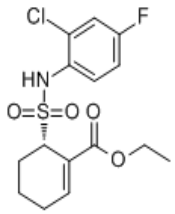
Product Data Sheet

Product Name: TAK-242 S enantiomer

CAS No.: 243984-10-3

Cat. No.: CS-1214

Structure



MWt: 361.82

Formula: C15H17ClFNO4S

Solubility: DMSO

Purity : >98%

Biological Activity:

S enantiomer of TAK-242. TAK-242 (Resatorvid), a small-molecule inhibitor of Toll-like receptor (TLR) 4 signaling. TAK-242 is in treatment of sepsis and septic shock.

References:

[1]. Naoko Matsunaga 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. Molecular Pharmacology January 2011 vol. 79 no. 1 34-41
[2]. Xie H, Zhou H, Wang H, Chen D, Xia L, Wang T, Yan J.Anti-β(2)GPI/β(2)GPI induced TF and TNF-α expression in monocytes involving both TLR4/MyD88 and TLR4/TRIF signaling pathways.Mol Immunol. 2012 Sep 7;53(3):246-254.
[3]. Jinno F, Kakehi M, Takeuchi T, Tagawa Y, Kondo T, Asahi S.Investigation of the unique metabolic fate of ethyl (6R)-6- [N- (2-chloro-4-fluorophenyl) sulfamoyl] cyclohex-1-ene-1-carboxylate (TAK-242) in rats and dogs using two types of 14C-labeled compounds having different labeled positions.Arzneimittelforschung. 2011;61(8):458-71.
[4]. Fenhammar J, Rundgren M, Fores...

Caution: Not fully tested. For research purposes only

ChemScene, LLC

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MSDS

1 Composition

Product Name: TAK-242 S enantiomer

Chemical Name:

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

CAS No.: 243984-10-3

Appearance: light yellow to yellow(solid)

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 Regulary 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

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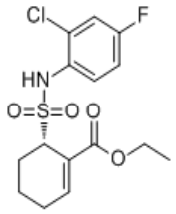
Certificate of Analysis

Product Name	TAK-242 S enantiomer
CAS No.	243984-10-3
Batch No.	03405
Structure	

Test Date	12/09/2013	**Retest Date**	12/08/2015

Items	Specifications	Results
Appearance	light yellow solid	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 LCMS	NLT 98.0%	99.86%
E.E.	NLT 98.0%	99.44%
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

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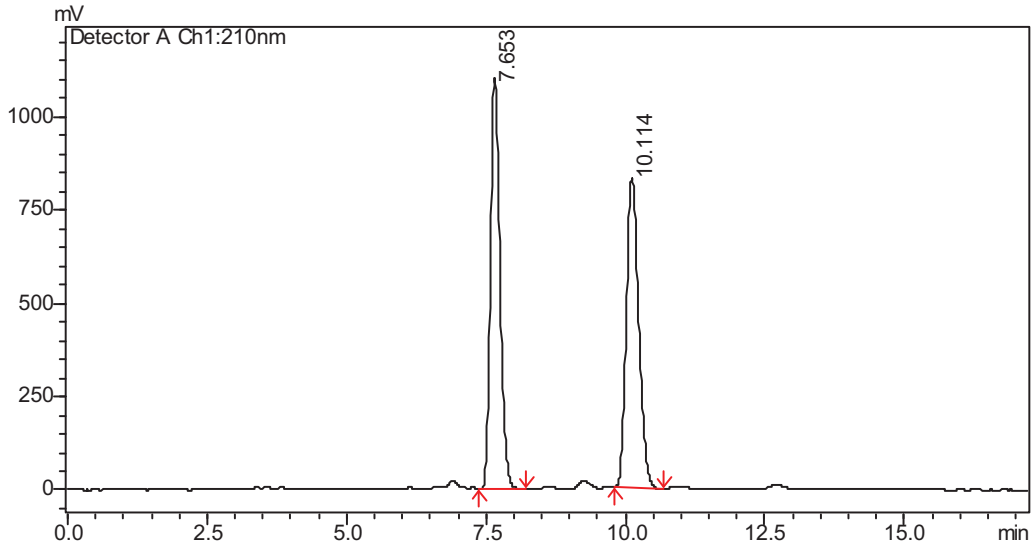
CHIRAL CHROMATOGRAPHY REPORT

Column	:	CHIRALCEL IC
Column size	:	0.46 cm I.D. × 25 cm L
Injection	:	1 ul
Mobile phase :		H/E=80/20(v/v)
Flow rate	:	1.0 ml/min
Wave length :		UV 210 nm
Temperature :		35 ℃
Sample solution	:	X mg/ml in mobile phase
Brand of solvents	:	Hexane,EtOH : HPLC grade
Sample structure	:	Racemate



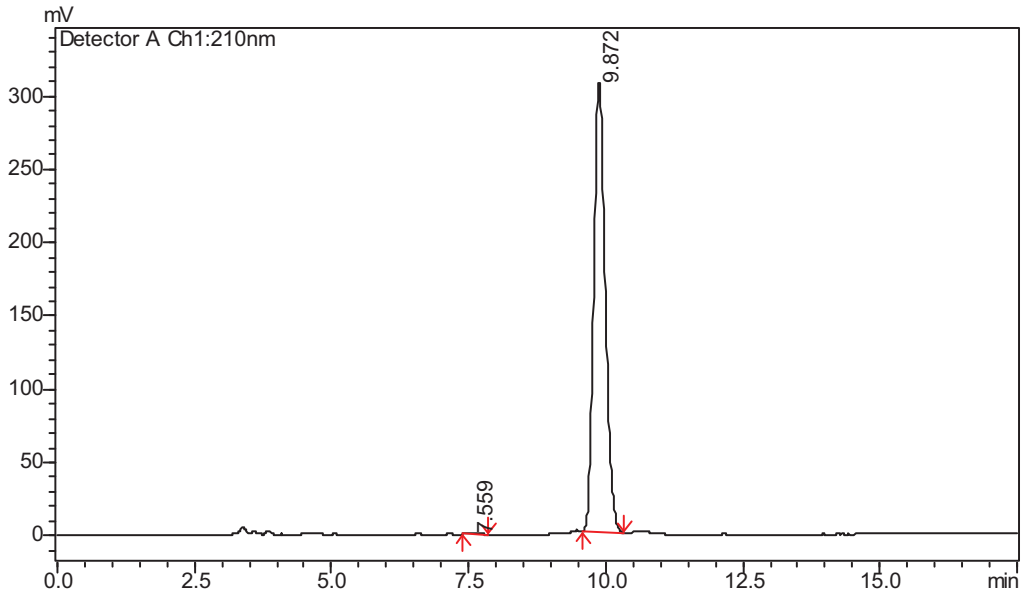
<Column Performance Report>

Peak No.	Time	Area	Area %	T Plate	Tailing	Resolution
1	7.653	13104927	50.3898	9047.262	1.251	--
2	10.114	12902199	49.6102	9422.108	1.209	6.665

Testing date: _____ Tested by: _____ Confirmd by: _____

CHIRAL CHROMATOGRAPHY REPORT

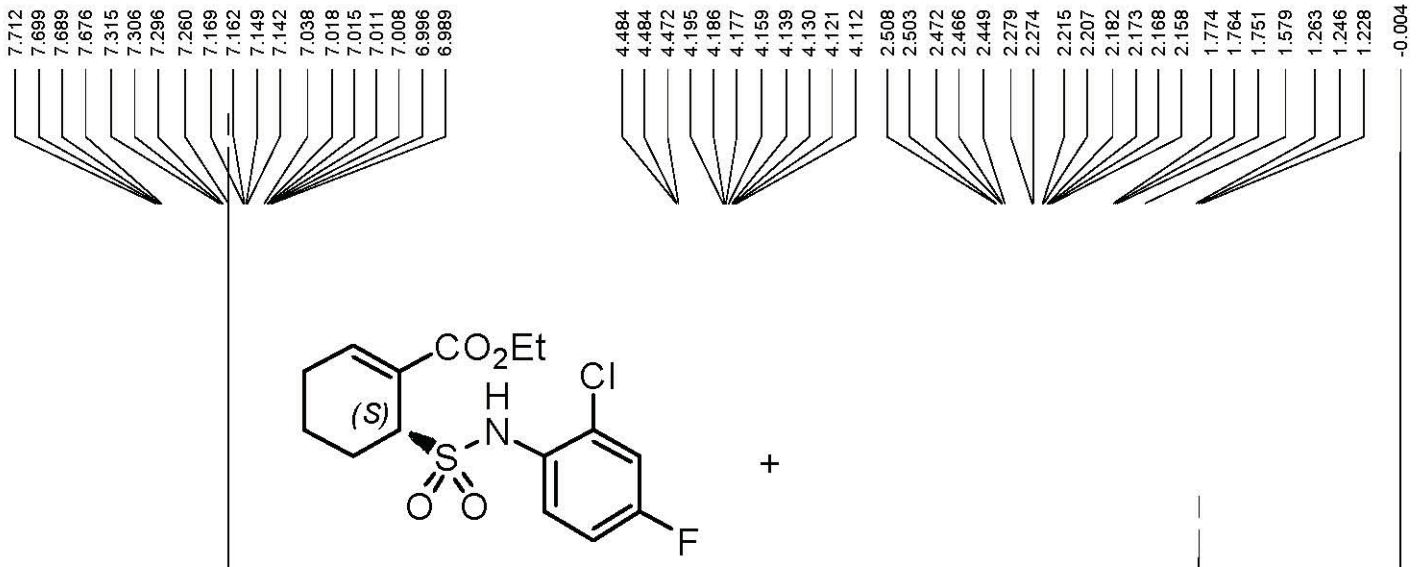
Column	:	CHIRALCEL IC
Column size	:	0.46 cm I.D. × 25 cm L
Injection	:	2 ul
Mobile phase :		H/E=80/20(v/v)
Flow rate	:	1.0 ml/min
Wave length :		UV 210 nm
Temperature :		35 ℃
Sample solution	:	X mg/ml in mobile phase
Brand of solvents	:	Hexane,EtOH : HPLC grade
Sample structure	:	Peak 2
Sample ID	:	PBL0498-017-P7
Batch No	:	HM-028_6-20101024



Peak No.	Time	Area	Area %	T Plate	Tailing	Resolution
1	7.5	59	12698	0.2807	14279.030	1.271	--
2	9.8	72	4510574	99.7193	10032.119	1.205	7.150

Testing date: _____ Tested by: _____ Confirmed by: _____

Sample ID: PBL0498-017-P7, Catalog No: CS-1214 Batch#03405, CDCl3



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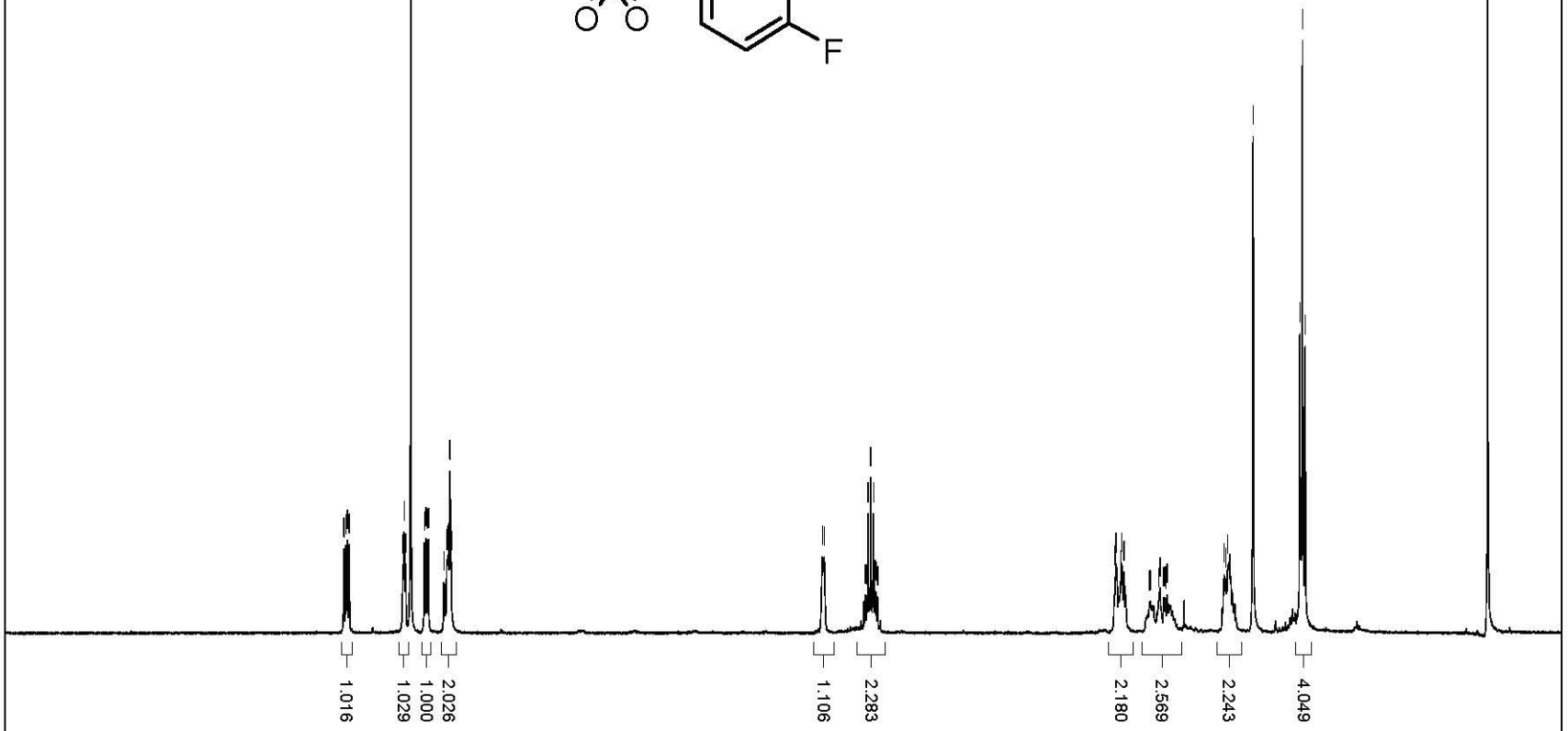
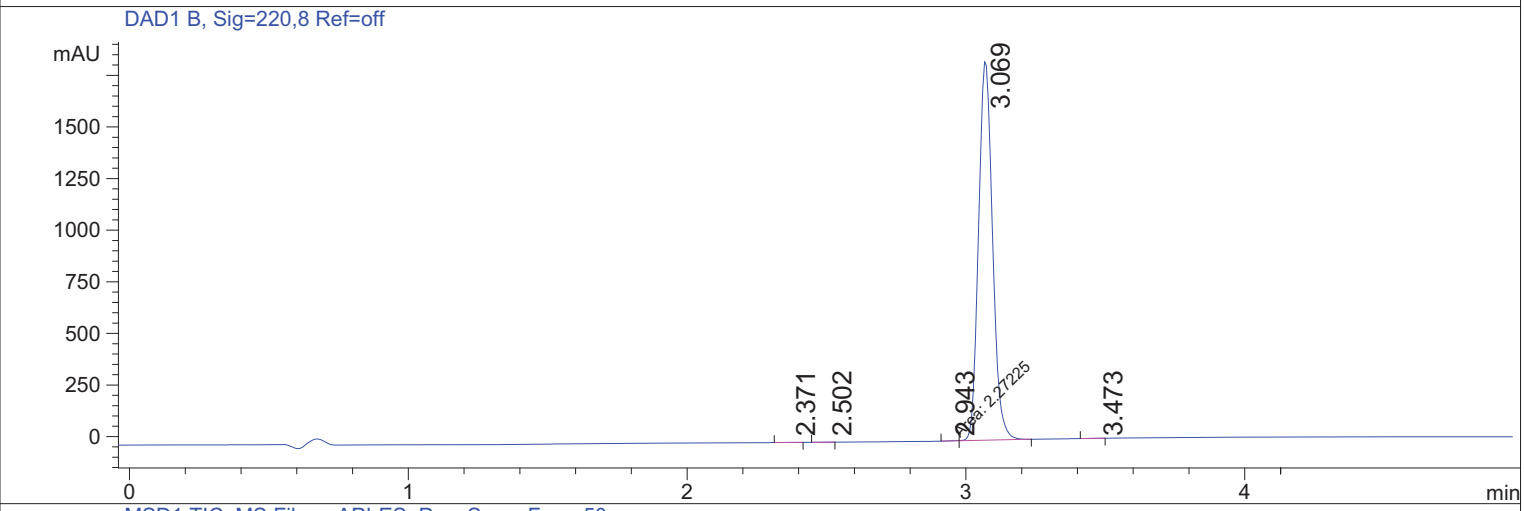
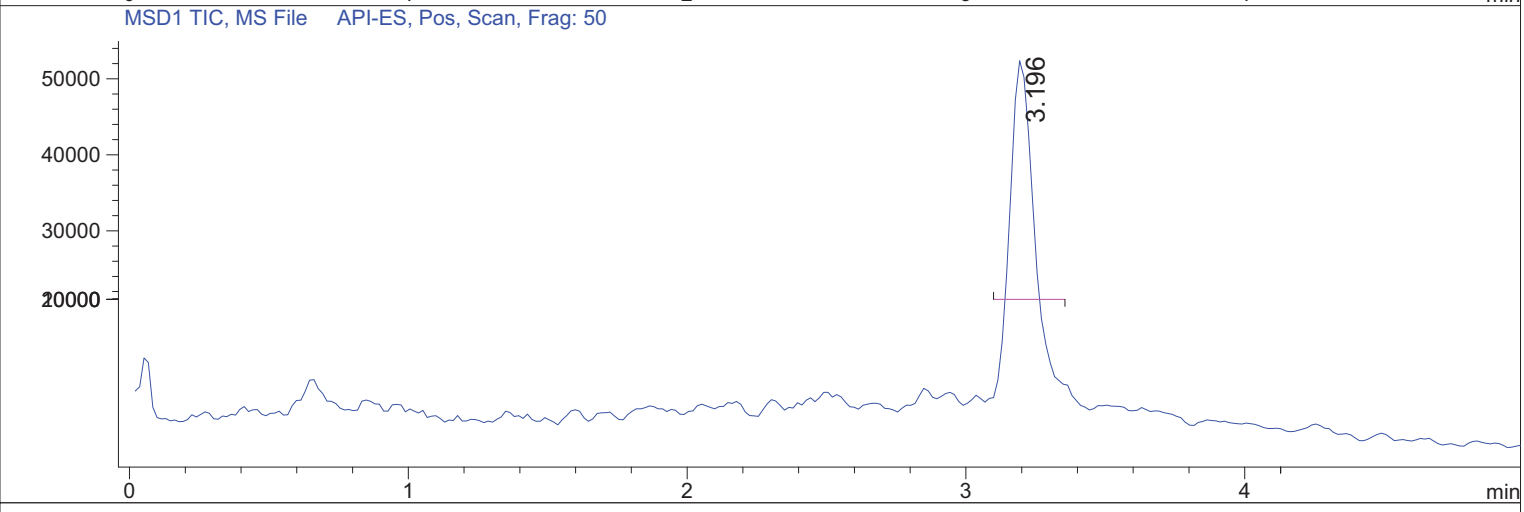


Date:
9 Dec 2013
Document's Title:
Catalog No:CS-1214 Batch#03405
Spectrum Title:
PBL0498-017-P7-CDCL3
Frequency (MHz):
(f1) 400.132
Original Points Count:
(f1) 24670

Actual Points Count:
(f1) 65536
Acquisition Time (sec):
(f1) 2.9999
Spectral Width (ppm):
(f1) 20.552
Pulse Program:
ZG30
Temperature:
293.96
Number of Scans:
17

Lot Number	: **PBL0498-017-P7**	**Location**	: **Vial 35**
Injection Date	: **09-Dec-13, 15:07:03**	**Seq. Line**	: **51**
Acq. Operator	:	**Inj Volume**	: **3 ul**
Acq. Method	: **E:\METHODS\METHODS\20101020\3-9A.M**		
Analysis Method	: **E:\METHODS\METHODS\20101020\80ACN10.M**		
Catalog No	: **CS-1214 Batch#03405**		
Test Type	:		





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

RetTime	Width	Area	Height	Area%	MSBase(+)
2.37	0.05	2.84	0.87	0.04	60.1
2.50	0.05	1.70	0.52	0.03	60.1
2.94	0.04	2.27	0.98	0.04	60.1
3.07	0.06	6404.96	1852.63	99.86	298.1
3.47	0.06	2.10	0.60	0.03	60.1

Ret. Time: 3.20 <<<< POSITIVE SPECTRA >>>>