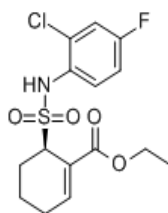


Product Data Sheet

Product Name: TAK-242
CAS No.: 243984-11-4
Cat. No.: CS-0408

Structure



MWt: 361.82
Formula: C₁₅H₁₇ClFNO₄S
Solubility: DMSO
Purity : >98%

Biological Activity:

TAK-242 (Resatorvid), a small-molecule-specific inhibitor of Toll-like receptor (TLR) 4 signaling, inhibits the production of lipopolysaccharide-induced inflammatory mediators by binding to the intracellular domain of TLR4.

IC₅₀ value: 1.1-11 nM [1]

Target: TLR4

in vitro: In RAW264.7 cells and mouse peritoneal macrophages, TAK-242 suppressed lipopolysaccharide (LPS)-induced production of NO, tumor necrosis factor-alpha (TNF-alpha), and interleukin (IL)-6, with 50% inhibitory concentration (IC₅₀) of 1.1 to 11 nM. TAK-242 also suppressed the production of these cytokines from LPS-...

References:

- [1]. Li M, et al. A novel cyclohexene derivative, ethyl (6R)-6-[N-(2-Chloro-4-fluorophenyl)sulfamoyl]cyclohex-1-ene-1-carboxylate (TAK-242), selectively inhibits toll-like receptor 4-mediated cytokine production through suppression of intracellular signaling. *Mol Pharmacol.* 2006 Apr;69(4):1288-95.
- [2]. Matsunaga N, et al. TAK-242 (resatorvid), a small-molecule inhibitor of Toll-like receptor (TLR) 4 signaling, binds selectively to TLR4 and interferes with interactions between TLR4 and its adaptor molecules. *Mol Pharmacol.* 2011 Jan;79(1):34-41.
- [3]. Tramullas M, et al. Toll-Like Receptor 4 Regulates Chronic Stress-Induced Visceral Pain in Mice. *Biol Psychiatry.* 2013 Nov 11. pii: S0006-3223(13)00985-2.
- [4]. Sha T, et al. Therapeutic effects of TAK-242, a novel selective Toll-like receptor 4 signal transduction inhibitor, in mouse endotoxin shock model. *Eur ...*

Caution: Not fully tested. For research purposes only

ChemScene, LLC

MSDS

1 Composition

Product Name: TAK-242

Chemical Name:

1-Cyclohexene-1-carboxylic acid, 6-[[2-chloro-4-fluorophenyl)amino]sulfonyl]-, ethyl ester, (6R)-

CAS No.: 243984-11-4

Appearance: light yellow to yellow(Oil)

Formula: C₁₅H₁₇ClFNO₄S

Solubility: DMSO

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 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 Regulatory 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.

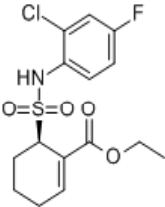
13 Other Information

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	TAK-242
CAS No.	243984-11-4
Batch No.	10094
Structure	

Test Date	11/15/2013	Retest Date	11/14/2015
------------------	------------	--------------------	------------

Items	Specifications	Results
Appearance	Light yellow to yellow Oil	Conforms
Identification	1H NMR 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 HPLC	NLT 98.0%	99.95%
E.E.	NLT 98.0%	98.00%
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

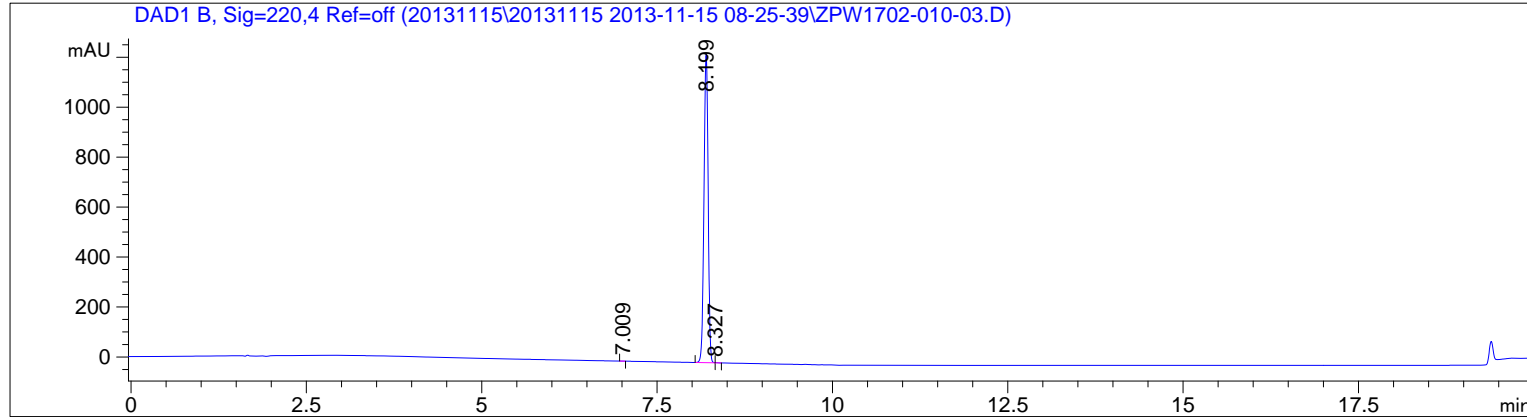
```
=====
Acq. Operator   :                               Seq. Line :   16
Acq. Instrument : Instrument 1                 Location  : Vial 10
Injection Date  : 11/15/2013 1:39:13 PM      Inj       :    1
                                                Inj Volume: 5.0 µl

Acq. Method     : D:\CHEM32\1\DATA\20131115\20131115 2013-11-15 08-25-39\30-90A,9MIN.M
Last changed    : 11/15/2013 1:00:32 PM
Analysis Method : D:\CHEM32\1\METHODS\30-90A,9MIN.M
Last changed    : 11/15/2013 2:04:22 PM
                  (modified after loading)

Method Info     : HPLC-06

Catalog No.    : CS-0408 Batch#10094
                  A-RP-65
=====
```

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=220,4 Ref=off

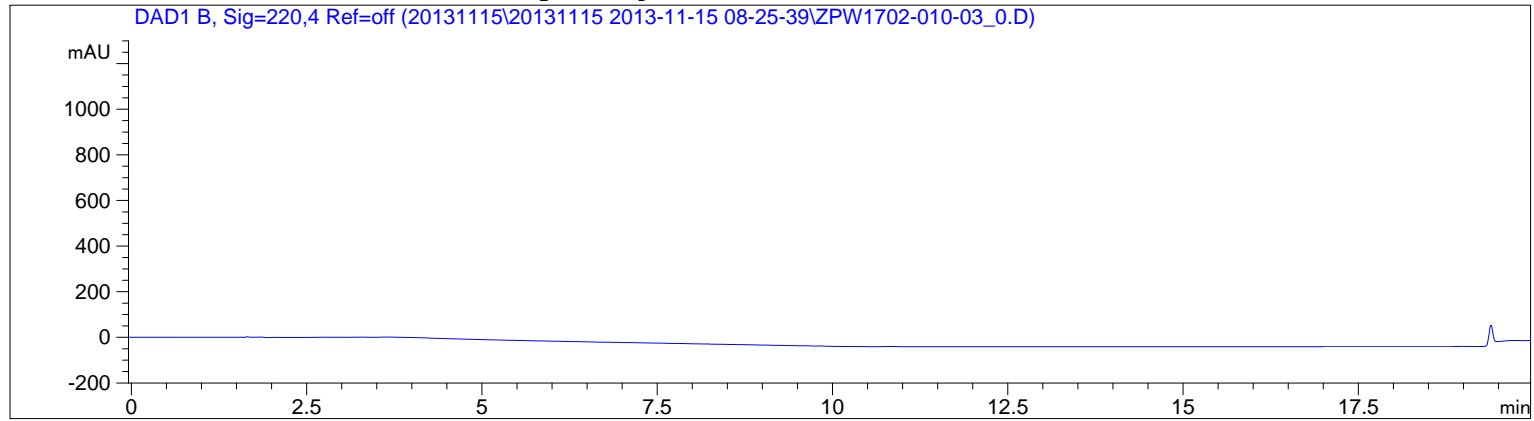
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.009	MM R	0.0549	6.88935e-1	2.09024e-1	0.0136
2	8.199	MF R	0.0679	5063.76221	1243.38977	99.9501
3	8.327	FM R	0.0561	1.83876	5.45899e-1	0.0363

Totals : 5066.28990 1244.14469

=====
*** End of Report ***

```
=====
Acq. Operator   :                               Seq. Line :   15
Acq. Instrument : Instrument 1                   Location  : Vial 1
Injection Date  : 11/15/2013 1:17:23 PM         Inj       :    1
                                                    Inj Volume: 5.0 µl
Acq. Method     : D:\CHEM32\1\DATA\20131115\20131115 2013-11-15 08-25-39\30-90A,9MIN.M
Last changed    : 11/15/2013 1:00:32 PM
Analysis Method : D:\CHEM32\1\METHODS\30-90A,9MIN.M
Last changed    : 11/15/2013 2:09:02 PM
                  (modified after loading)
Method Info     : HPLC-06
Catalog No.    : CS-0408 Batch#10094 (BLANK)
                  A-RP-65
=====
```

Additional Info : Peak(s) manually integrated



```
=====
                          Area Percent Report
=====
```

```
Sorted By           :      Signal
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

No peaks found

```
=====
*** End of Report ***
=====
```

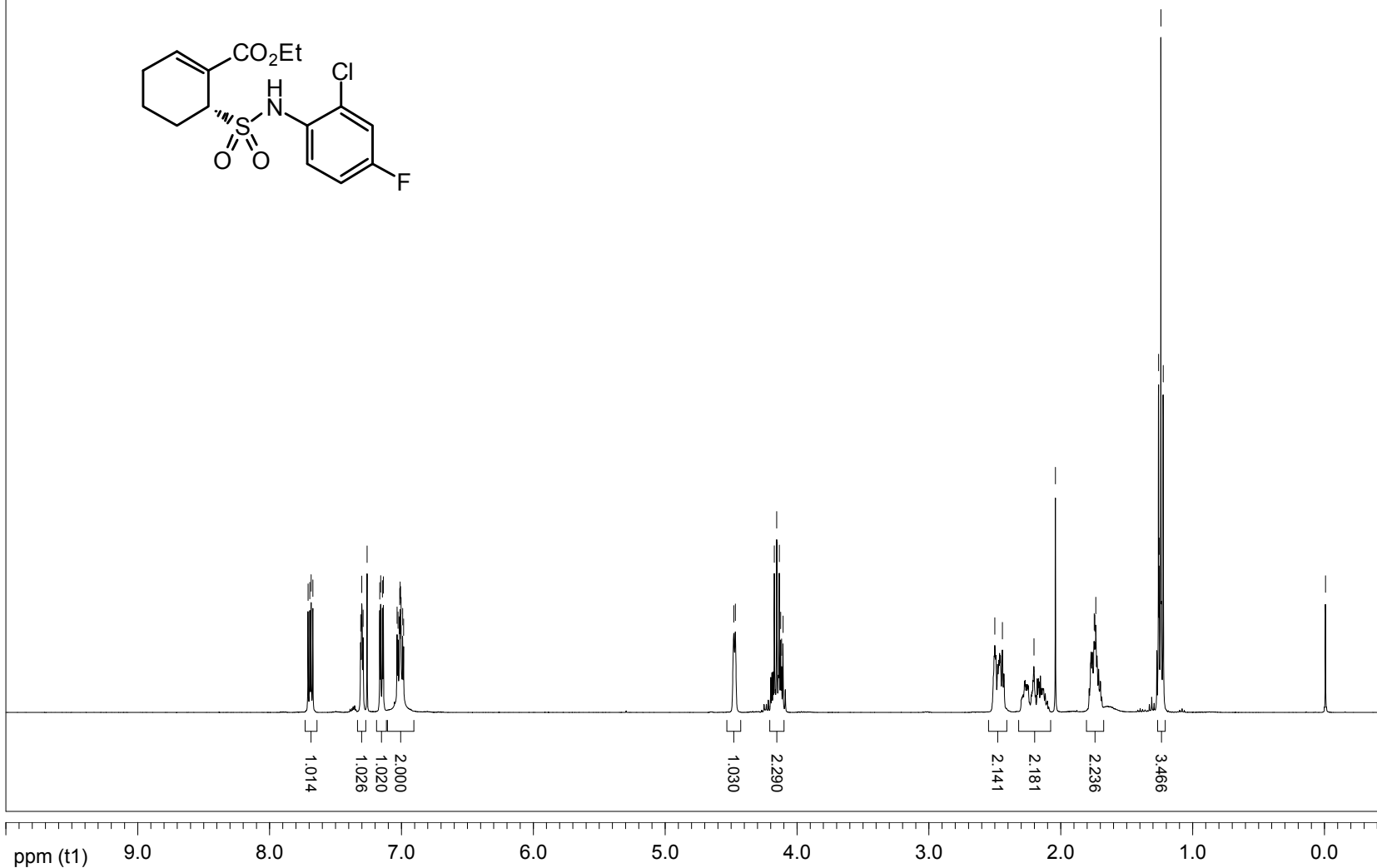
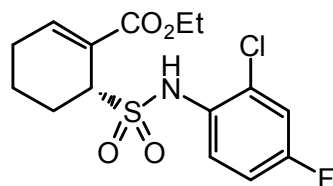
Sample ID: ZPW1702-010-03, Catalog No.: CS-0408 Batch#10094, CDCl₃

7.708
7.694
7.685
7.671
7.309
7.300
7.290
7.260
7.164
7.157
7.144
7.137
7.033
7.026
7.013
7.010
7.006
7.003
6.991
6.983

4.479
4.467
4.172
4.153
4.134
4.124
4.116
4.106

2.499
2.442
2.203
2.040
1.747
1.741
1.734
1.258
1.253
1.240
1.222

-0.008



Date:

15 Nov 2013

Document's Title:

Catalog No.: CS-0408

Batch#10094

Spectrum Title:

zpw1702-010-03-cdcl3-131115

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

CHIRAL CHROMATOGRAPHY REPORT

Column : CHIRALPAK IC

Column size : 0.46 cm I.D. × 15 cm L

Injection : 0.1ul

Mobile phase : Hexane/EtOH=80/20(v/v)

Flow rate : 1.0 ml/min

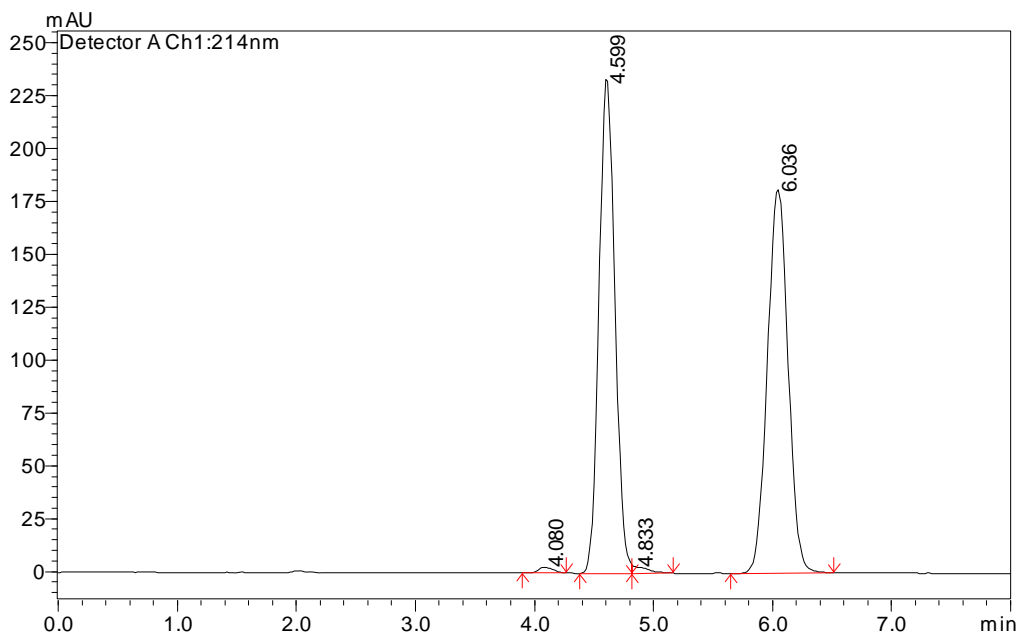
Wave length : UV 214nm

Temperature : 35°C

Sample solution : X mg/ml in mobile phase

Sample ID : Racemate

< Chromatogram >



<Column Performance Report>

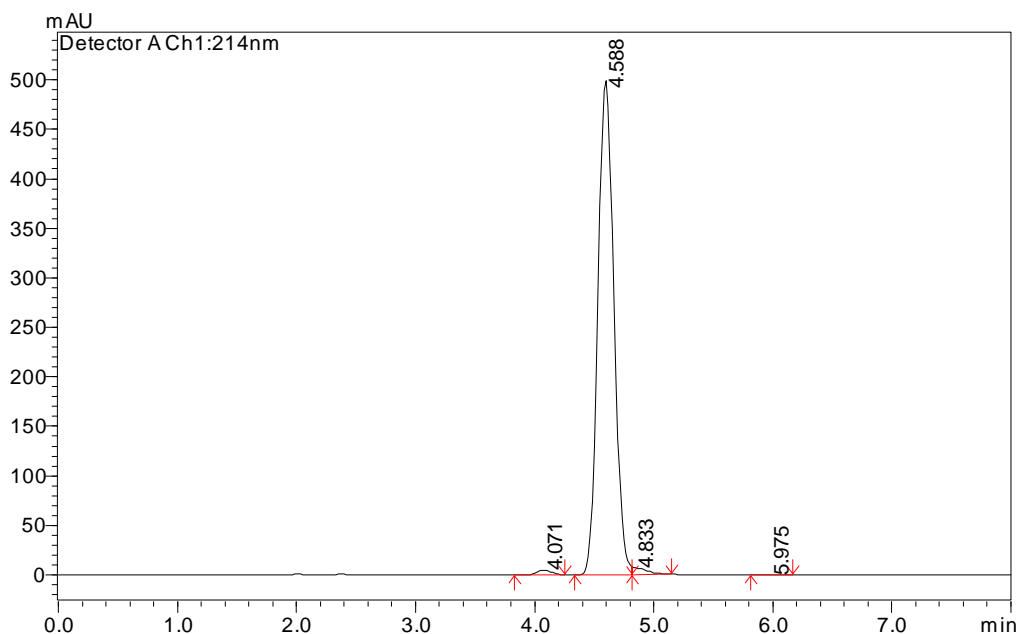
Peak No.	Time	Area	Area %	T Plate	Tailing	Resolution
1	4.080	22988	0.5192	4108.478	1.218	--
2	4.599	2180580	49.2470	4448.323	1.159	1.959
3	4.833	28280	0.6387	--	--	--
4	6.036	2195995	49.5951	4893.782	1.067	--

Testing date: 2013/11/15 Tested by: _____ Confirmed by: _____

CHIRAL CHROMATOGRAPHY REPORT

Column	: CHIRALPAK IC
Column size	: 0.46 cm I.D. × 15 cm L
Injection	: 0.2ul
Mobile phase	: Hexane/EtOH=80/20(v/v)
Flow rate	: 1.0 ml/min
Wave length	: UV 214nm
Temperature	: 35°C
Sample solution	: X mg/ml in mobile phase
Sample ID	: ZPW1702-010-03
Batch NO.	: HM-028_5-20131115

< Chromatogram >



<Column Performance Report>

Peak No.	Time	Area	Area %	T Plate	Tailing	Resolution
1	4.071	38592	0.8120	4379.332	1.188	--
2	4.588	4655139	97.9470	4387.341	1.158	1.978
3	4.833	56541	1.1896	--	--	--
4	5.975	2440	0.0513	6036.455	1.171	--

Testing date: 2013/11/15 Tested by: _____ Confirmed by: _____