

Certificate of Analysis

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Product Name: NF 546

Catalog No.: 3892

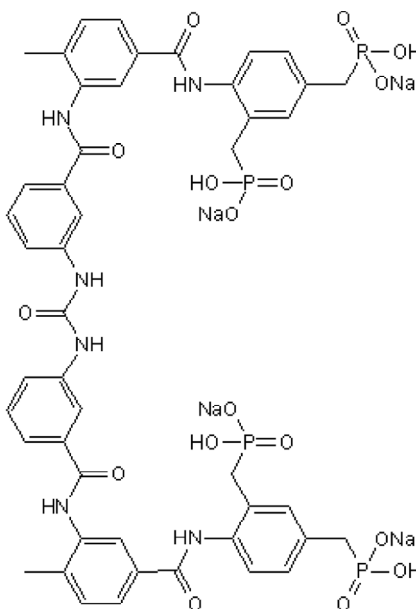
Batch No.: 3

CAS Number: 1006028-37-0

IUPAC Name: 4,4'-(Carbonylbis(imino-3,1-phenylene-carbonylimino-3,1-(4-methyl-phenylene)carbonylimino))-bis(1,3-xylene-alpha,alpha'-diphosphonic acid tetrasodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₇H₄₄N₆Na₄O₁₇P₄·13.5H₂O
Batch Molecular Weight: 1424.01
Physical Appearance: Off White solid
Solubility: water to 10 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 96.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	39.64	5.03	5.9
Found	39.65	4.79	6.01

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

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Description:

NF 546 is a P2Y₁₁ agonist (pEC₅₀ = 6.27). Exhibits selectivity for P2Y₁₁ over a range of P2Y and P2X receptors. Also inhibits DNA-binding activity of HMGA2 (IC₅₀ = 5.49 μM).

Physical and Chemical Properties:

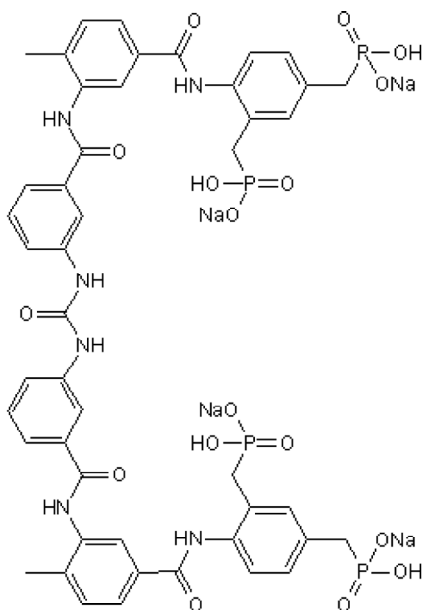
Batch Molecular Formula: C₄₇H₄₄N₆Na₄O₁₇P₄·13.5H₂O

Batch Molecular Weight: 1424.01

Physical Appearance: Off White solid

Minimum Purity: ≥95%

Batch Molecular Structure:



References:

Su et al (2020) Identification of HMGA2 inhibitors by AlphaScreen-based ultra-high-throughput screening assays. *Sci.Rep.* **10** 18850. PMID: 33139812.

Meis et al (2010) NF546 [4,4'-(carbonylbis(imino-3,1-phenylene-carbonylimino-3,1-(4-methyl-phenylene)carbonylimino))-bis(1,3-xylene-γ,γ'-diphosphonic acid) tetrasodium salt] is a non-nucleotide P2Y₁₁ agonist and stimulates release of interleukin J.Pharmacol.Exp.Ther. **332** 238. PMID: 19815812.

Storage: Store at -20°C

Solubility & Usage Info:

water to 10 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.

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