

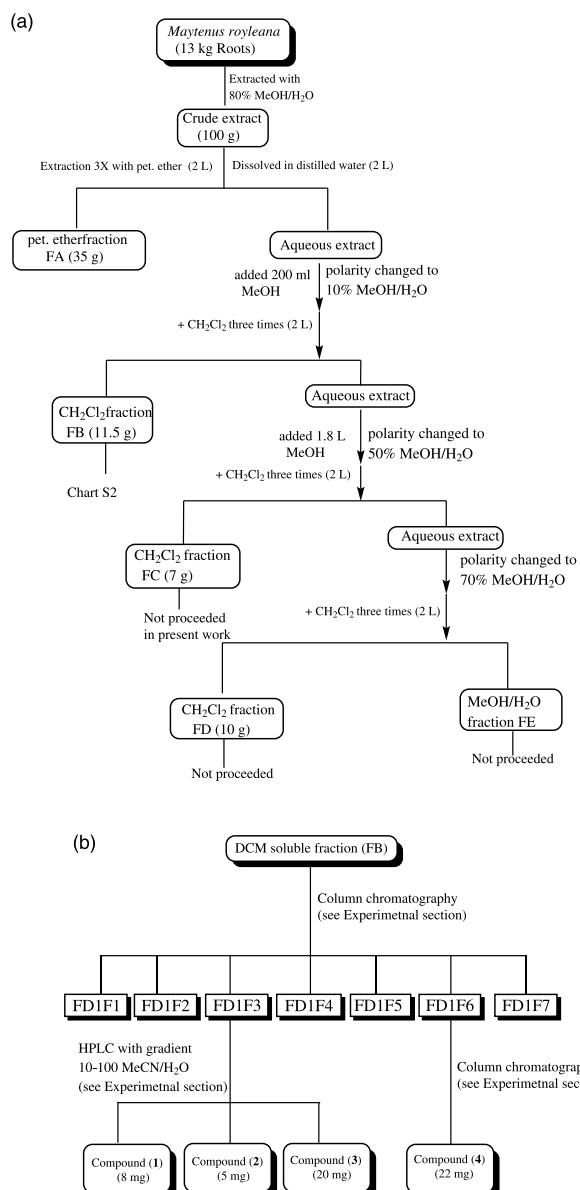
# Supplementary Information

## Ficusonic Acid: a New Cytotoxic Triterpene Isolated from *Maytenus royleanus* (Wall. ex M. A. Lawson) Cufodontis

**Ala Ud Din,\*<sup>a</sup> Ghias Uddin,<sup>a</sup> Nusrat Hussain<sup>b</sup> and Mohammad Iqbal Choudary<sup>b</sup>**

<sup>a</sup>*Center for Phytomedicine and Medicinal Organic Chemistry, Institute of Chemical Sciences,  
 University of Peshawar, Peshawar-25120, Pakistan*

<sup>b</sup>*International Center for Chemical and Biological Sciences, HEJ Research Institute of Chemistry,  
 University of Karachi, Karachi-75270, Pakistan*



**Figure S1.** Extraction (a) and isolation (b) schemes of *Maytenus royleanus*.

\*e-mail: allauddin77@yahoo.com

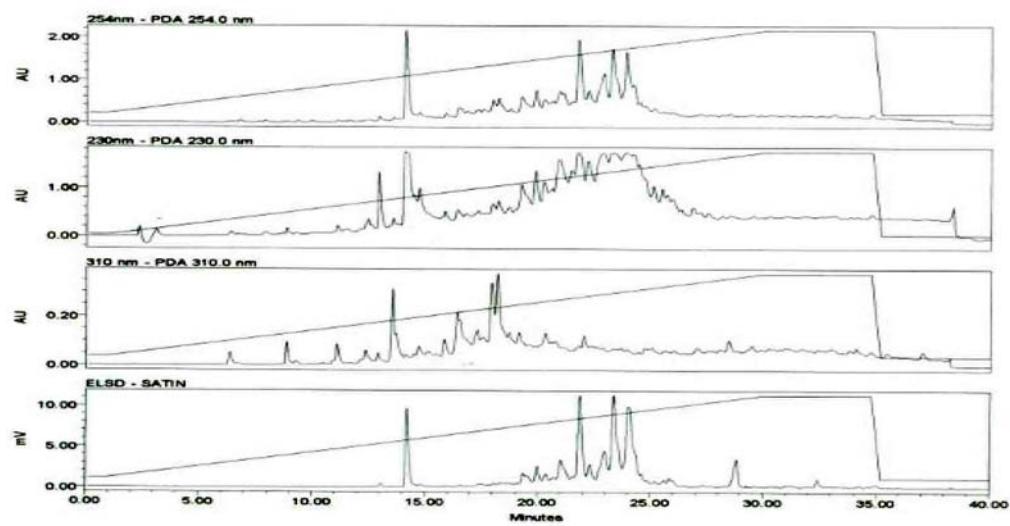


Figure S2. LCMS profile of fraction FB (MR7FD).

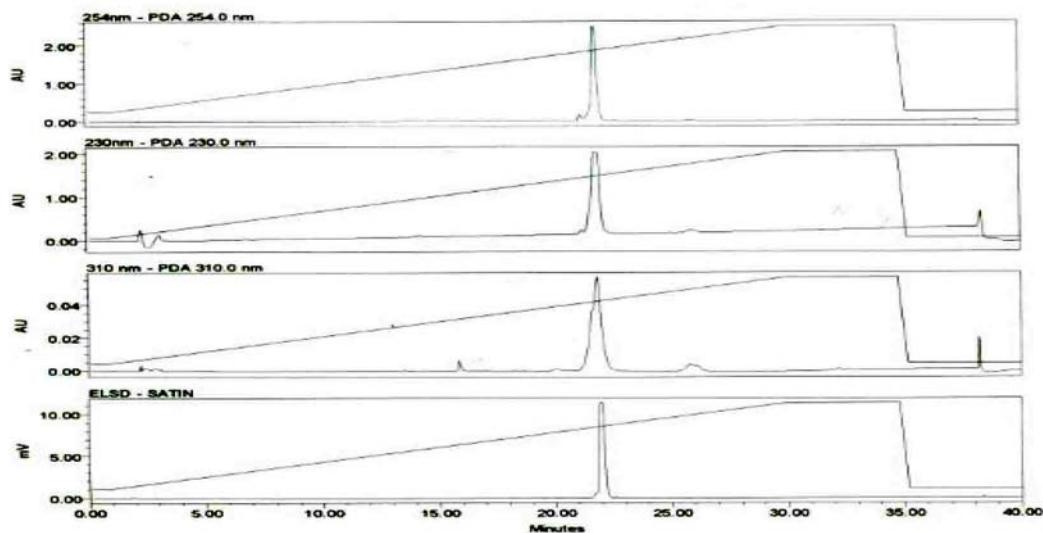
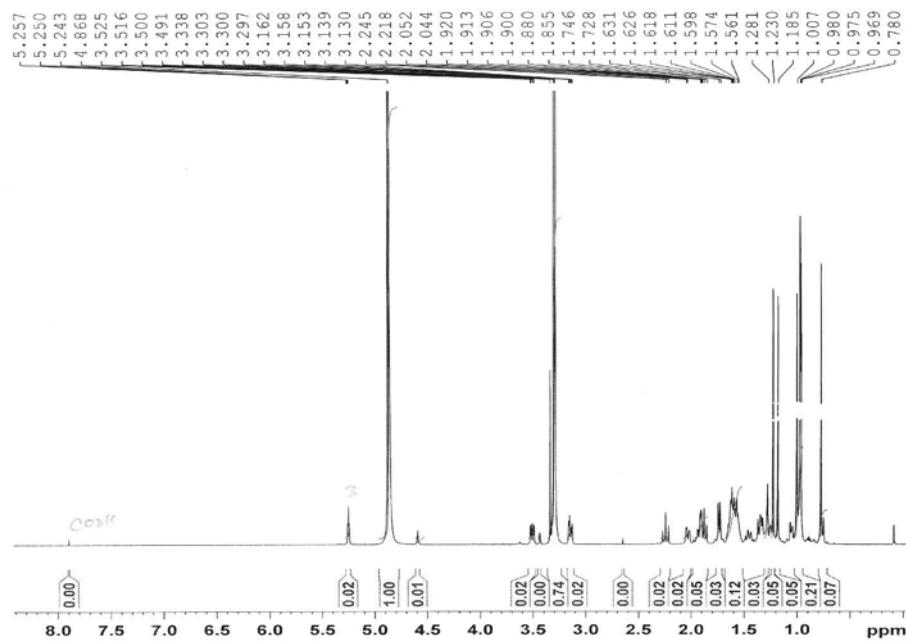
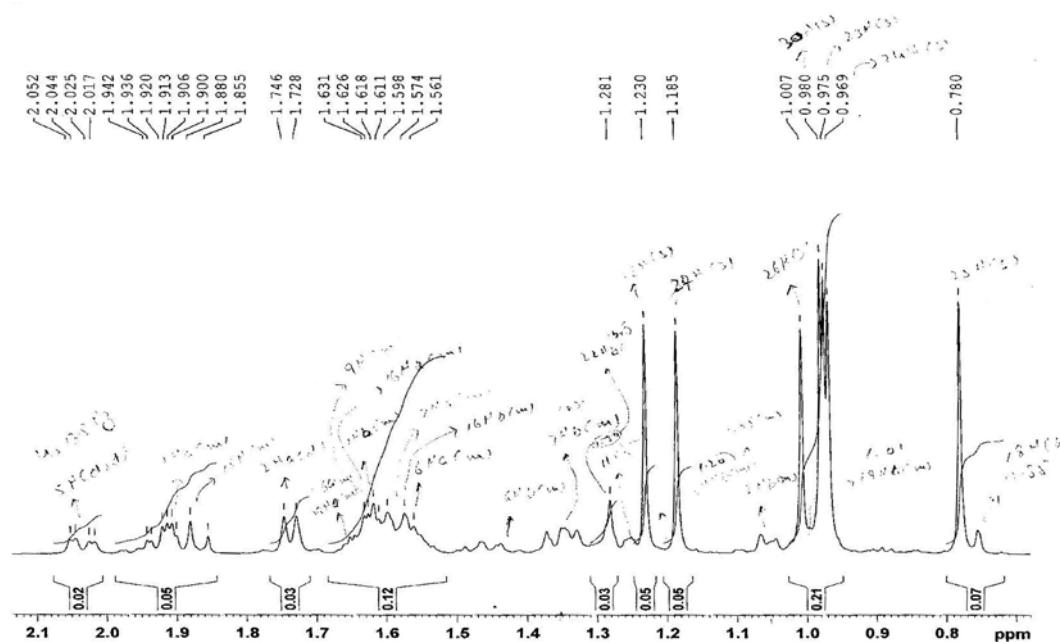
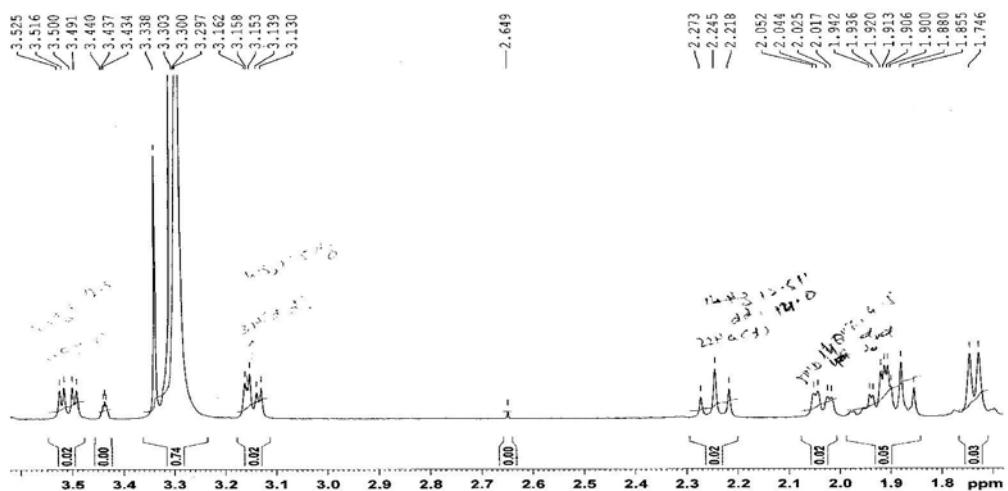
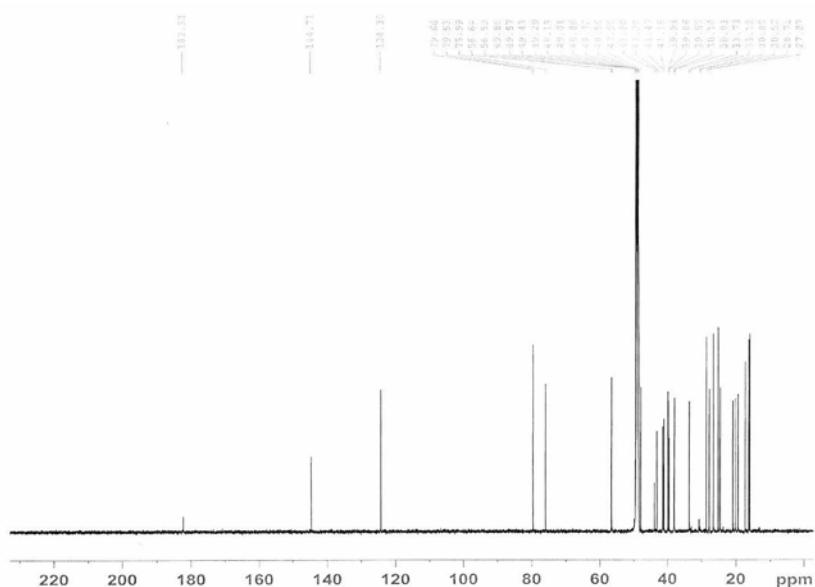


Figure S3. The LCMS data of compound 1.

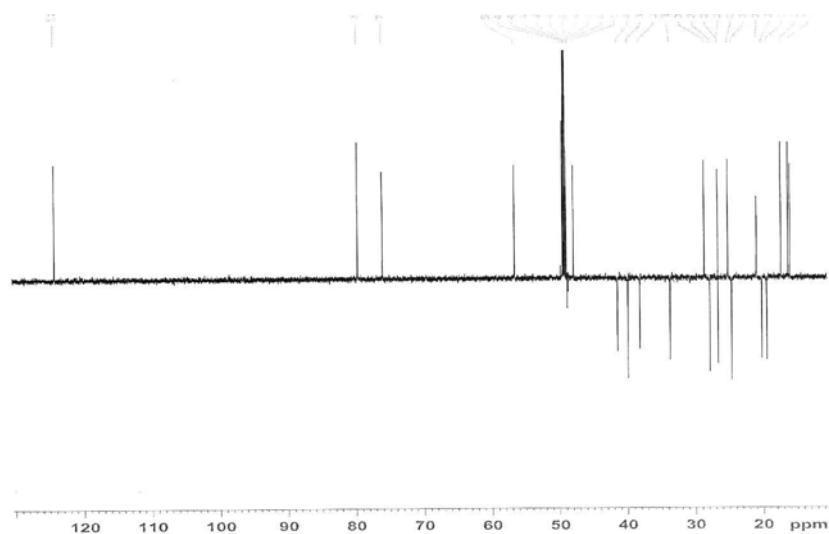
**Figure S4.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**.**Figure S5.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**.



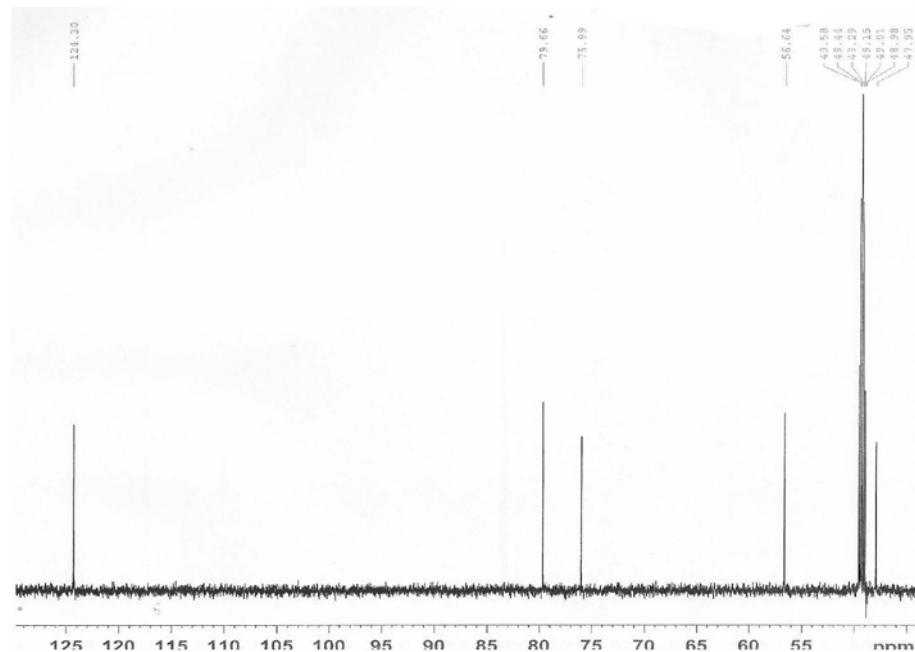
**Figure S6.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**.



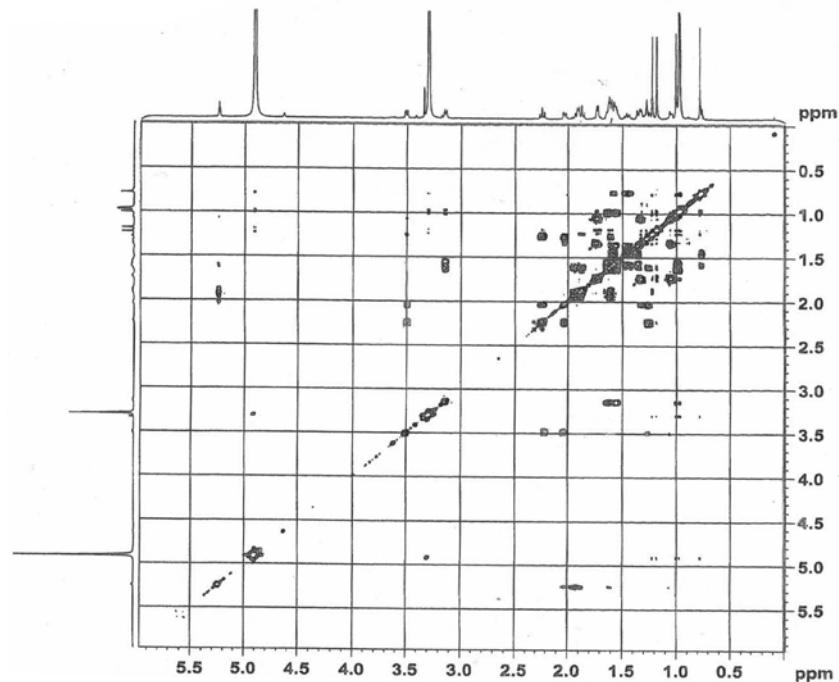
**Figure S7.**  $^{13}\text{C}$  NMR spectrum (125MHz,  $\text{CD}_3\text{OD}$ ) of compound 1.



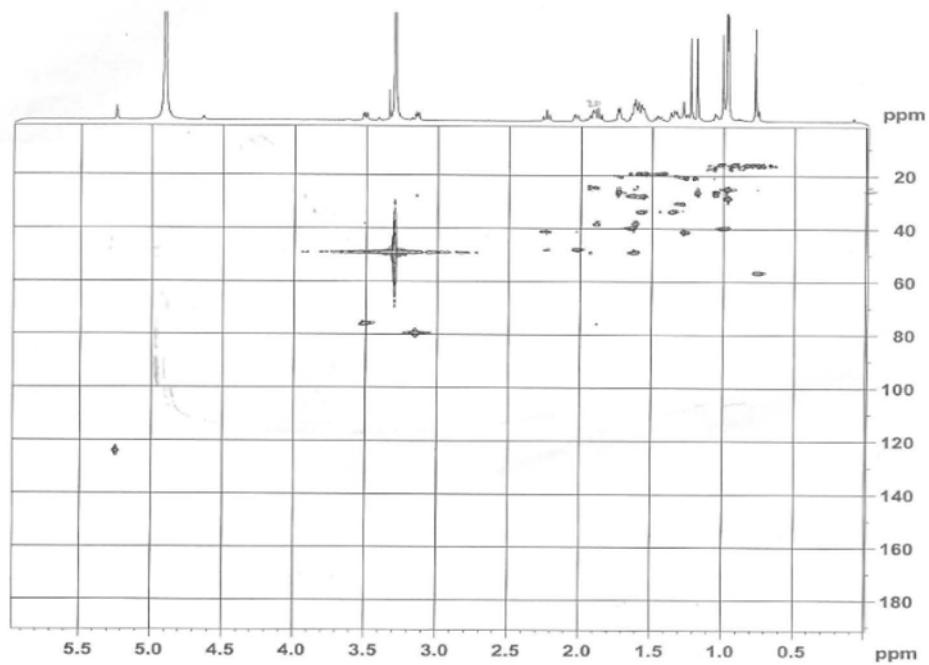
**Figure S8.**  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ ) of compound 1.



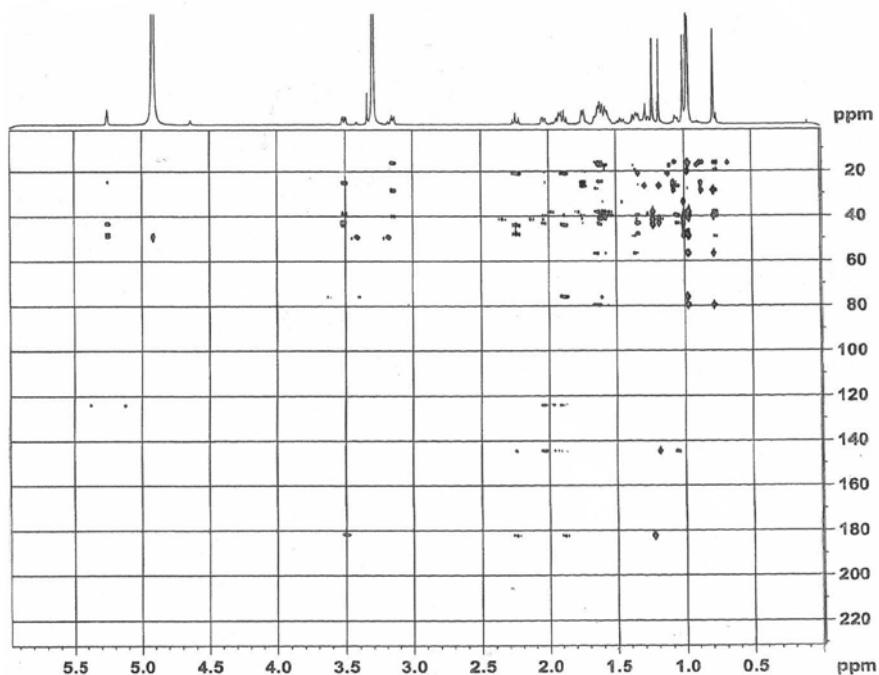
**Figure S9.**  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ ) of compound 1.



**Figure S10.** gCOSY spectrum ( $\text{CD}_3\text{OD}$ ) of compound **1**.



**Figure S11.** HMQC ( $\text{CD}_3\text{OD}$ ) spectrum of compound **1**.

**Figure S12.** gHMBC spectrum ( $\text{CD}_3\text{OD}$ ) of compound 1.

[Data Information]  
Creation Date 5/21/2011 9:39 AM

[Measurement Information]  
Instrument Name Polarimeter  
Model Name P-2000  
Serial No. a060061232  
Polarizer Glan-Taylor Prism  
Faraday Cell Quartz  
Accessory RSC-200  
Accessory S/N B044761260

Light Source WI  
Monitor wavelength 589 nm  
D.I.T. 5 sec  
No. of cycle 1  
Cycle interval 0 sec  
Temp. Monitor Cell  
Temp. Corr. Factor None  
Aperture(S) 8.0mm  
Aperture(L) Auto  
Mode Optical Rotation  
Factor 1

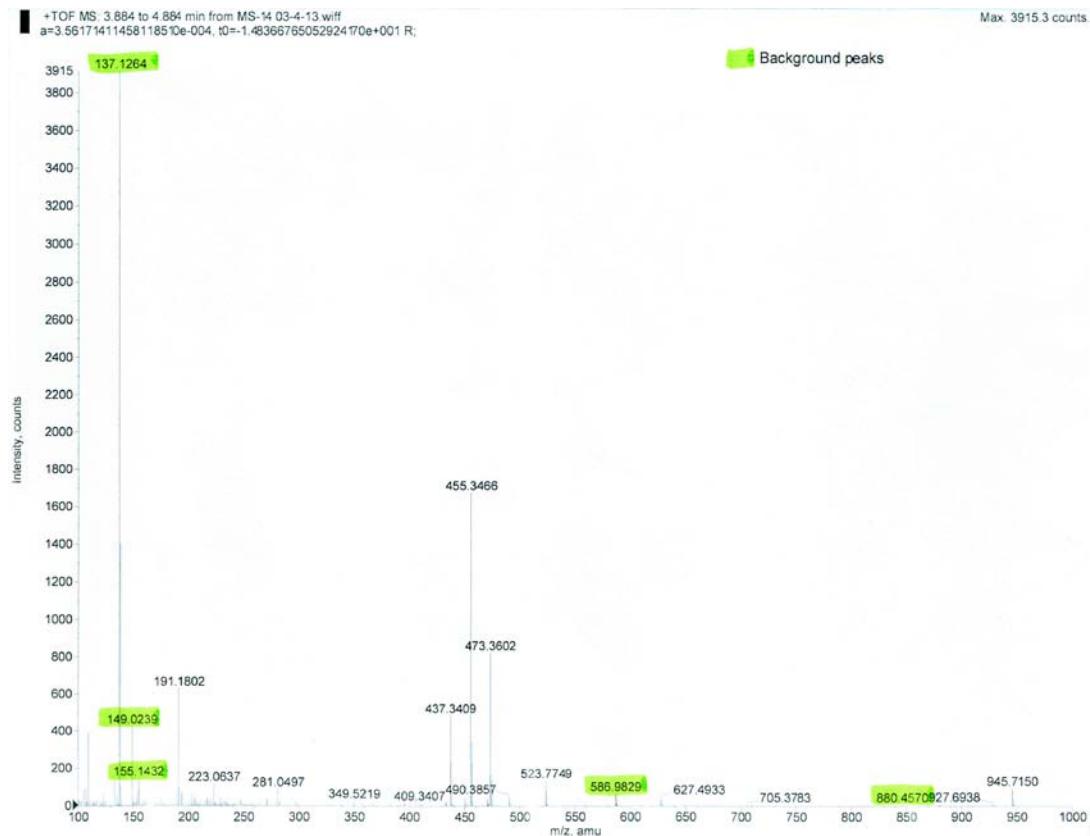
$\text{MR7FD} = \alpha_D^{29.7} = -115$

$\text{MR7FD} = \beta_D^{29.7} = -76$

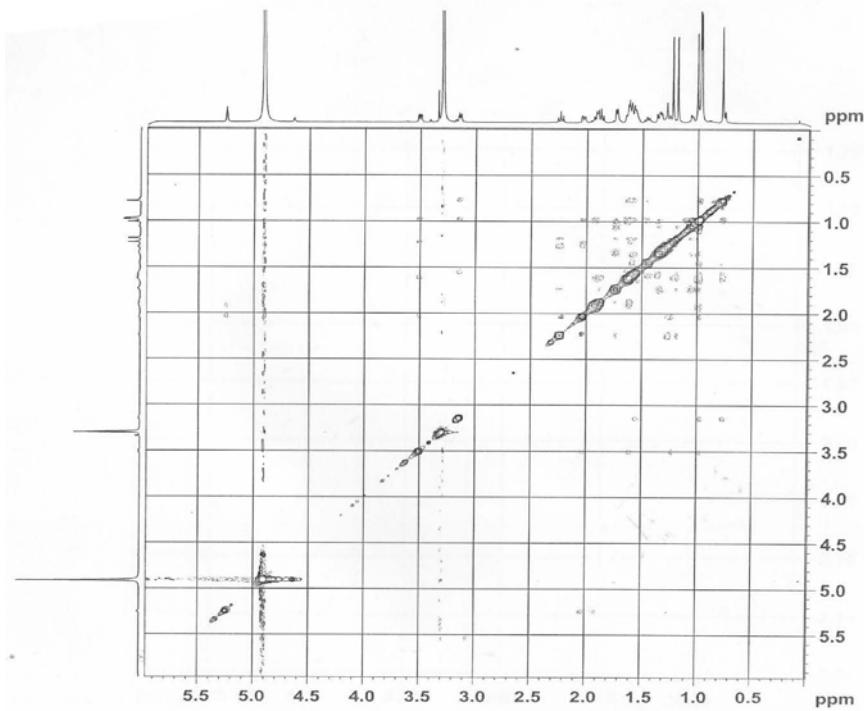
No.	Sample Name	Measurement Date	PMT Voltage[V]	Temperature[C]	Optical Rotation Monitor	Optical Rotation[deg]	Comment
1	Blank	5/21/2011 9:34 AM	211	29.67	-0.3068		
2	MR7FD-2A <sup>+</sup>	5/21/2011 9:36 AM	212	29.70	-0.3172	-0.0104	Alauddin
3	MR7FD-2A	5/21/2011 9:36 AM	215	29.71	-0.3166	-0.0098	Alauddin
4	MR7FD-2A	5/21/2011 9:36 AM	212	29.72	-0.3160	-0.0092	Alauddin
5	MR7FD-2A	5/21/2011 9:36 AM	211	29.72	-0.3165	-0.0097	Alauddin
6	MR7FD-B	5/21/2011 9:38 AM	209	29.73	-0.3190	-0.0122	Alauddin
7	MR7FD-B	5/21/2011 9:38 AM	210	29.74	-0.3187	-0.0119	Alauddin
8	MR7FD-B	5/21/2011 9:39 AM	212	29.75	-0.3154	-0.0086	Alauddin
9	MR7FD-B	5/21/2011 9:39 AM	209	29.76	-0.3111	-0.0043	Alauddin
10	MR7FD-B	5/21/2011 9:39 AM	212	29.77	-0.3128	-0.0060	Alauddin
11	MR7FD-B	5/21/2011 9:39 AM	211	29.78	-0.3111	-0.0043	Alauddin

Path length = 10mm  
vol = 2 ml

**Figure S13.** Optical rotation data of compound 1.



**Figure S14.** HRESI-MS (+ve) data of compound **1**.



**Figure S15.** gNOESY spectrum ( $\text{CD}_3\text{OD}$ ) of compound **1**.




  
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**AND**  
**DR. PANJWANI CENTER FOR MOLECULAR MEDICINE AND DRUG RESEARCH**  
**THIRD WORLD CENTER**  
**UNIVERSITY OF KARACHI**

**RESULTS OF IMMUNOMODULATORY/CYTOTOXICITY STUDIES**

Date: 1-2-12

Submitted By: D.I. Alauddin.....Lab. No/intercom No:.....

Name of Supervisor:..... Institution: H.E.J. UOK.....

Name of Assay: Anticancer Assay..... Amount Used (mg):.....

Proposed Implications of the Immunomodulatory/Cytotoxicity Activity:.....

Sample Code	Conc. (mg/ml)	% Inhibition/Stimulation	$IC_{50 \pm SD}$ ( $\mu M$ )
MR-5			35.613 ± 0.23
MR-6			34.46 ± 0.01
MR-13			10.212 ± 0.25
MR-TED-2A			35.612 ± 0.48
Doxorubicin (AS Standard)			0.912 ± 0.12

Remarks: All the compound shows weak cytotoxic effect towards prostate cancer cell line (PC-3).

.....Saminia.....  
Evaluated By \_\_\_\_\_

Section Incharge \_\_\_\_\_

Note: These studies are done on collaborative basis; both collaborators will share data for relevant publication.

**Figure S16.** Cytotoxic activity (PC-3) of compound 1.




  
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Date: 1-2-12

Submitted By: D.I. Alauddin.....Lab. No/intercom No:.....

Name of Supervisor:..... Institution: H.E.J. UOK.....

Name of Assay: Anticancer Assay..... Amount Used (mg):.....

Proposed Implications of the Immunomodulatory/Cytotoxicity Activity:.....

Sample Code	Conc. (mg/ml)	% Inhibition/Stimulation	$IC_{50 \pm SD}$ ( $\mu M$ )
MR-5			32.64 ± 0.30
MR-6			22.60 ± 0.41
MR-13			34.29 ± 0.39
MR-TED-2A			20.47 ± 0.01
Doxorubicin (AS Standard)			3.10 ± 0.20

Remarks: Compounds codes no. MR-5 and MR-TED-2A shows moderate cytotoxic effect toward S. cervix (C3) cancer cell line (HeLa).

.....Saminia.....  
Evaluated By \_\_\_\_\_

Section Incharge \_\_\_\_\_

Note: These studies are done on collaborative basis; both collaborators will share data for relevant publication.

**Figure S17.** Cytotoxic activity (HeLa) of compound 1.