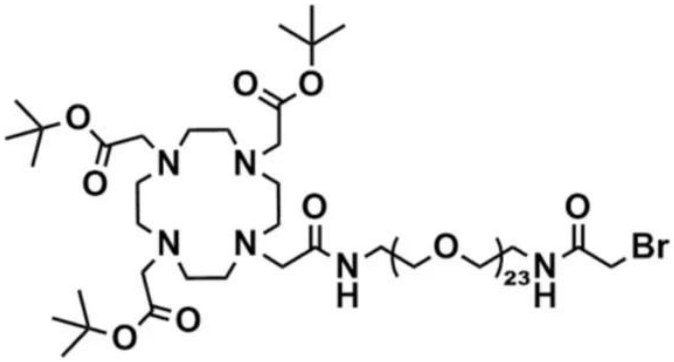
www.vectorlabs.com
Email: customerservice@vectorlabs.com
Telephone: (650) 697-3600

DOTA TRIS(TBE)-AMIDO-DPEG®$_{23}$-BROMOACETAMIDE

SKU: QBD-11153



DESCRIPTION

DOTA-tris(TBE)-amido-dPEG®23-bromoacetamide, product number QBD-11153, combines the macrocycle 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid (DOTA) through a single molecular weight, discrete polyethylene glycol (dPEG®) linker to a thiol-reactive bromoacetyl group that couples to the dPEG® linker via an amide bond. The dPEG® linker contains 75 atoms and is 85.2 Å long from the terminal amide adjacent to the DOTA moiety to the methylene group adjacent to the bromine atom. This product is useful in radioimaging and radiotherapeutic applications.

The bromoacetate moiety (present as the bromoacetamide in QBD-11153) reacts chemoselectively, but not chemospecifically, with free thiol groups to form stable thioether bonds. The rate and specificity of bromoacetate for free thiols depends upon the pH of the reaction and the relative availability (compared to thiols) of other groups with which the bromoacetate moiety can react (for example, surface-accessible amines).

DOTA is a highly popular bifunctional chelator used in a variety of diagnostic and therapeutic applications for the delivery of radionuclides, particularly lanthanide radionuclides and certain rare earth radioisotopes such as yttrium. DOTA is the preferred ligand for treatments using trivalent lanthanides because it binds the metal ions to form thermodynamically stable, kinetically inert complexes. Importantly, this product has the DOTA group protected by three

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tert-butyl ester groups and cannot chelate metals until those protecting groups are removed (using, for example, trifluoroacetic acid). However, this compound can be introduced at an early stage in a drug development process and left protected until the final step before chelation. This allows users to extensively manipulate and develop the product without putting the DOTA moiety's performance at risk.

The long, flexible, single molecular weight dPEG® linker between the DOTA and the bromoacetate groups serves many purposes. First, each ethylene glycol unit in the dPEG® chain acquires up to three molecules of water through hydrogen bonding resulting in improved water solubility for conjugate molecules. Second, in aqueous environments such as blood, dPEG® increases the hydrodynamic volume of dPEG® conjugates. With larger hydrodynamic volumes, conjugates are less susceptible to renal excretion, meaning that lower doses of the diagnostic or therapeutic agent are needed for the efficacious performance of the conjugate. Third, dPEG® is non-immunogenic, and its large hydrodynamic volume helps reduce the immunogenicity of conjugated molecules.

SPECIFICATIONS

CAS Number	N/A
Molecular Weight	1748.98; single compound
Chemical Formula	C78H151BrN6O31
Purity	> 95%
Unit Size	50 mg, 100 mg, 500 mg
Solubility	Methylene Chloride, Acetonitrile, Methanol, Dimethylformamide, or Dimethylacetamide
Spacers	dPEG® Spacer is 75 atoms and 85.2 Å
Storage Instructions	-20°C; Always let come to room temperature before opening; be careful to limit exposure to moisture and restore under an inert atmosphere; stock solutions can be prepared with dry solvent and kept for several days (freeze when not in use). dPEG® pegylation compounds are generally hygroscopic and should be treated as such. This will be less noticeable with liquids, but the solids will become tacky and difficult to manipulate, if care is not taken to minimize air exposure.
Shipping Instructions	Ambient

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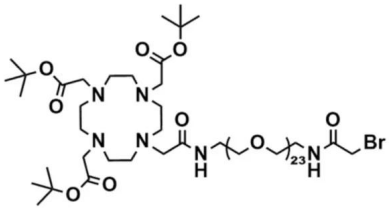
DOCUMENTS

- Safety Data Sheet
- Datasheet

GALLERY IMAGES



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