

**Product Name:** NF 546

**Catalog No.:** 3892

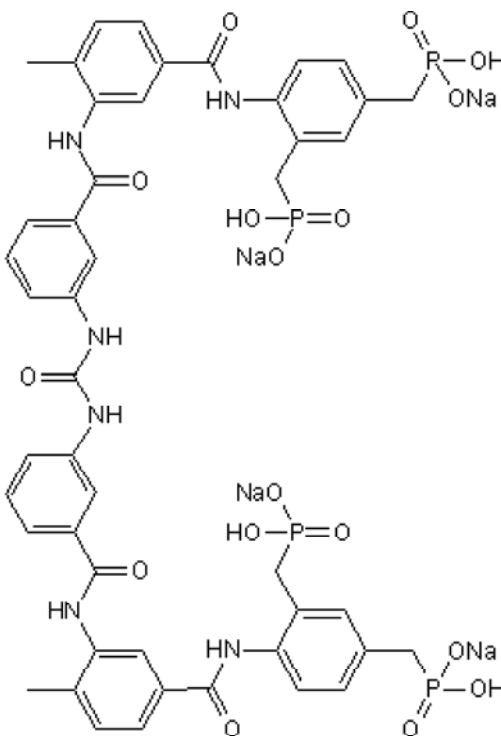
**Batch No.:** 3

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:** C<sub>47</sub>H<sub>44</sub>N<sub>6</sub>Na<sub>4</sub>O<sub>17</sub>P<sub>4</sub>·13.5H<sub>2</sub>O  
**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 98.9% purity  
**<sup>1</sup>H 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:**

P2Y<sub>11</sub> agonist (pEC<sub>50</sub> = 6.27). Exhibits selectivity for P2Y<sub>11</sub> over a range of P2Y and P2X receptors. Also inhibits DNA-binding activity of HMGA2 (IC<sub>50</sub> = 5.49 μM).

**Physical and Chemical Properties:**

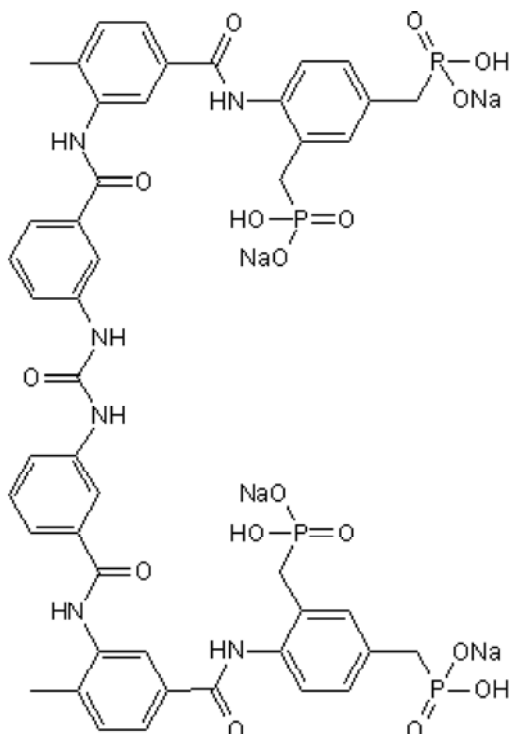
Batch Molecular Formula: C<sub>47</sub>H<sub>44</sub>N<sub>6</sub>Na<sub>4</sub>O<sub>17</sub>P<sub>4</sub>·13.5H<sub>2</sub>O

Batch Molecular Weight: 1424.01

Physical Appearance: Off White solid

**Minimum Purity:** ≥95%

**Batch Molecular Structure:**



**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. Our standard recommendations are:

**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:**

**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 P2Y<sub>11</sub> agonist and stimulates release of interleukin J.Pharmacol.Exp.Ther. **332** 238. PMID: 19815812.

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