Supplementary material A

Certificate of Analysis of Sparganin A (cyclo (Tyr-Leu))

Product Name: 04010028241

Sequence: cyclo(YL) (Remark:haid-to-tail cyclization)

Sequence(Three Letters Code): cyclo(Tyr-Leu) (Remark:haid-to-tail cyclization)

Purity: 99.81%

Molecular Weight: 276.35

Solubility: 1mg/ml in 25%ACN/75%H_2O

Test	Specification	Result
Purity:	HPLC	Conforms
	(See attached RP-HPLC chromatogram)	
MS Analysis:	ESI-MS	Conforms
	(See attached MS spectrum)	
Counter Ion:	Trifluoroacetate	Conforms
Appearance:	Lyophilized powder or Crystallization	Conforms

Quality Assurance By: _____ **Position**: _Manager_ **Date**: _2018-11-05_

Important: The peptides can be used for research only. Most of the peptides are lyophilized white or faint yellow powder while fluorescent modified ones have special colors. The state of peptides with strong hydrophilic properties may be crystalline or liquid which does not affect for use. Before experiment, please choose proper solvent for your experiment to dissolve peptides. If peptides cannot be dissolved under harsh conditions, we can carry out feasibility study. Storage conditions:-20ºC, seal, avoid light, dry.

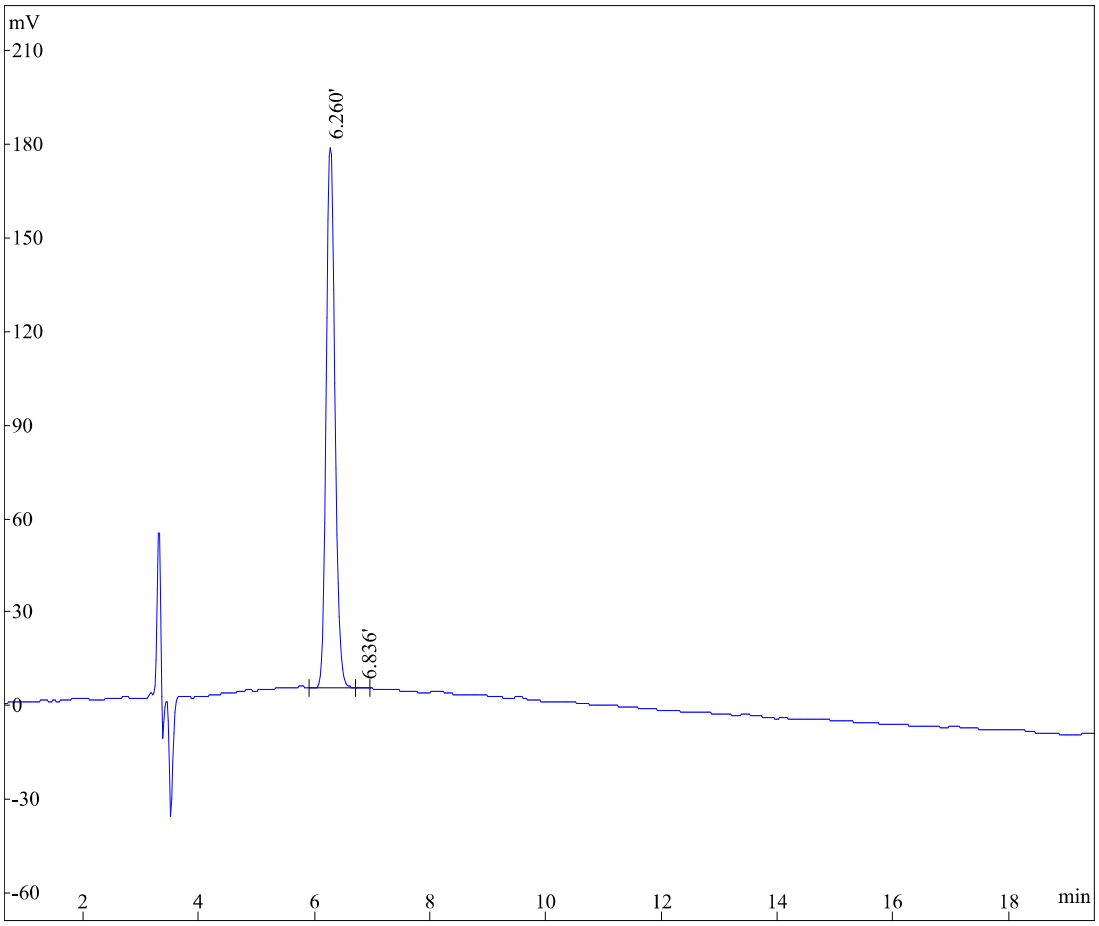
Please test the sample within two weeks after receiving it.

HPLC Analysis Report

Measurement:	Peak Area	Run Time:	20min
Calculation Type:	Percent	Wavelength :	220nm
Flow Rate :	1.0ml/min	Inj.Vol:	10uL
Column:	Kromasil 100-5C18,4.6mmX250mm,5 micron	Column Temp: 25℃	
Buffer A :	0.1%TFA in Acetonitrile	Buffer B:	0.1%TFA in water

Gradient(linear):

	A	B
0.0min	18%	82%
20min	38%	62%
20.1min	100%	0%



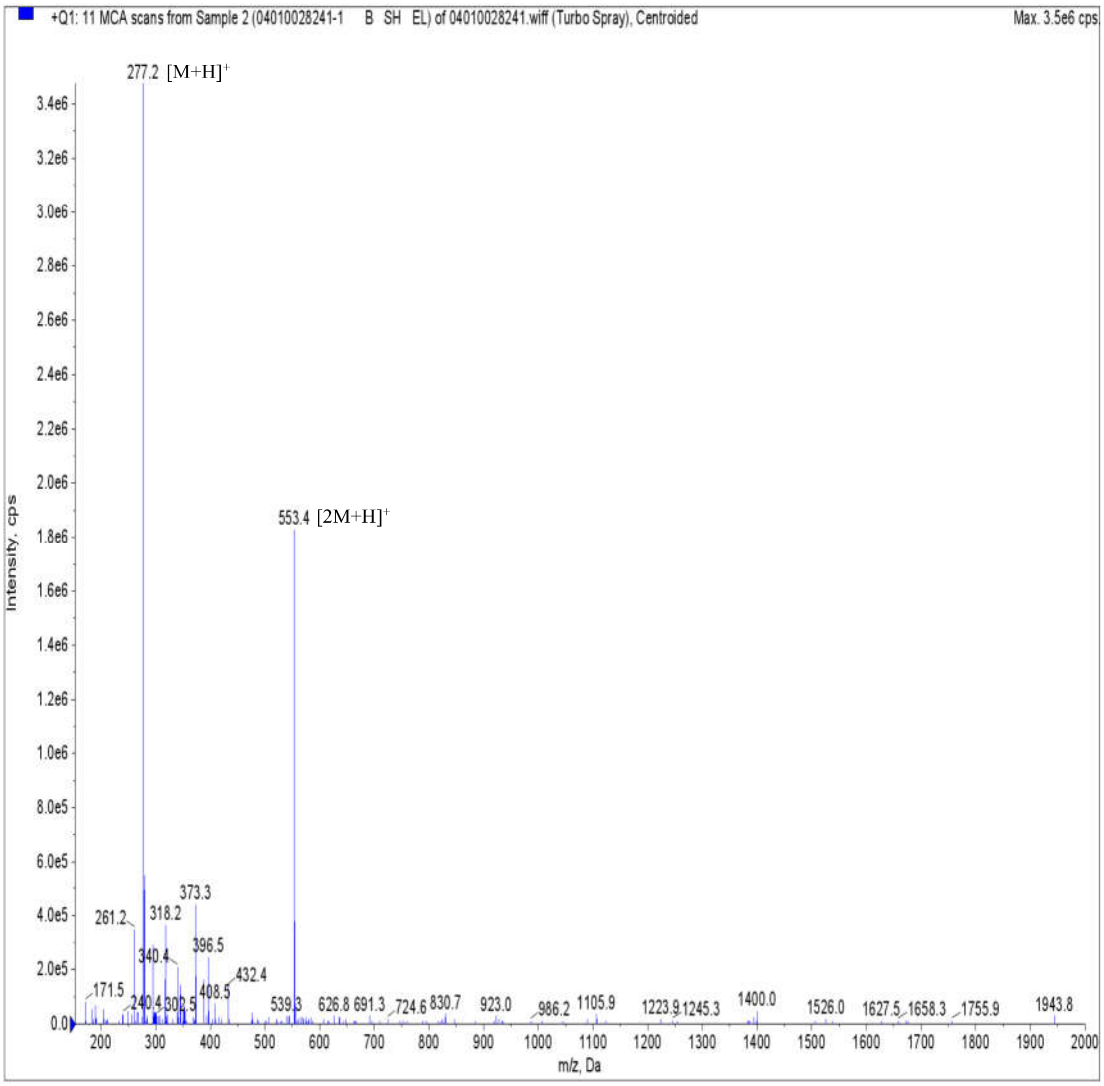
Rank	Time	Name	Conc.	Area
1	6.260		99.81	1632454
2	6.836		0.1886	3084
Total			100	1635538

MS Analysis Report

Ion Source: ESI Nebulizer Gas (NEB): 12.00

Curtain Gas(CUR): 6.00 Ionspray Voltage(IS): ±4500

Temperature(TEM): 0.00 Run Time: 0.5-1min



Supplementary material B

Table The results of molecular docking score of targets with Sparganin A (cyclo(Tyr-Leu))

Gene name	PDB ID	Total score
FLT3	6il3	7.5293
TNF	5yoy	7.2241
PTGS2	5kir	7.1925
SLC23A1	5vnn	6.9739
KLKB1	6O1S	6.9247
CYP2C9	5X23	6.9195
EPO	1eer	6.8649
SERPINC1	4EB1	6.8426
SPP1	3cxd	6.8083
GUCY1A1	4ni2	6.8074
SERPINA1	5NBU	6.8064
ITGB3	6BXJ	6.7364
CRP	4n9h	6.6167
NPPB	3N56	6.5964
P2Y12	4NTJ	6.5699
GP1BA	3p72	6.5262
PROC	3f6u	6.4348
CYP2C19	4gqs	6.3976
ACE	6H5W	6.3549
F7	5pa8	6.3294
F5	6cqn	6.3015
MMP9	6ESM	6.2834
COL4A1	6MPX	6.2226
CSF2	6BFQ	6.1999
CYP3A5	6mjm	6.1655
HGF	5COE	6.1406
AVP	2BN2	6.1207
FUT4	2de0	6.0568
UBIAD1	4tq3	6.0501
IL11	4MHL	6.0427
AGT	6I3F	6.0122
PIP4K2A	2YBX	6.007
F2	6BJR	5.9687
KDR	6GQO	5.9395
MERTK	5u6c	5.9197
OXT	2hnu	5.865
SERPINE1	6I8S	5.8438
VEGFA	6d3o	5.7943
EDNRB	6IGK	5.771
NQO1	6FY4	5.7104
ADAMTS13	3ghm	5.6989
SELP	1g1q	5.6701
PTGER3	6M9T	5.6232
FLT1	5T89	5.5924
REN	6I3F	5.5343
CASP3	6CKZ	5.4785
GAS6	5vxz	5.457
CASP8	5H31	5.444
FOS	1S9K	5.4304
HMOX1	6EHA	5.4048
F10	5vof	5.3568
GNAQ	4ekc	5.3101
PF4	4RAU	5.2821
FGA	5cfa	5.2782
NOS2	5TP6	5.2612
PLAT	5ZLZ	5.2403
PLAU	6NMB	5.2253
CD2	2j7i	5.2194
APP	6HAR	5.2084
ADORA1	6D9H	5.1831
MMP3	4G9L	5.1488
ITGAV	6DJP	4.989
P2RY12	4pxz	4.9312
KLF4	2wbs	4.919
LTF	2PMS	4.8734
MMP2	3AYU	4.8641
POMC	4XNH	4.8473

BCL2L1	6IJQ	4.8461
P2RY1	4XNV	4.7912
HMOX2	5UC8	4.7899
TYRO3	1rhf	4.7412
F9	6mv4	4.6438
F3	2hft	4.5654
APC	5Z8H	4.3996
S100B	5D7F	4.395
CNTF	1CNT	4.378
FCGR2A	3ry4	4.351
BCL2	6GL8	4.2924
VWF	6n29	4.2748
BAX	6EB6	4.0258
EDN1	6DK5	3.986
PDE3A	5K1I	3.9724
ITGA2B	2N9Y	3.633
SIRT1	4ZZH	3.6223
FERMT3	2ys3	3.4687
VKORC1	3kp8	3.2532
THBD	5to3	3.218
PROS1	1Z6C	2.675

Supplementary material C

Figure Sparganin A is bound to residues outside the active pocket of targets