

# PRODUCT INFORMATION

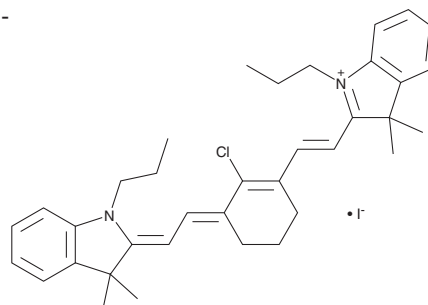


## IR 780

Item No. 31632

**CAS Registry No.:** 207399-07-3  
**Formal Name:** 2-[2-[2-chloro-3-[2-(1,3-dihydro-3,3-dimethyl-1-propyl-2H-indol-2-ylidene)ethylidene]-1-cyclohexen-1-yl]ethenyl]-3,3-dimethyl-1-propyl-3H-indolium, monoiodide

**MF:** C<sub>36</sub>H<sub>44</sub>ClN<sub>2</sub> • I  
**FW:** 667.1  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 783 nm  
**Ex./Em. Max:** 780/799 nm  
**Supplied as:** A crystalline solid  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

IR 780 is supplied as a crystalline solid. A stock solution may be made by dissolving the IR 780 in the solvent of choice, which should be purged with an inert gas. IR 780 is soluble in the organic solvent chloroform at a concentration of approximately 10 mg/ml. IR 780 is slightly soluble in ethanol, DMSO, and dimethyl formamide.

### Description

IR 780 is a heptamethine cyanine fluorescent probe for *in vivo* imaging of tumor cells.<sup>1</sup> It displays excitation/emission maxima of 780/799 nm, respectively.<sup>2</sup> IR 780 is transported into tumor cells, an effect that can be blocked by the organic anion transporting polypeptide (OATP) inhibitor sulfobromophthalein (bromosulfalein; Item No. 21058), and targeted to the mitochondria.<sup>1</sup> It has an additive effect on the increase in reactive oxygen species (ROS) production induced by sonodynamic therapy (SDT) in 4T1 breast cancer cells when used at a concentration of 16 μM.<sup>3</sup> IR 780 (0.2 mg/kg, i.v.) preferentially accumulates in tumor tissue in MCF-7, HeLa, and MG-63 mouse xenograft models and in a syngeneic mouse model of chemically induced lung tumors, and its fluorescence is detectable for up to 20 days. It also has an additive effect on the SDT-induced reduction in tumor growth in an 4T1 murine mammary carcinoma model. IR 780 has been incorporated into heparin-folic acid-IR 780 nanoparticles for use in photothermal therapy.<sup>4</sup>

### References

1. Zhang, C., Liu, T., Su, Y., *et al.* A near-infrared fluorescent heptamethine indocyanine dye with preferential tumor accumulation for *in vivo* imaging. *Biomaterials* **31**(25), 6612-6617 (2010).
2. Baeten, J., Niedre, M., Dunham, J., *et al.* Development of fluorescent materials for diffuse fluorescence tomography standards and phantoms. *Opt. Express* **15**(14), 8681-8694 (2007).
3. Li, Y., Zhou, Q., Deng, Z., *et al.* IR-780 dye as a sonosensitizer for sonodynamic therapy of breast tumor. *Sci. Rep.* **6**, 25968 (2016).
4. Yue, C.H., Liu, P., Zheng, M., *et al.* IR-780 dye loaded tumor targeting theranostic nanoparticles for NIR imaging and photothermal therapy. *Biomaterials* **34**(28), 6853-6861 (2013).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

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