

# Cytotoxic Effects of Pinnatane A Extracted from *Walsura pinnata* (Meliaceae) on Human Liver Cancer Cells

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**Table S1:** <sup>1</sup>H (600 MHz) and <sup>13</sup>C (150 MHz) Nuclear Magnetic Resonance (NMR) data of pinnatane A in CDCl<sub>3</sub>.

Position	Pinnatane A		3 $\beta$ -hydroxy-5-glutinen-28-oic acid (Elfita <i>et al.</i> , 2009)	
	$\delta_H$ (ppm), <i>J</i> (Hz)	$\delta_C$ (ppm)	$\delta_H$ (ppm), <i>J</i> (Hz)	$\delta_C$ (ppm)
1	1.45, <i>m</i>	18.3	1.44	18.3
	1.50, <i>m</i>		1.52	
2	1.67, <i>m</i>	27.8	1.67	27.8
	1.85, <i>m</i>		1.82	
3	3.47, <i>dd</i> (3.2, 2.3)	76.3	3.45, <i>br s</i>	76.3
4	-	40.8	-	40.8
5	-	141.6	-	141.5
6	5.64, <i>d</i> (5.8)	121.7	5.6	121.7
7	1.77, <i>m</i>	23.5	1.75	23.4
	1.95, <i>m</i>		1.95	
8	1.52, <i>m</i>	47.7	1.5	47.7
9	-	35.1	-	35.1
10	2.00, <i>m</i>	49.4	1.98	49.9
11	1.36, <i>m</i>	34.5	1.36	34.5
	1.53		1.51	
12	1.39, <i>m</i>	30.9	1.35	30.9
	1.47, <i>m</i>		1.45	
13	-	38.7	-	38.6
14	-	37.2	-	37.1
15	1.21, <i>m</i>	32.5	1.2	32.4
	1.25, <i>m</i>			
16	1.50, <i>m</i>	35.8	1.48	35.8
17	-	44.7	-	44.7
18	2.43, <i>dd</i> (13.2, 4.5)	37.8	2.37, <i>dd</i> (13.1, 3.8)	37.7
19	1.17, <i>m</i>	34.9	1.14	34.8
	1.31, <i>m</i>		1.29	
20	-	28.5	-	28.5
21	1.47, <i>m</i>	32.8	1.46	32.8
22	1.67, <i>m</i>	29.4	1.65	29.5
	2.29, <i>dd</i> (14.9, 9.7)		2.29, <i>dd</i> (14.7, 9.5)	
23	1.04, <i>s</i>	28.9	1.01, <i>s</i>	28.9
24	1.14, <i>s</i>	25.4	1.12, <i>s</i>	25.4
25	0.82, <i>s</i>	15.6	0.80, <i>s</i>	15.6
26	0.93, <i>s</i>	20.3	0.89, <i>s</i>	20.3
27	1.04, <i>s</i>	18.2	0.96, <i>s</i>	18.2
28	-	182.6	-	184.8
29	0.98, <i>s</i>	34.3	0.91, <i>s</i>	34.3
30	0.94, <i>s</i>	29.8	1.01, <i>s</i>	29.7

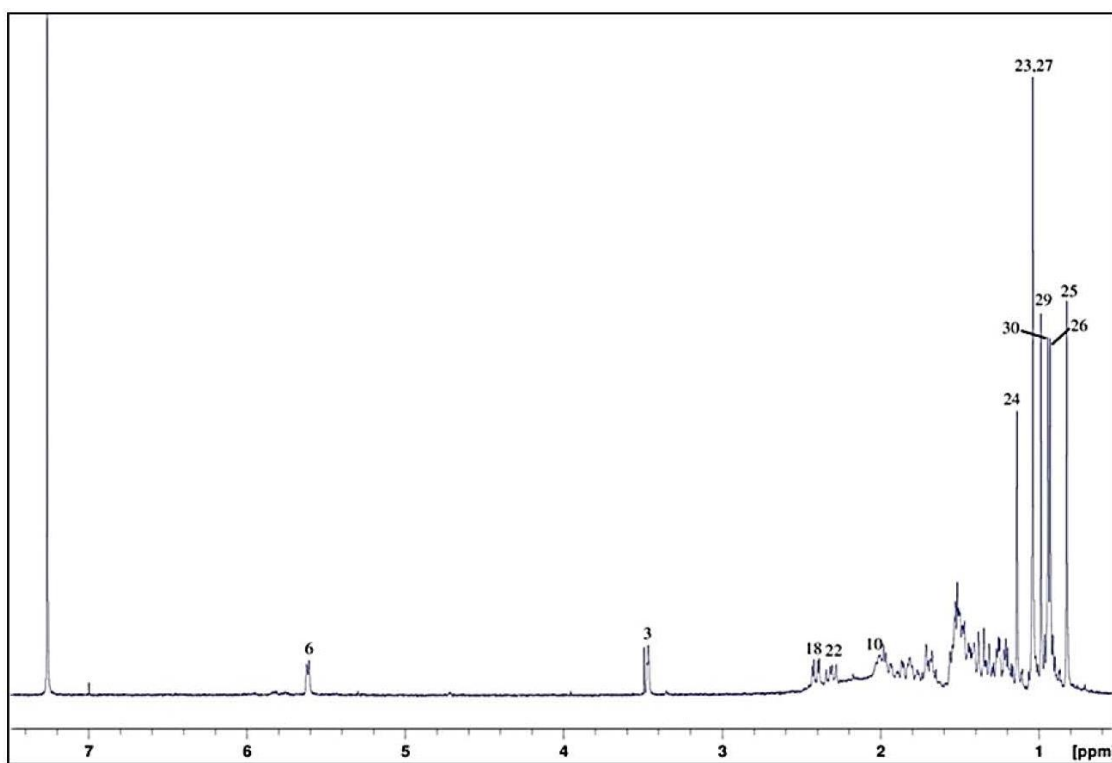


Figure S1:  $^1\text{H}$  (600 MHz) NMR spectrum of pinnatane A.

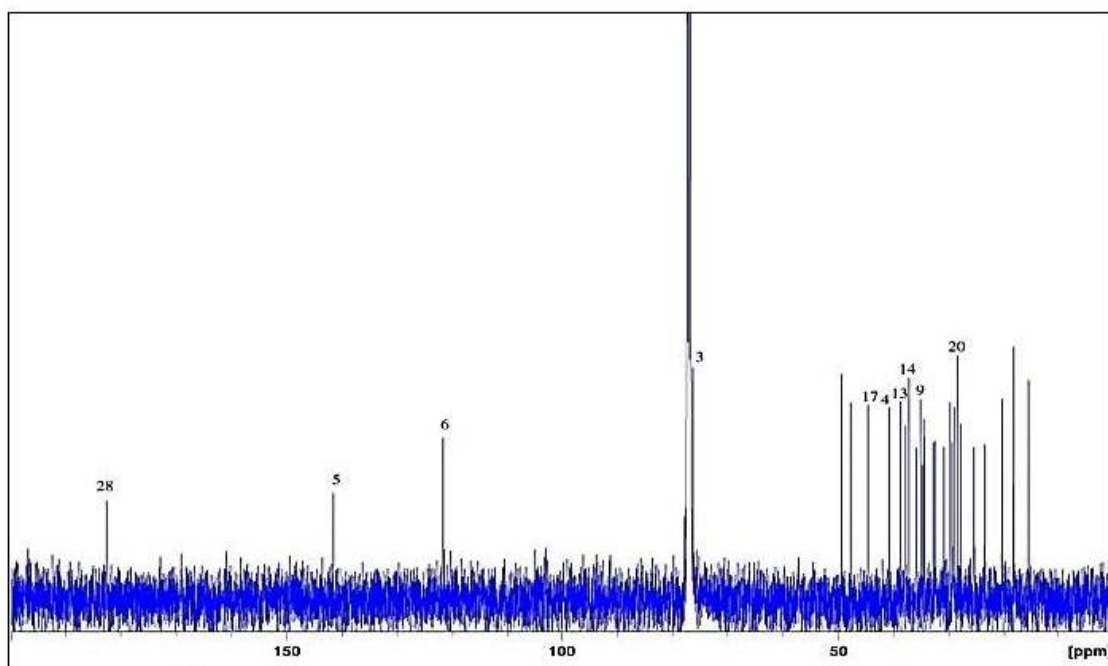
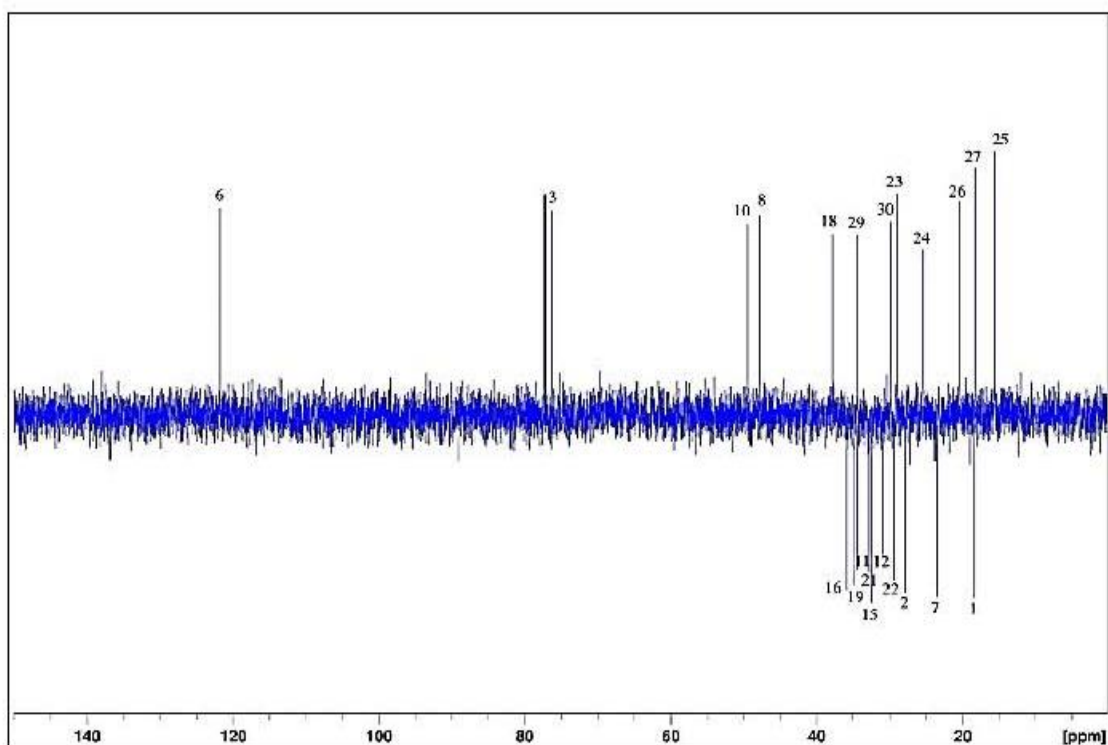
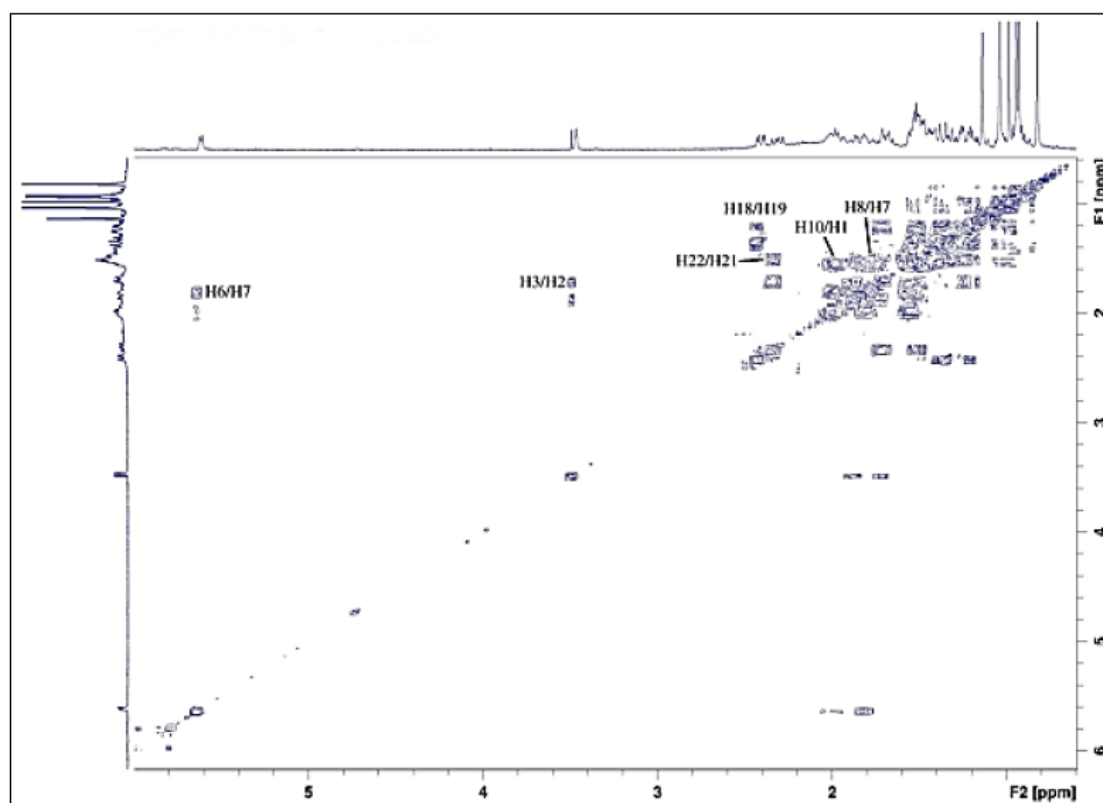


Figure S2:  $^{13}\text{C}$  (150 MHz) NMR spectrum of pinnatane A.



**Figure S3:** Distortionless enhancement by polarization transfer -135 (DEPT-135) spectrum of pinnatane A.



**Figure S4** Homonuclear correlation spectroscopy (COSY) spectrum of pinnatane A.

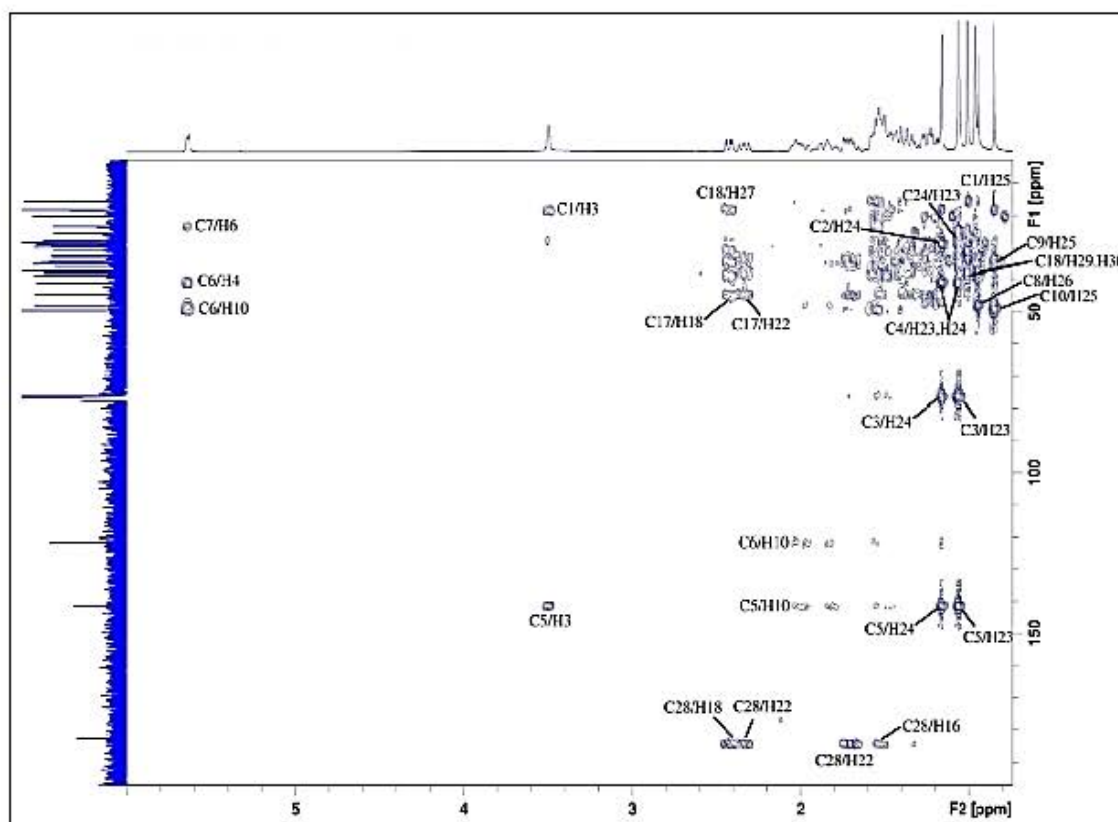


Figure S5: Heteronuclear multiple bond correlation (HMBC) spectrum of pinnatane A.

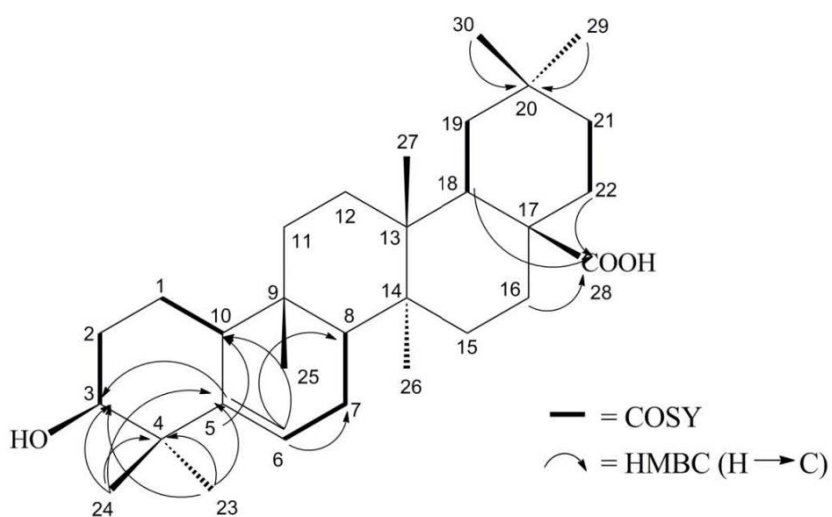


Figure S6: Selected COSY and HMBC correlations of pinnatane A.

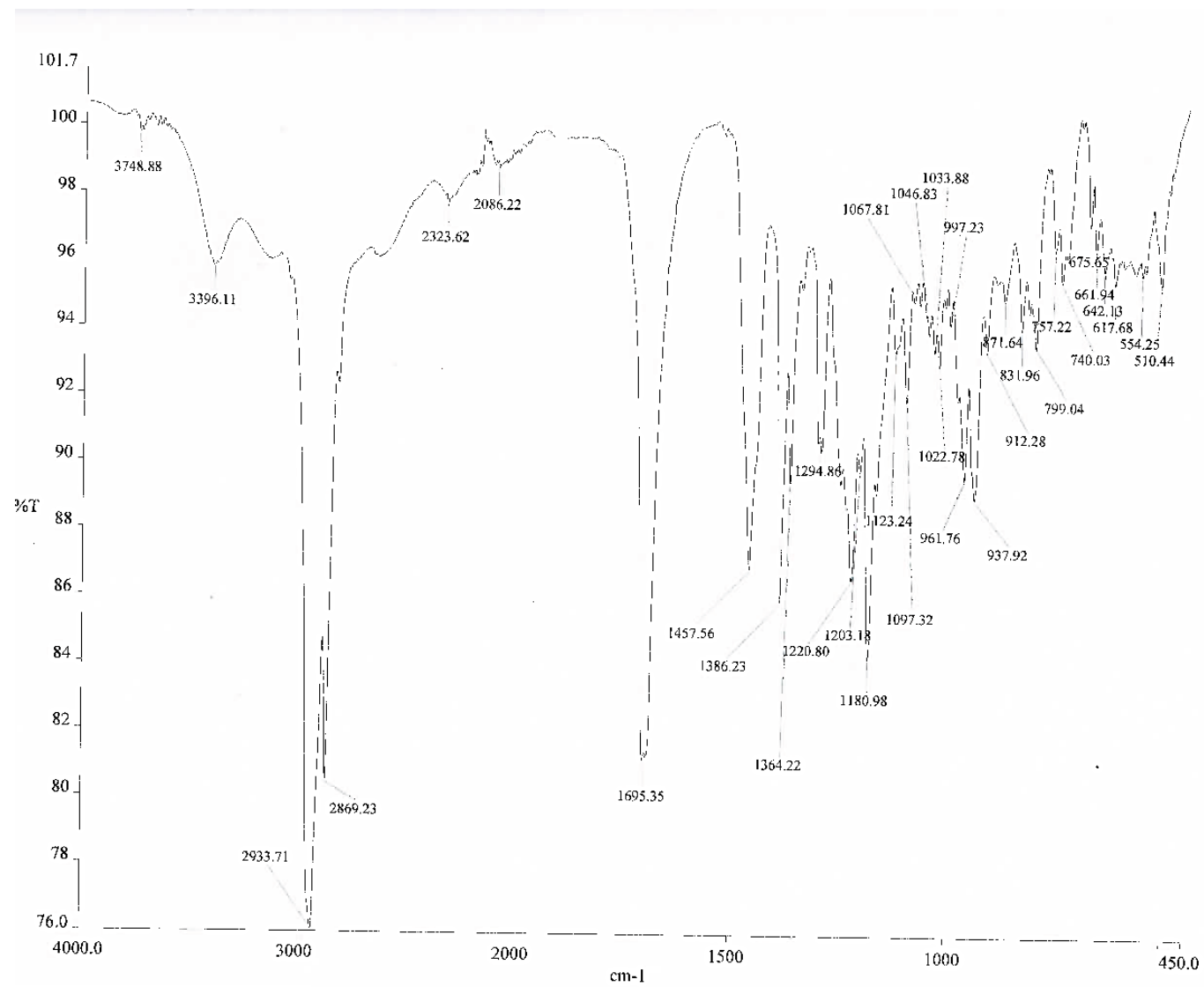
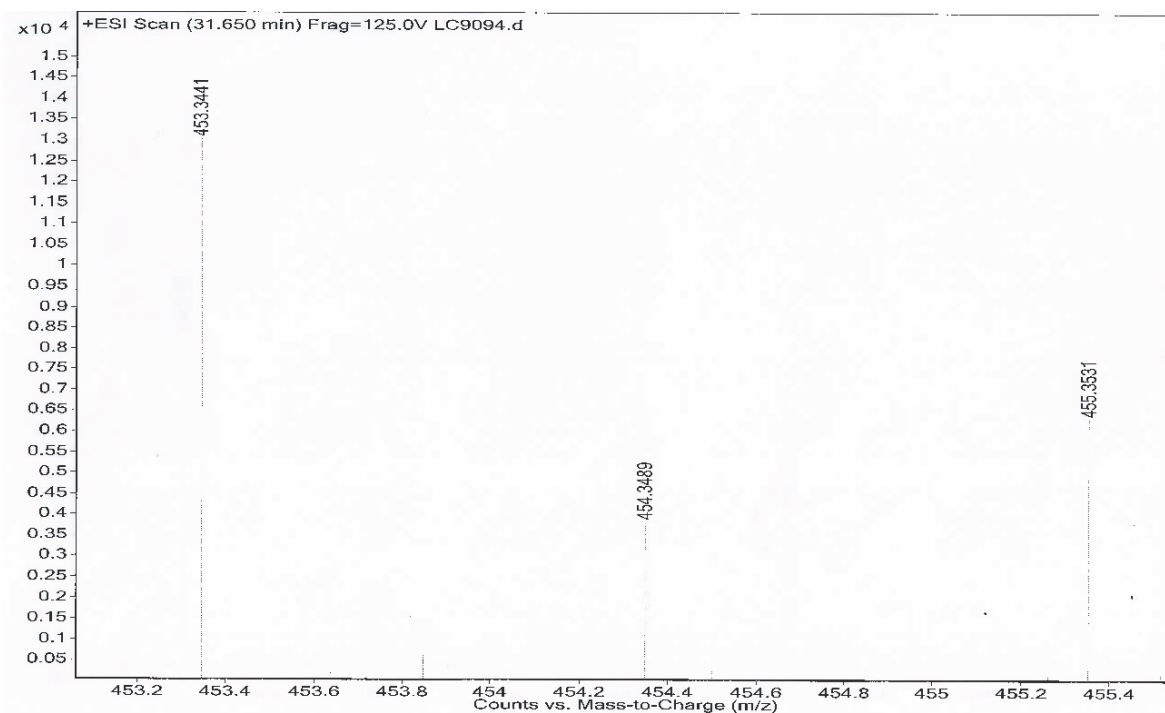


Figure S7: Infrared (IR) spectrum of pinnatane A



**Figure S8:** Liquid chromatography–mass spectrometry (LC-MS) spectrum of pinnatane A.

Related references:

1. Elfita, E.; Muharni, M.; Latief, M.; Darwati, D.; Widiyantoro, A.; Supriyatna, S.; Bahti, H.H.; Dachriyanus, D.; Cos, P.; Maes, L., et al. Antiplasmodial and other constituents from four Indonesian *Garcinia* spp. *Phytochemistry*, 2009. 70(7): pp. 907-12. DOI: 10.1016/j.phytochem.2009.04.024.
2. Mohamad, K.; Yusoff, M.; Awang, K.; Ahmad, K.; Ng, S.W. Pinnatane A from the bark of *Walsura pinnata* Hassk. *Acta Crystallogr Sect E Struct Rep Online*, 2009. 65(Pt 6): pp. o1317. DOI: 10.1107/s1600536809015955.
3. Yusoff, M. Chemical constituents of *Walsura pinnata* Hassk., in Department of Chemistry. 2012, University of Malaya, Kuala Lumpur, Malaysia (Dissertation). url: <http://studentsrepo.um.edu.my/5775/> (accessed on 15 August 2018). pp. 96-99.
4. Mahdzir, M.A.; Shilpi, J.A.; Mahmud, N.; Ramasamy, S.; Awang, K. Chemical constituents from *Walsura pinnata* (Meliaceae). *Nat Prod Commun*, 2017. 12(9): pp. 1397-1400.