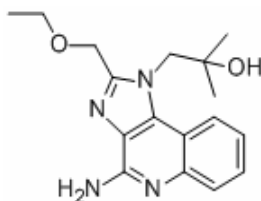


Product Data Sheet

Product Name: Resiquimod
CAS No.: 144875-48-9
Cat. No.: CS-1706
Structure



MWt: 314.38
Formula: C₁₇H₂₂N₄O₂
Solubility: DMSO ≥ 10 mg/mL (warmed to 60 °C)
Purity : >98%

Biological Activity:

Resiquimod (R-848) is a potent synthetic agonist of TLR7/TLR8 that possesses antiviral and antitumoral activities. Resiquimod belongs to the class of imidazoquinolinamines compounds with immunomodulatory effects. It increases the levels of cytokines such as TNF- α , IL-6 and IFN- α .

IC50 Value:

Target: TLR7/TLR8

in vitro: Resiquimod, like CD40, stimulates antibody secretion, cytokine production, protection from apoptosis, and CD80 upregulation. In addition, it shows synergy with signals delivered by the B cell antigen receptor and heightens CD40-mediated B cell activation, demonstra...

References:

- [1]. Bishop GA, et al. The immune response modifier resiquimod mimics CD40-induced B cell activation. *Cell Immunol.* 2001 Feb 25;208(1):9-17.
- [2]. Brugnolo F, et al. The novel synthetic immune response modifier R-848 (Resiquimod) shifts human allergen-specific CD4+ TH2 lymphocytes into IFN-gamma-producing cells. *J Allergy Clin Immunol.* 2003 Feb;111(2):380-8.
- [3]. Pockros PJ, et al. Oral resiquimod in chronic HCV infection: safety and efficacy in 2 placebo-controlled, double-blind phase IIa studies. *J Hepatol.* 2007 Aug;47(2):174-82.
- [4]. McCluskie MJ, et al. Treatment of intravaginal HSV-2 infection in mice: a comparison of CpG oligodeoxynucleotides and resiquimod(R-848). *Antiviral Res.* 2006 Feb;69(2):77-85.

Caution: Not fully tested. For research purposes only

ChemScene, LLC

MSDS

1 Composition

Product Name: Resiquimod
Chemical Name:
1H-Imidazo[4,5-c]quinoline-1-ethanol, 4-amino-2-(ethoxymethyl)- α , α -dimethyl-

CAS No.: 144875-48-9
Appearance: white to off-white(Solid)
Formula: C17H22N4O2
Solubility: DMSO \geq 10 mg/mL (warmed to 60 °C)

2 Handling and Storage

HANDLING- Do not breathe dust. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.
STORAGE- Please store the product under the recommended conditions in the Certificate of Analysis.

3 Stability and Reactivity

STABILITY- Stable under normal handling conditions.
MATERIALS TO AVOID- Strong oxidizing agents.
REACTIVITY- May emit toxic gasses like Carbon monoxide, Carbon dioxide, Nitrogen oxides upon thermal decomposition.

4 Hazards Identification

Special indication of hazards to humans and the environment.
Irritating to eyes, respiratory system and skin.

5 First Aid

INHALATION- If inhaled, remove to fresh air. If not breathing give, artificial respiration. If breathing is difficult, give oxygen.
SKIN CONTACT- In case of contact, immediately wash skin with soap and copious amounts of water.
EYE CONTACT- In case of contact, immediately flush eyes with copious amounts of water for at least 15 minutes.
INGESTION- If swallowed, wash out mouth with water provided person is conscious. Call a physician.

6 Fire Fighting Measures

EXTINGUISHING MEDIA
Water spray- Carbon dioxide, dry chemical powder, or appropriate foam.
SPECIAL RISKS
Specific Hazard(s)- Emits toxic fumes under fire conditions.
SPECIAL PROTECTIVE EQUIPMENT FOR FIREFIGHTERS
Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

7 Accident Release Measure

PROCEDURE(S) OF PERSONAL PRECAUTION(S)-Wear respirator, chemical safety goggles, rubber boots, and heavy rubber gloves.
METHODS FOR CLEANING UP-Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

8 Accident Release Measure

No data available.

9 Toxicological Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

10 Regular Information

CLASSIFICATION- Substance not yet fully tested.
SAFETY PHASES- 26-36 (In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing.) 36/37/38 (Irritating to eyes, respiratory system and skin.)

11 Disposal Considerations

As specific country, federal, state and local environmental regulations vary and change frequently we suggest you contact a local, authorized waste disposal contractor for adequate disposal.

12 Transport Information

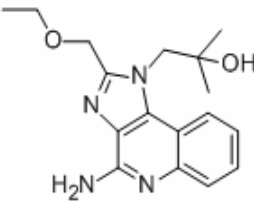
RID/ADR- Non-hazardous for road transport.
IMDG- Non-hazardous for sea transport.
IATA - Non-hazardous for air transport.

13 Other Information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. ChemScene LLC shall not be held liable for any damage resulting from handling or from contact with the above product.

Caution: Not fully tested. For research purposes only
ChemScene, LLC

Certificate of Analysis

Product Name	Resiquimod
CAS No.	144875-48-9
Batch No.	10284
Structure	

Test Date	12/03/2013	Retest Date	12/02/2015
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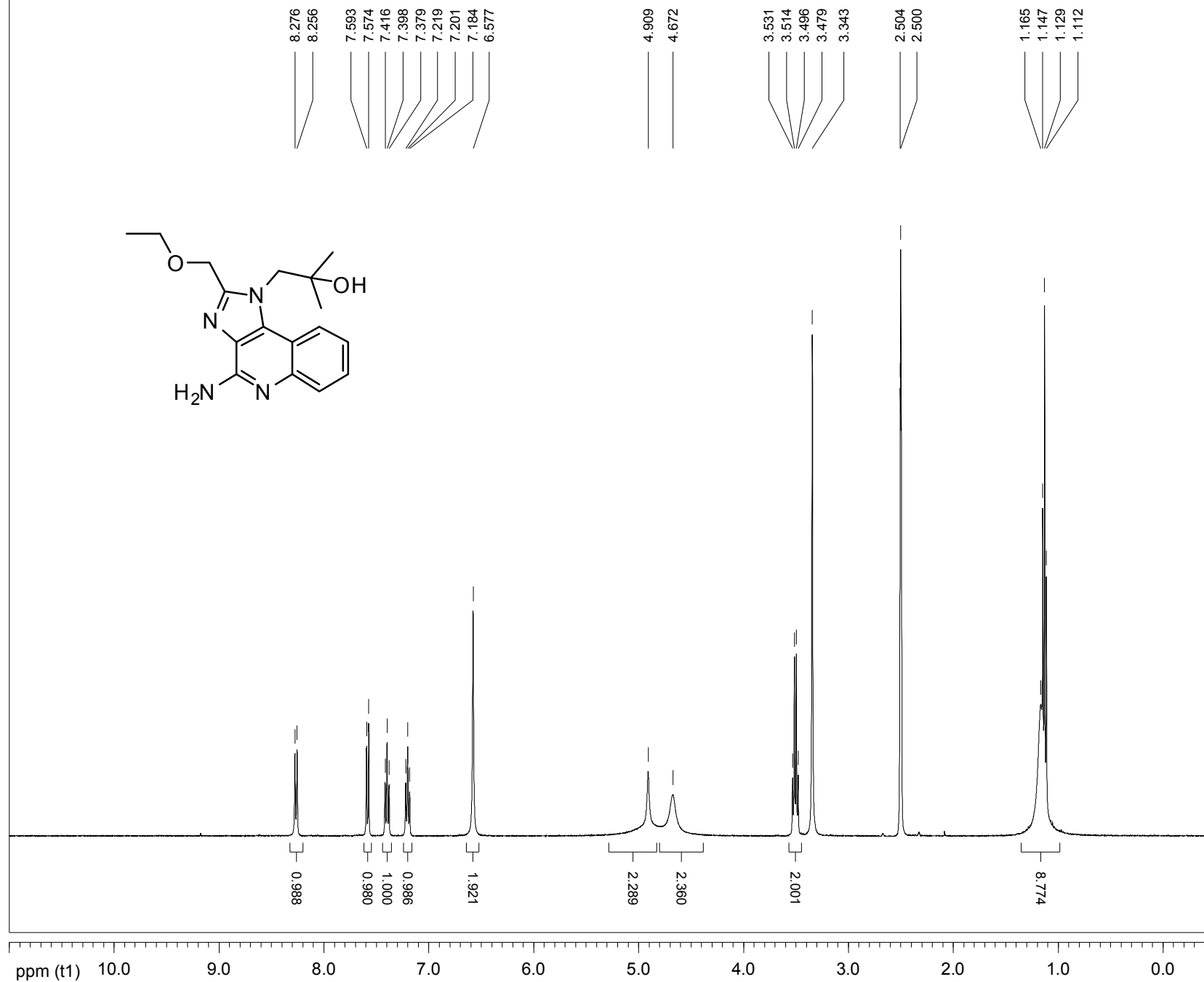
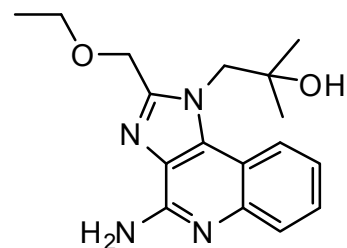
Items	Specifications	Results
Appearance	White to off-white Solid	Conforms
Identification	1H NMR spectrum of sample corresponds to that of standard preparation	Conforms
	Mass spectrum of sample corresponds to that of standard preparation	Conforms
	The retention time of the major peak in the chromatogram of sample corresponds to that in the chromatogram of standard preparation	Conforms
Purity by LCMS	NLT 98.0%	98.95%
Conclusion	The product tested complies with the specifications.	
Storage condition: Store in a tightly closed container, in a cool and dry place.		

Caution: Not fully tested. For research purposes only

ChemScene, LLC

11 Deer Park Drive, Suite 102D, Monmouth Junction, NJ 08852
Tel: 732-484-9848 Fax: 888-484-5008 Email: info@chemscene.com Web: www.chemscene.com

Sample ID: BIZ2013-D03-ZLQ1, Catalog No: CS-1706 Batch#10284, DMSO



Date:

3 Dec 2013

Document's Title:

Catalog No: CS-1706

Batch#10284

Spectrum Title:

biz2013-d03-zlq1-dms0-131203

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

(f1) 3.2768

Spectral Width (ppm):

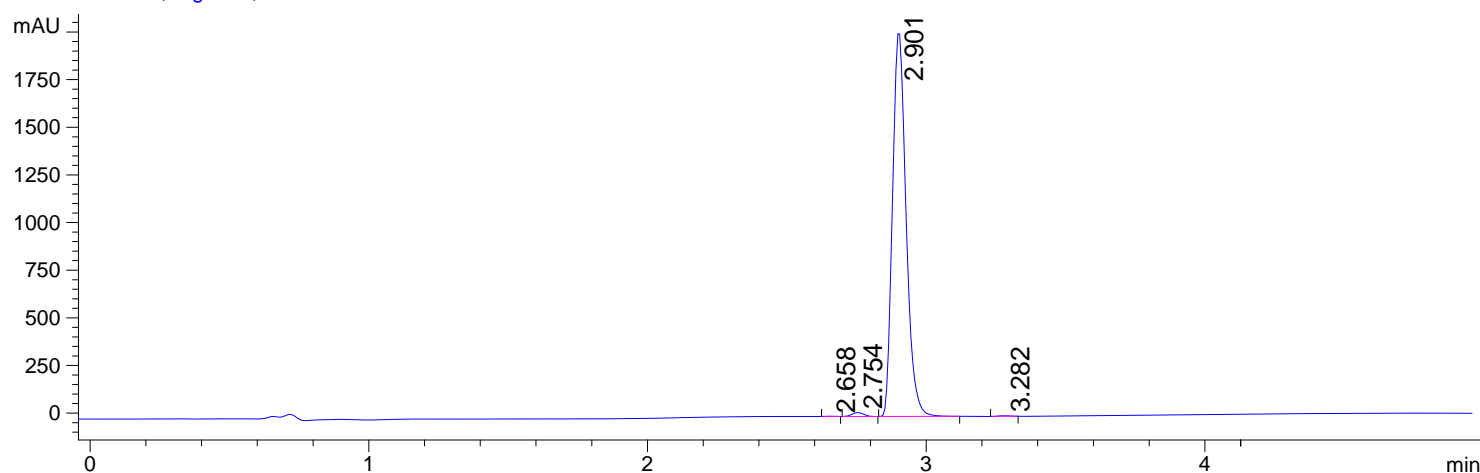
(f1) 24.992

Pulse Program:

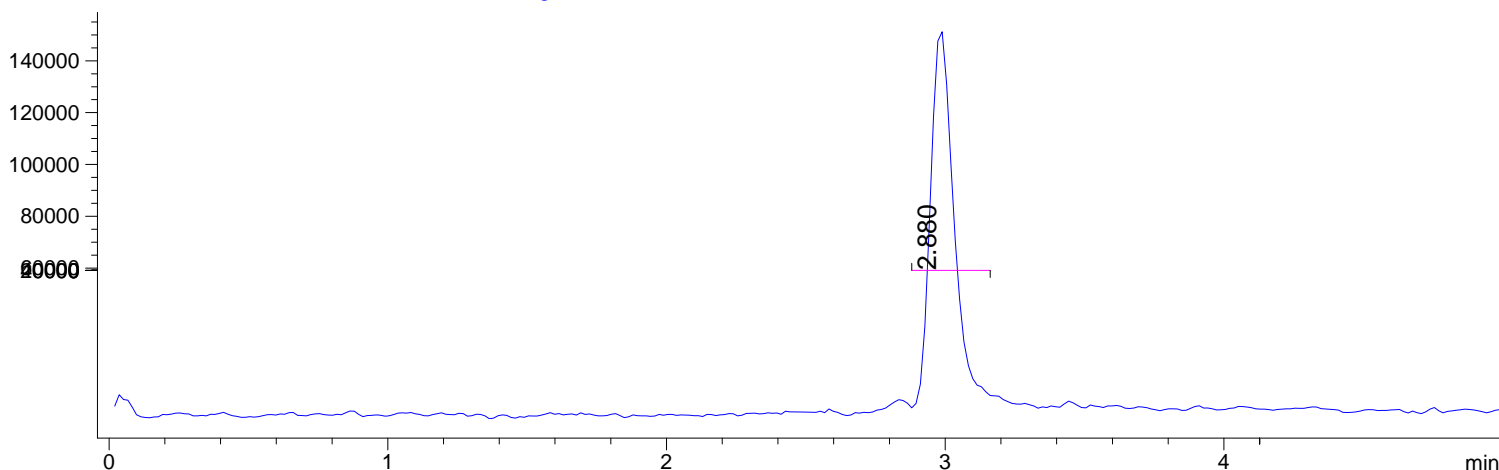
Unknown

Lot Number : BIZ2013-D03-ZLQ1 Location : Vial 40
Injection Date : 03-Dec-13, 16:44:08 Seq. Line : 70
Acq. Operator : SY Inj Volume : 1 ul
Acq. Method : E:\METHODS\METHODS\20101020\1-8A.M
Analysis Method : E:\METHODS\METHODS\20101020\BL1B.M
Catalog No : CS-1706 Batch#10284
Test Type :

DAD1 B, Sig=220,8 Ref=off



MSD1 TIC, MS File API-ES, Pos, Scan, Frag: 50



Integration Results for DAD1 B, Sig=220,8 Ref=off

RetTime	Width	Area	Height	Area%	MSBase (+)
2.66	0.04	2.11	0.93	0.03	ND
2.75	0.05	61.58	20.84	0.89	ND
2.90	0.06	6832.57	2039.72	98.95	315.2
3.28	0.04	9.06	3.37	0.13	ND

Ret. Time: 2.88 <<<< POSITIVE SPECTRA >>>>

