



# **Certificate of Analysis**

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Product Name: CRANAD 2 Catalog No.: 4803 Batch No.: 1

CAS Number: 1193447-34-5

IUPAC Name: (T-4)-[(1E,6E)-1,7-Bis[4-(dimethylamino)phenyl]-1,6-heptadiene-3,5-dionato-kO<sup>3</sup>,kO<sup>5</sup>]difluoroboron

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{23}H_{25}BF_2N_2O_2$ 

**Batch Molecular Weight:** 410.26 **Physical Appearance:** Black solid

**Solubility:** DMSO to 5 mM with gentle warming

Storage: Store at -20°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**HPLC:** Shows 99.6% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.34 6.14 6.83 Found 67.04 6.12 6.9

## **Product Information**

Print Date: Jun 17th 2024

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 $IUPAC\ Name: (T-4)-[(1E,6E)-1,7-Bis[4-(dimethylamino)phenyl]-1,6-heptadiene-3,5-dionato-kO^3,kO^5] diffuoroboron$ 

#### **Description:**

Key information: CRANAD 2 is a curcumin derivatized near-infrared probe that binds to  $A\beta40$  aggregates. Penetrates the blood-brain barrier. Used for: amyloid- detection in vitro, tissue and in vivo. Shown to bind to plaques in APP-PS1 transgenic mice, in vitro. Detects senile plaques in 19-month-old Tg2576 mice in vivo. Application: Fluorescence microscopy, epifluorescence microscopy. Properties and Photophysical Data: CRANAD 2 binds to  $A\beta40$  aggregates (Kd = 38 nM) and elicits upon interacting with A $\beta$  aggregates, an emission blue shift (from 805 nm to 715 nm). When unbound in PBS, excitation and emission maxima ( $\lambda$ ) ar... Please see product specific page on www.tocris.com for full description.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C23H25BF2N2O2

Batch Molecular Weight: 410.26 Physical Appearance: Black solid

Minimum Purity: ≥98%

#### **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:

DMSO to 5 mM with gentle warming

#### 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:

**Ni** et al (2021) *In-vitro* and *in-vivo* characterization of CRANAD-2 for multi-spectral optoacoustic tomography and fluorescence imaging of amyloid-beta deposits in Alzheimer mice. Photoacoustics **23** 100285. PMID: 34354924.

Ran et al (2011) Non-conjugated small molecule FRET for differentiating monomers from higher molecular weight amyloid beta species. PLoS One. 6 e19362. PMID: 21559413.

Ran et al (2009) Design, synthesis, and testing of difluoroboron-derivatized curcumins as near-infrared probes for in vivo detection of amyloid-beta deposits. J.Am.Chem.Soc. 131 15257. PMID: 19807070.

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