5*E*,7*Z*)-7-(1,1-Dimethyl-3-(4-sulfonatobutyl)-1,3-dihydro-2*H*-benzo[*e*]indol-2-ylidene)hepta-1,3,5-trien-1-yl-1,2,3,4,5,6,7-*d*₇)-1,1-dimethyl-1*H*-benzo[*e*]indol-3-ium-3-yl)butane-1-sulfonate

Description:

ICG-d7 is a partially deuterated form of near-infrared fluorescent dye Indocyanine Green (ICG; Cat. No. 7510). Operates in the 700 - 900 nm wavelength range; also exhibits fluorescence emission in the shortwave infrared window (SWIR; 1,000 - 2,000 nm) which enables in vivo imaging. ICG-d7 shows improved stability in aqueous solutions over ICG with the same fluorescence brightness, and similar absorption and emission maxima in both DMSO and FBS. Excitation maximum = 794 nm; emission maximum = 818 nm.

Physical and Chemical Properties:

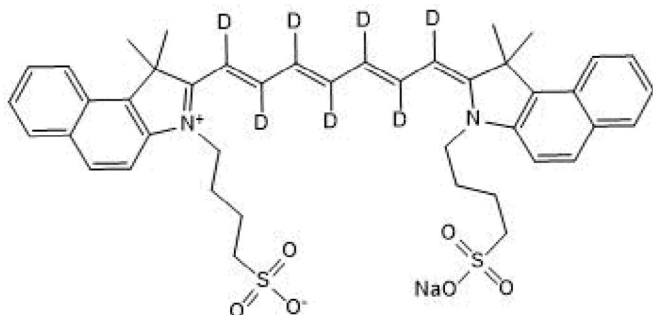
Batch Molecular Formula: C₄₃H₄₀D₇N₂O₆S₂Na

Batch Molecular Weight: 782.01

Physical Appearance: Red metallic solid

Minimum Purity: ≥95%

Batch Molecular Structure:



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:

water to 10 mM

DMSO to 10 mM

In solution, this compound undergoes slow deuterium/protium exchange such that the total Atom%D diminishes over time. It is therefore recommended that solutions are used immediately following preparation.

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.

Licensing Information:

Sold under license from the University of Notre Dame

References:

Li and Smith (2021) Deuterated indocyanine green (ICG) with extended aqueous storage shelf-life: chemical and clinical implications. *Chemistry* 27 14535. PMID: 34403531.

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