Supporting Information

***Rec. Nat. Prod*. 10:4 (2016) 397-406**

The First Solid-phase Synthesis and Structural Studies on Phakellistatin 15

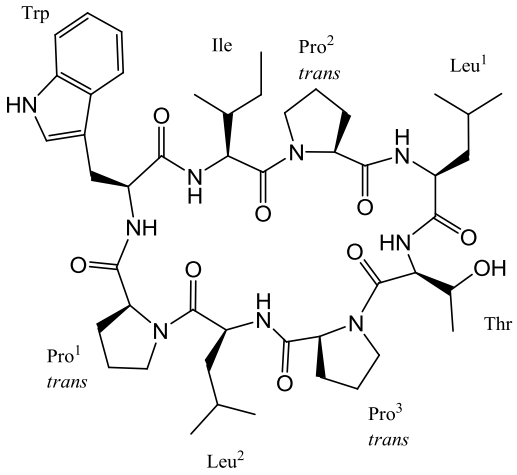
Farzana Shaheen[1*], Muhammad Asad Ziaee[1], Syed Abid Ali[1], Shabana U. Simjee[1,2] Aqeel Ahmed[2] and M. Iqbal Choudhary[1,2,3]

[1]*H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan*

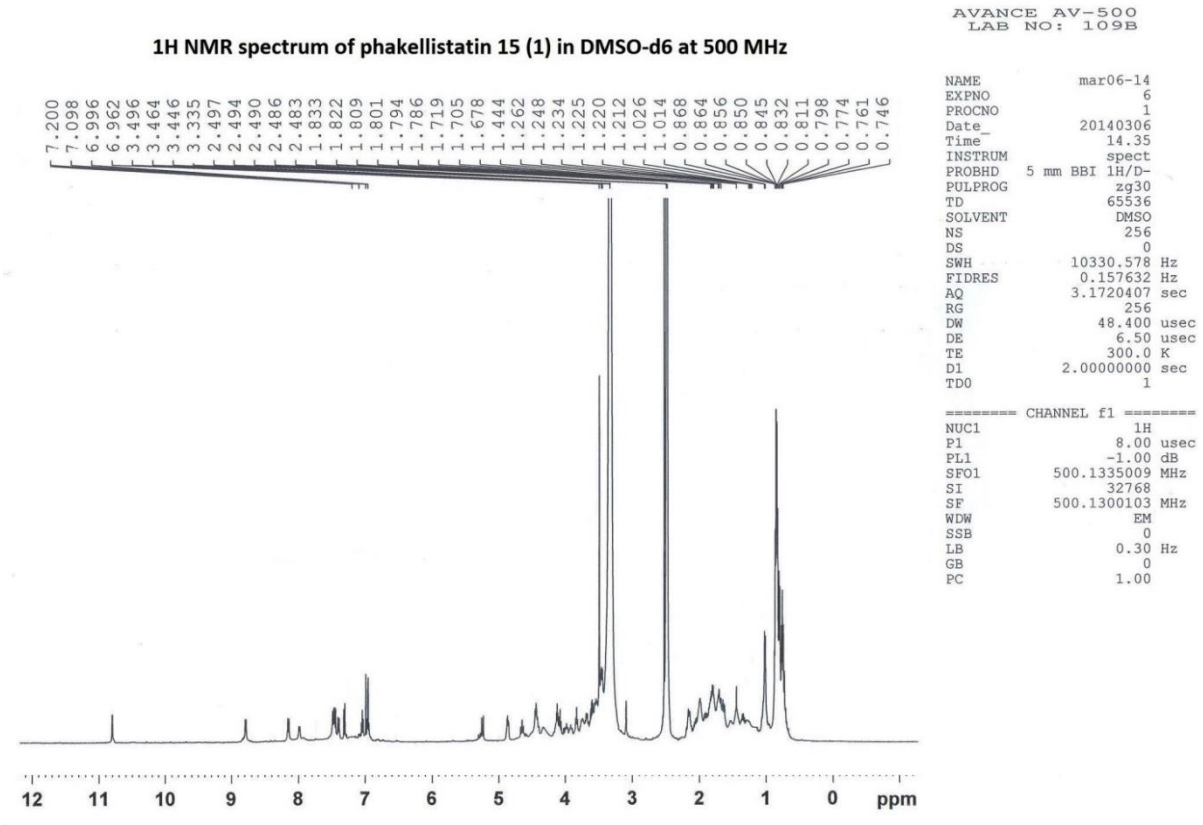
[2]*Dr. Panjwani Center for Molecular Medicine and Drug Research,, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan*

[3]*Department of Biochemistry, Faculty of Science, King Abdulaziz University, Jeddah-21412, Saudi Arabia*

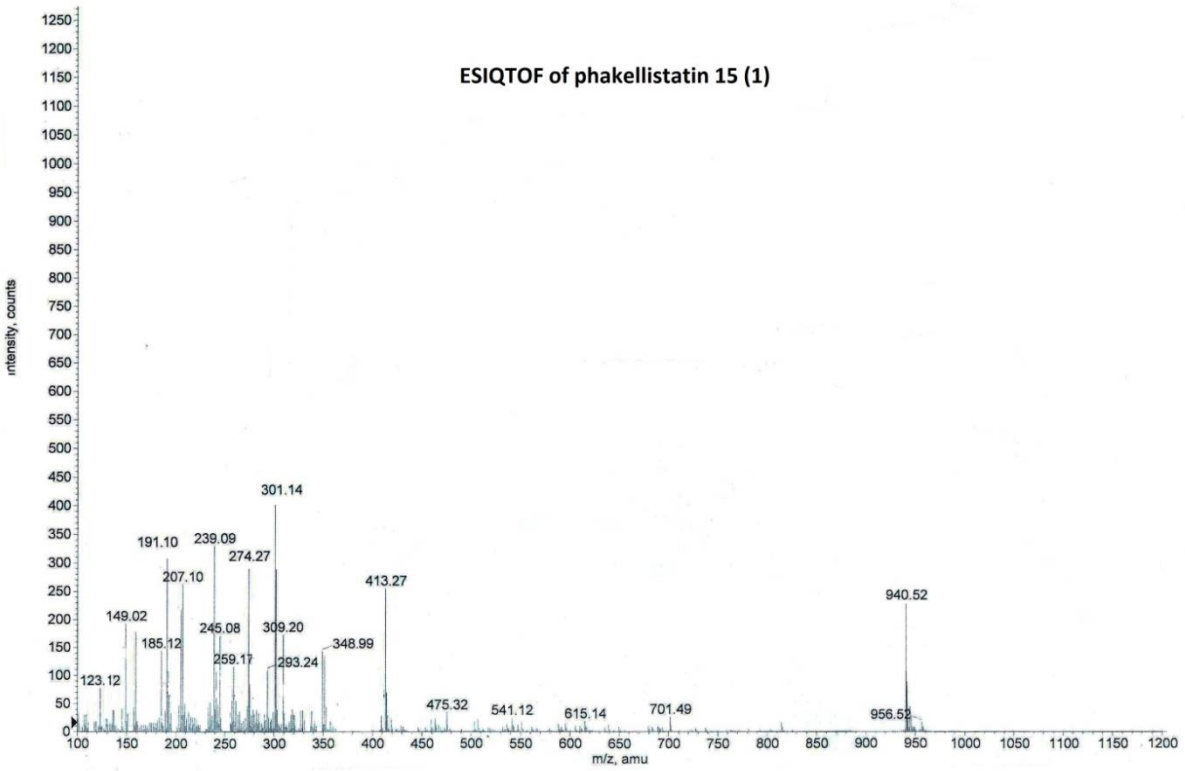
Table of Contents **Page**



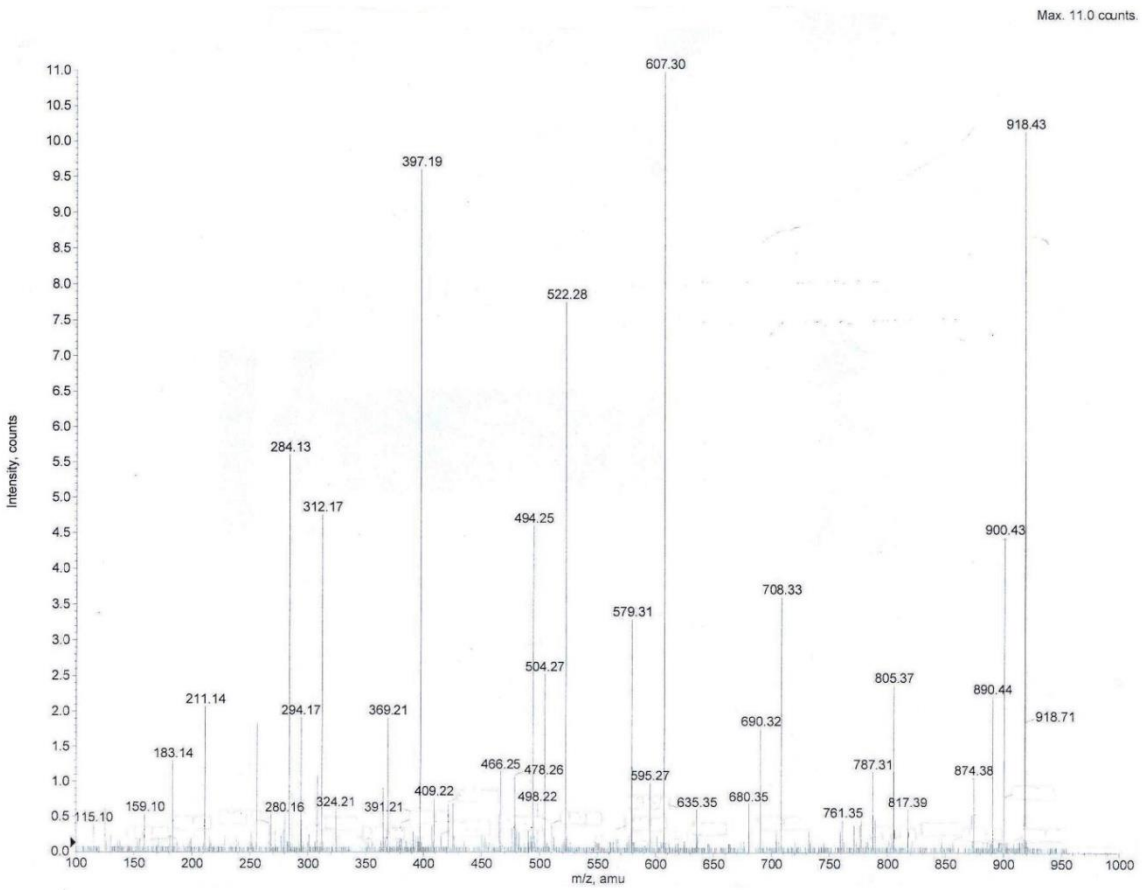
1



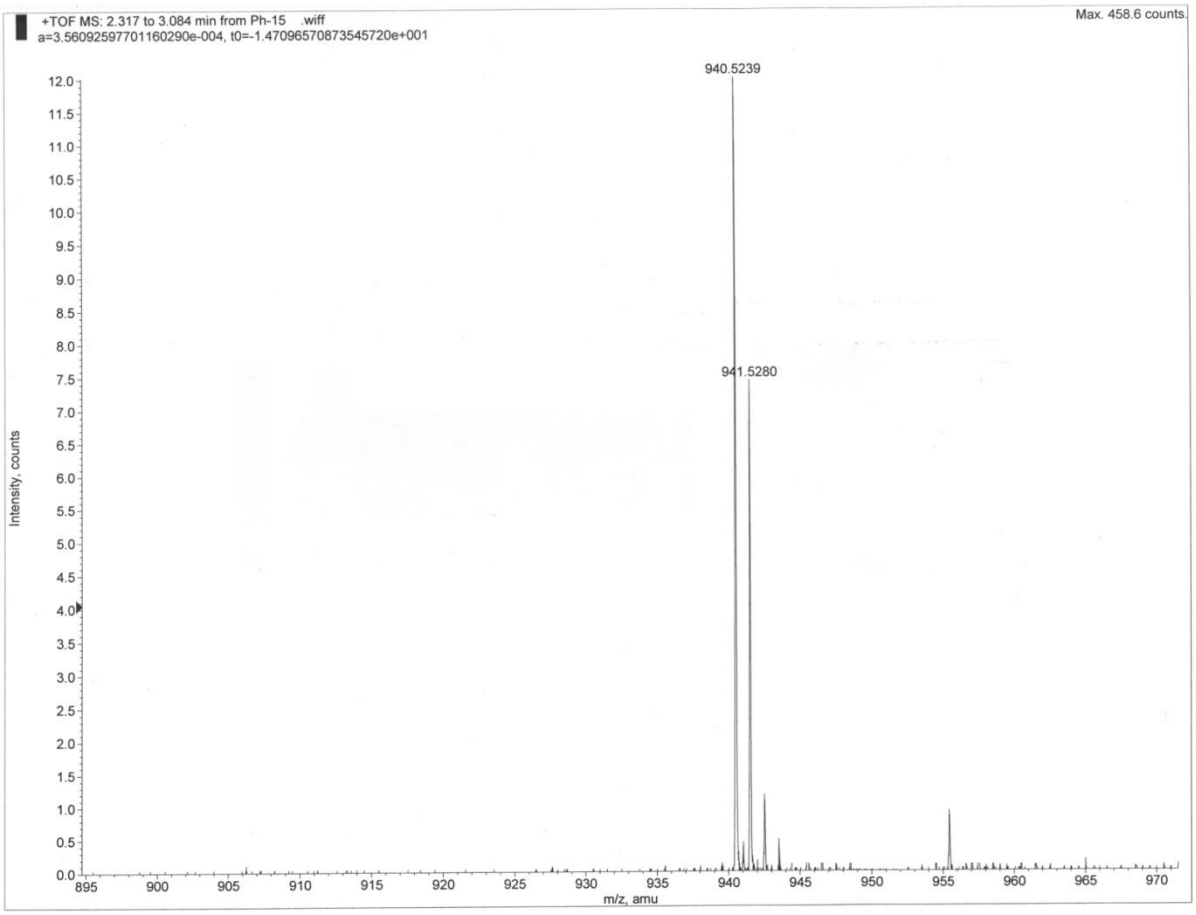
S1: [1]HNMR Spectra of synthetic phakellistatin 15 (**1**)



S2: ESIMS Spectra of synthetic phakellistatin 15 (**1**)



S3: ESIMSMS Spectra of peak 918 of synthetic phakellistatin 15 (**1**)



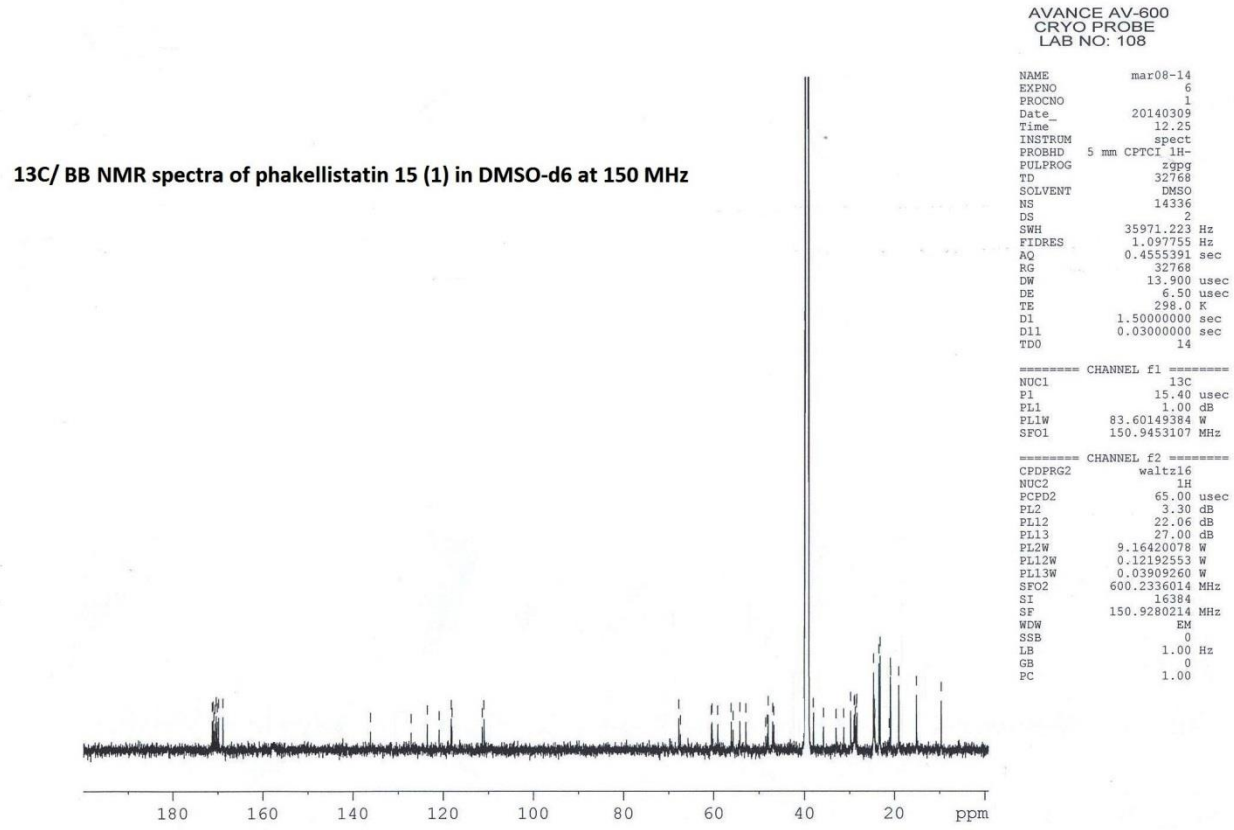
Elemental composition calculator

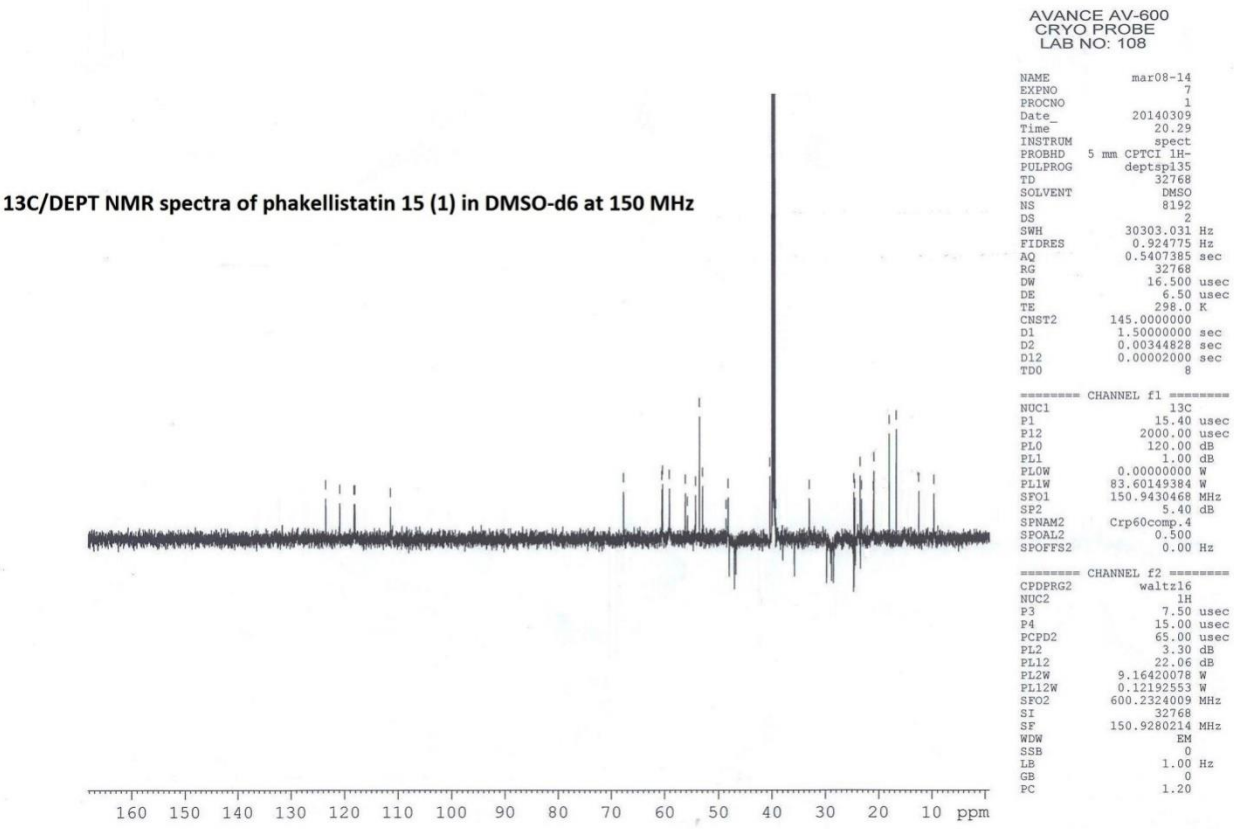
Target m/z: +940.5239 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 100
Min DBE: -0.5000 Max DBE: +50.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: Ph-15 .wiff

	Elements	Min Number	Max Number
1	C	0	50
2	H	0	80
3	N	0	10
4	O	0	10
5	Na	0	1

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C48 H71 N9 O9 Na	940.5272	-3.3453	-3.5569	17.5
2	C50 H73 N6 O10 Na	940.5285	-4.6880	-4.9845	17.0
3	C50 H70 N9 O9	940.5296	-5.7506	-6.1142	20.5
4	C49 H68 N10 O9	940.5170	6.8254	7.2570	21.0
5	C49 H71 N7 O10 Na	940.5160	7.8880	8.3868	17.5
6	C47 H69 N10 O9 Na	940.5146	9.2307	9.8144	18.0

S4:HR-ESIMS Spectra of synthetic phakellistatin 15 (**1**)

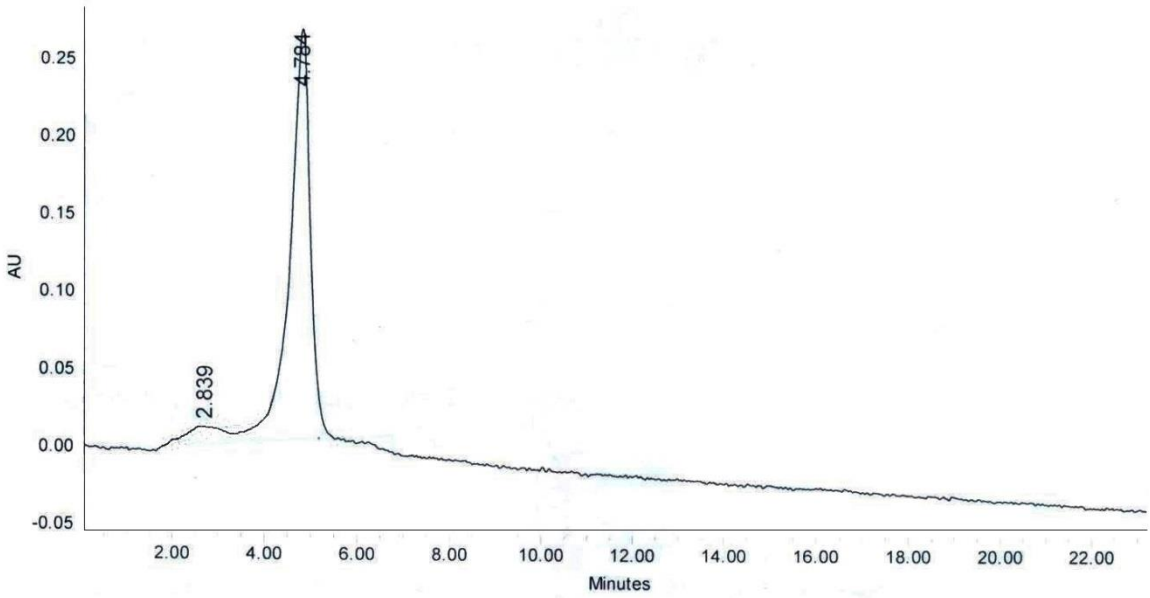




S5: ^{13}C Spectra of synthetic phakellistatin 15 (**1**)

SAMPLE INFORMATION

Sample Name:	Ph-15(iv)	Acquired By:	Maria
Sample Type:	Unknow n	Date Acquired:	8/13/2014 11:26:10 AM
Vial:	1	Acq. Method Set:	ASAD
Injection #:	1	Date Processed:	8/13/2014 12:24:17 PM
Injection Volume:	100.00 ul	Processing Method:	Default
Run Time:	40.0 Minutes	Channel Name:	WvIn Ch1
Sample Set Name:		Proc. Chnl. Descr.:	PDA 282.0 nm



Processed Channel: PDA 282.0 nm

	Processed Channel	Retention Time (min)	Area	% Area	Height
1	PDA 282.0 nm	2.839	268667	3.66	13830
2	PDA 282.0 nm	4.784	7067404	96.34	256522

S6: HPLC Profile of synthetic phakellistatin 15 (**1**)