Certificate of Analysis

Product Name: **RMR-Tre** **Catalog No.: 8013** **Batch No.: 1**

IUPAC Name: 3-(6-(5-(2,2-Dicyanovinyl)thiophen-2-yl)-3,4-dihydroquinolin-1(2*H*)-yl)-*N*-(((2*R*,3*S*,4*S*,5*R*,6*R*)-3,4,5-trihydroxy-6-(((2*R*,3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2*H*-pyran-2-yl)oxy)tetrahydro-2*H*-pyran-2-yl) methyl)propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{32}H_{38}N_4O_{11}S$

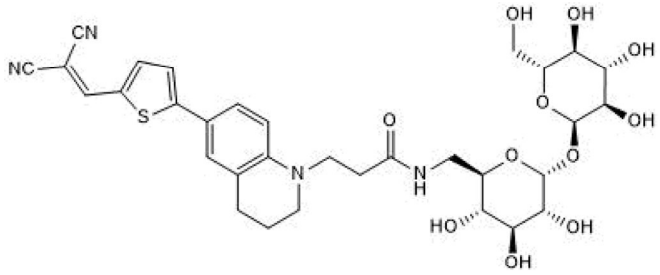
Batch Molecular Weight: 686.73

Physical Appearance: Dark brown solid

Solubility: DMSO to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 95.0% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

UV Spectrum: Consistent with structure

λ_{max}: 538 nm (Glycerol)

λ_{ex}: 578 nm (Glycerol)

λ_{em}: 673 nm (Glycerol)

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Description:

RMR-Tre is a far-red fluorogenic trehalose specific probe for live mycobacteria imaging. It enables fast, no-wash, low-background fluorescence detection of live mycobacterial outer membrane. RMR-Tre contains a molecular rotor fluorophore that brightly emits signal in the far-red region upon trehalose-guided metabolic integration into the mycomembrane. It exhibited up to a 100- fold enhancement in Mycobacterium tuberculosis labeling compared to existing fluorogenic trehalose probes. Excitation and emission maxima (λ) are 549 nm and 571 nm, respectively.

Physical and Chemical Properties:

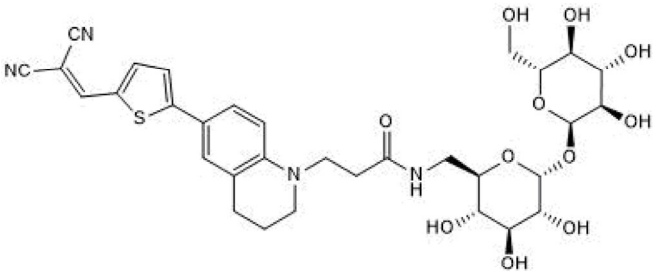
Batch Molecular Formula: $C_{32}H_{38}N_4O_{11}S$

Batch Molecular Weight: 686.73

Physical Appearance: Dark brown solid

Minimum Purity: ≥95%

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:

DMSO to 10 mM

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 Central Michigan University

References:

Banahene *et al* (2023) A far-red molecular rotor fluorogenic trehalose probe for live mycobacteria detection and drug-susceptibility testing. Angew.Chem.Int.Ed.Engl. ***62*** e202213563. PMID: 36346622.

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