

Supporting Information

Rec. Nat. Prod. 7:4 (2013) 302-306

Ixorene, a new Dammarane Triterpene from the Leaves of *Ixora coccinea* Linn.

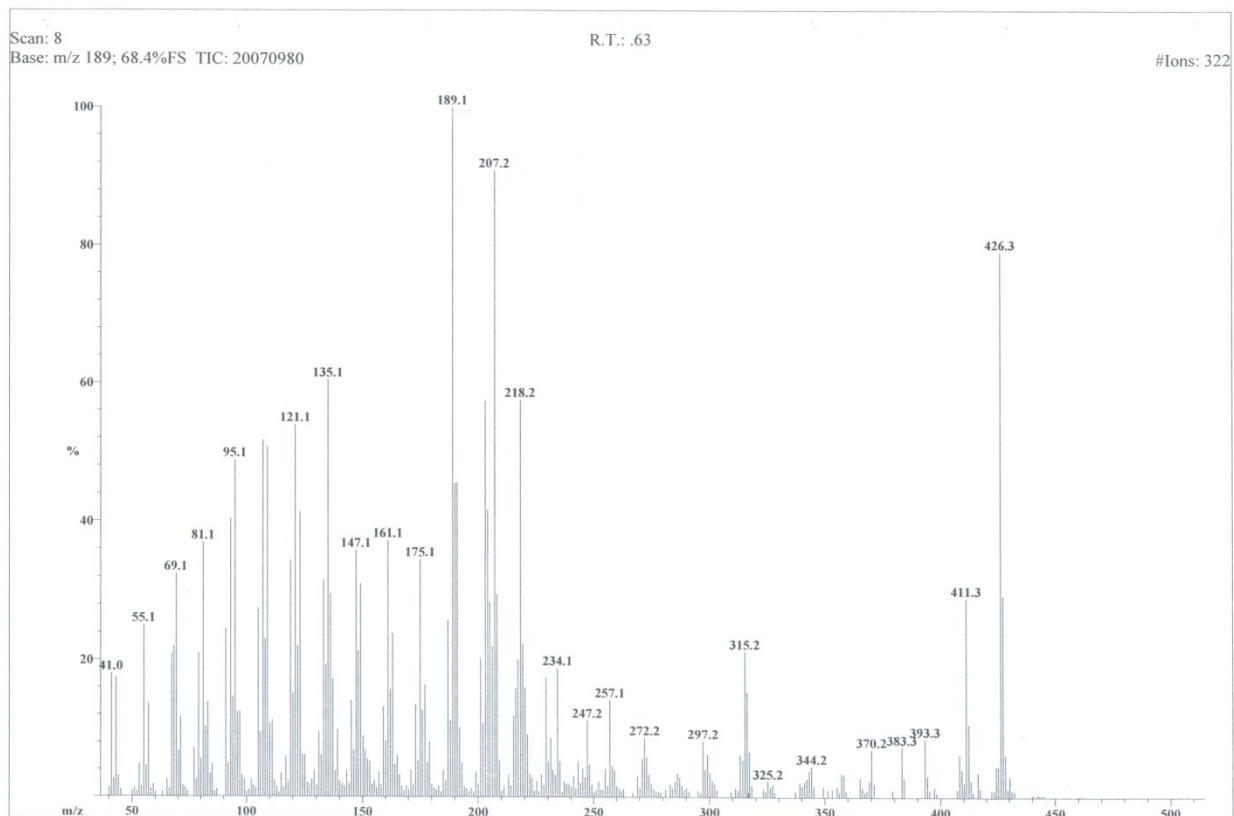
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File: IXB2 Date Run: 05-24-2012 (Time Run: 11:52:15)
Sample: SALMAN/DR.M ALI/FEDERAL URDU UNI/KHI
Instrument: JEOL MSRoute
Inlet: My Inlet Ionization mode: EI+



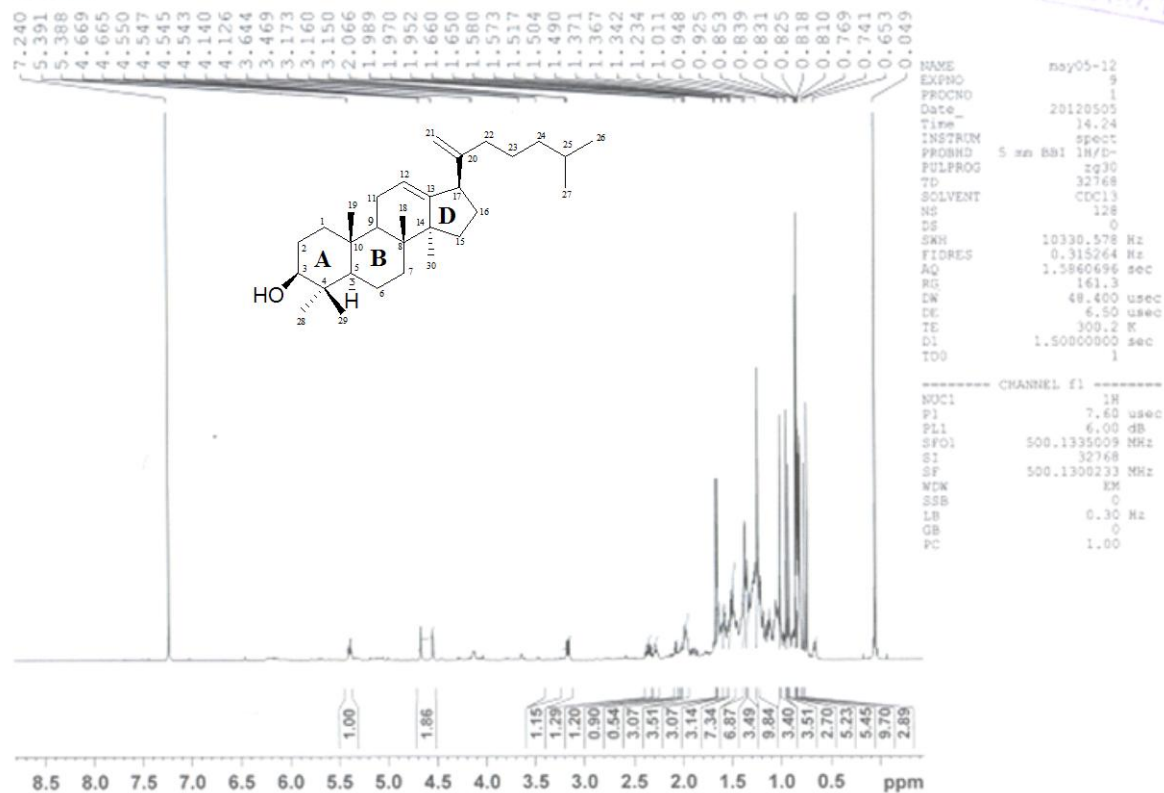
S1: EI-MS Spectrum of Compound 1 (ixorene)

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Compos
285.2456	2.7111					
296.2467	2.0425					
297.2584	41.4233	297.2582	0.6	0.2	6.5	C ₂₂ H ₃₃
298.2648	16.2098	298.2661	-4.3	-1.3	6.0	C ₂₂ H ₃₄
299.2758	8.4551	299.2739	6.3	1.9	5.5	C ₂₂ H ₃₅
300.2854	0.9935					
301.2833	0.5651					
304.9824	0.8184					
309.2586	1.0247	309.2582	1.2	0.4	7.5	
311.2738	1.8409	311.2739	-0.2	-0.1	6.5	C ₂₃ H ₃₃
312.2798	1.0953	312.2817	-6.1	-1.9	6.0	C ₂₃ H ₃₅
313.2572	1.4813					C ₂₃ H ₃₆
313.2808	1.4314					
314.2547	0.8078					
315.2717	2.4562	315.2688	9.2	2.9	5.5	C ₂₂ H ₃₅
316.2726	1.5915					
317.2873	0.8667	317.2844	8.9	2.8	4.5	C ₂₂ H ₃₇
318.9792	0.7374					
323.2677	1.5682					
324.2803	1.8635	324.2817	-4.2	-1.4	7.0	C ₂₄ H ₃₆
325.2858	5.6486					
326.2933	4.7857					
327.2986	2.3034					
330.9792	2.8264					
337.2822	0.9417					
338.2948	1.8774	338.2974	-7.5	-2.5	7.0	C ₂₅ H ₃₈
339.3030	29.1699	339.3052	-6.4	-2.2	6.5	C ₂₅ H ₃₉
340.3043	9.1185					
341.3037	1.7963	341.3056	-5.4	-1.9	1.5	C ₂₁ H ₄₁
342.9792	3.0582					
344.3054	0.7214	344.3079	-7.2	-2.5	5.0	C ₂₄ H ₄₀
351.3119	2.2709					
352.3164	3.3323	352.3130	9.7	3.4	7.0	C ₂₆ H ₄₀
353.3228	2.2497	353.3208	5.5	1.9	6.5	C ₂₆ H ₄₁
354.3335	0.5056					
354.9792	0.8805					
358.3301	0.6679					
363.3035	0.7349	363.3052	-4.6	-1.7	8.5	C ₂₇ H ₃₉
365.3287	60.8683					
366.3311	18.2840	366.3287	6.6	2.4	7.0	C ₂₇ H ₄₂
367.3370	3.4380	367.3365	1.4	0.5	6.5	C ₂₇ H ₄₃
379.3305	1.7851					
380.3467	1.1860	380.3443	6.4	2.4	7.0	C ₂₈ H ₄₄
380.9760	1.7590					
381.3594	1.0786					
383.3354	0.8008					
391.3423	1.9894					
392.3378	1.4422					
392.9760	2.7453					
393.3537	28.1351	393.3521	4.0	1.6	7.5	C ₂₉ H ₄₅
394.3582	9.6657	394.3600	-4.3	-1.7	7.0	C ₂₉ H ₄₆
395.3590	2.4598					
399.2840	1.0140					
400.2918	0.6625					
401.2777	0.5540					
404.9760	1.1043					
406.3651	4.4119					
407.3667	2.8757	407.3678	-2.7	-1.1	7.5	C ₃₀ H ₄₇
408.3780	60.6281	408.3756	5.8	2.4	7.0	C ₃₀ H ₄₈
409.3837	18.1972	409.3834	0.7	0.3	6.5	C ₃₀ H ₄₉
410.3834	4.2956					
411.3646	2.8638	411.3627	4.7	1.9	6.5	C ₂₉ H ₄₇ O ₁
412.3764	0.9738					
414.3466	0.5409	414.3498	-7.6	-3.1	6.0	C ₂₈ H ₄₆ O ₂
419.3593	0.5122					
422.3683	0.5807					
424.3771	0.9129	424.3707	6.4	0.7	6.0	C ₃₀ H ₄₉ O ₁
425.3672	0.7281	425.3631	9.6	4.1	2.5	C ₃₀ H ₅₀ O ₁
426.3864	7.7918	426.3862	0.6	0.3	6.0	C ₃₀ H ₅₀ O ₁

S2: HREI-MS Spectrum of Compound 1 (ixorene)

AMBREEN/DR.M.ALI/IXB2/
F.U.UNI/

AVANCE AV-500
LAB NO: 109-B



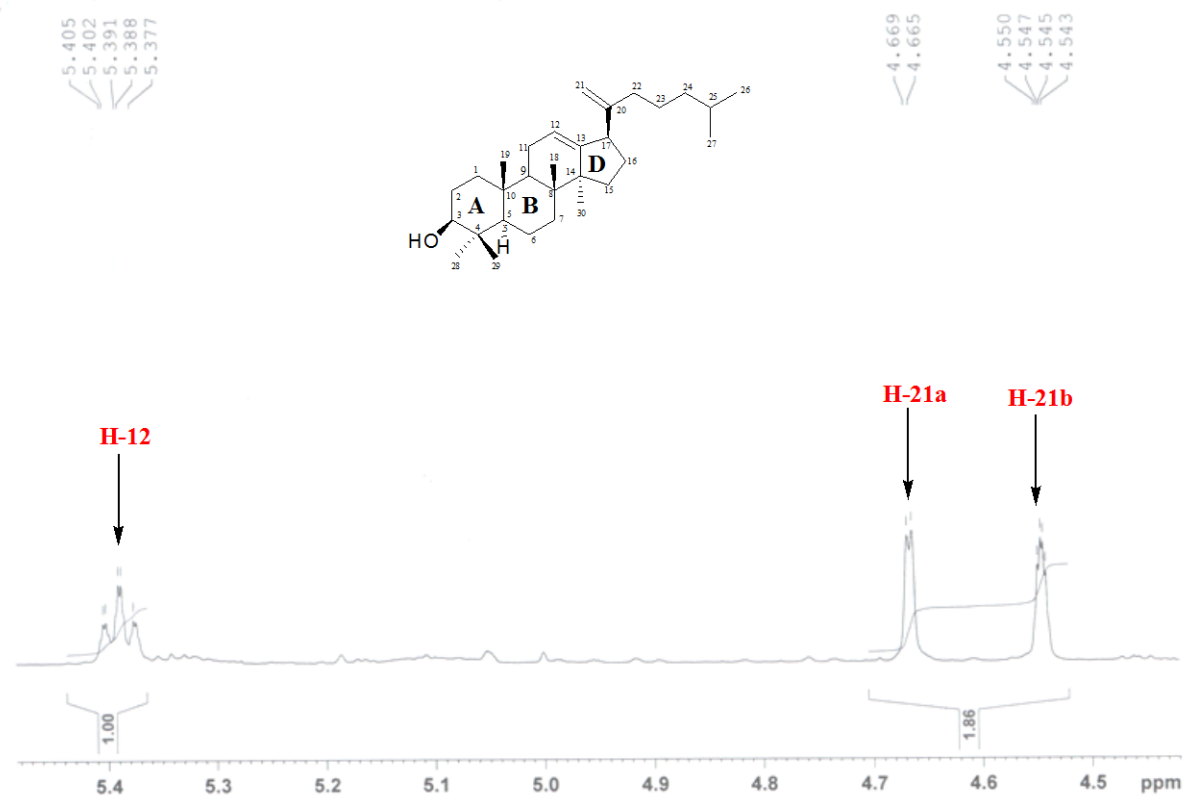
S3: $^1\text{H-NMR}$ (500 MHz, CDCl_3) Spectrum of Compound **1** (ixorene)

17\beta-dammara-12,20-diene-3 β -ol (**1**). Yellow solid, $[\alpha]_{\text{D}}^{24}$: +57.6 (*c* 0.0052, CDCl_3)

$^1\text{H-NMR}$ (CDCl_3 , 500 MHz), δ : 5.39 (1H, td, H-12), 4.69 (1H, d, H-21a), 4.54 (1H, d, H-21b), 3.16 (1H, dd, H-3 α), 2.35 (1H, m, H-17), 1.01 (6H, s, H-19/H-30), 0.94 (3H, s, H-28), 0.92 (3H, s, H-18), 0.85 (3H, d, H-26), 0.82 (3H, d, H-27), 0.75 (3H, s, H-29). $^{13}\text{C-NMR}$ (CDCl_3 , 125 MHz), δ : 150.97 (C-20), 140.31 (C-13), 123.15 (C-12), 109.31 (C-21), 79.03 (C-3), 48.01 (C-17), 27.99 (C-28), 22.70 (C-26), 19.75 (C-27), 18.02 (C-29), 16.01 (C-30), 14.57 (C-18), 15.37 (C-19).

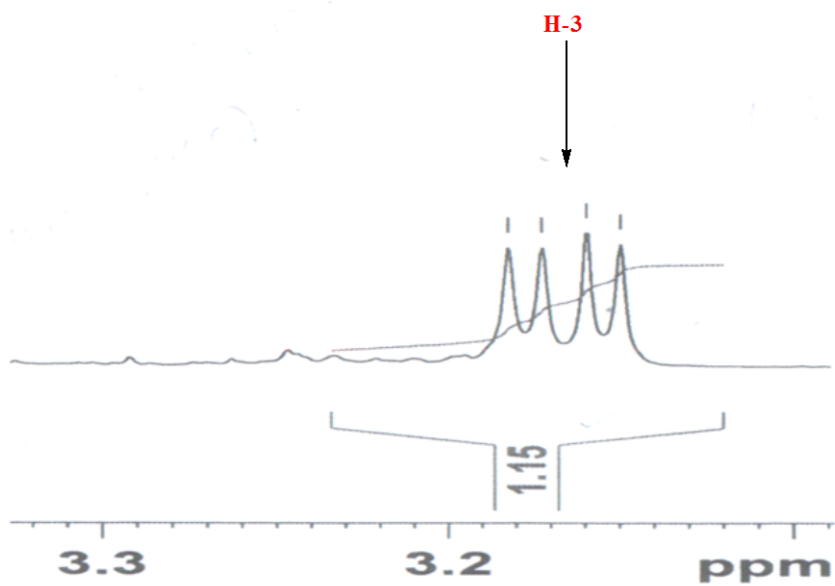
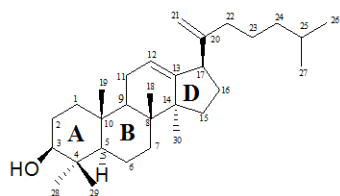
UV λ_{max} (MeOH) nm ($\log_{10}\epsilon$): 230(4.0), 244(4.1). IR ν_{max} (KBr) cm^{-1} : 3406, 2927, 2857, 1675, 1550, 1463, 1380, 915. HR EIMS m/z (rel. intensity, %): 426.3864 (M^+ , calcd. for $\text{C}_{30}\text{H}_{50}\text{O}$, 426.3862, 8), 408.3780 (M^+ , $-\text{H}_2\text{O}$, calcd. for $\text{C}_{30}\text{H}_{48}$, 408.3756, 61), 394.3582 ($\text{M}^+ - \text{CH}_3 - \text{OH}$, calcd. for $\text{C}_{29}\text{H}_{46}$, 394.3600, 10), 207.1774 (calcd. for $\text{C}_{14}\text{H}_{23}\text{O}$, 207.1749, 90), 190.1775 (calcd. for $\text{C}_{14}\text{H}_{22}$, 190.1772, 32), 189.1657 (calcd. for $\text{C}_{14}\text{H}_{21}$, 189.1643, 100). EIMS m/z (rel. intensity, %): 426 (M^+ , $\text{C}_{30}\text{H}_{50}\text{O}$, 79), 218 ($\text{C}_{16}\text{H}_{26}$, 58), 207 ($\text{C}_{14}\text{H}_{23}\text{O}$, 90), 189 ($\text{C}_{14}\text{H}_{21}$, 100), 147 ($\text{C}_{11}\text{H}_{15}$, 36), 133 ($\text{C}_{10}\text{H}_{13}$, 32), 107 (C_8H_{11} , 51), 71 (C_5H_{11} , 10).

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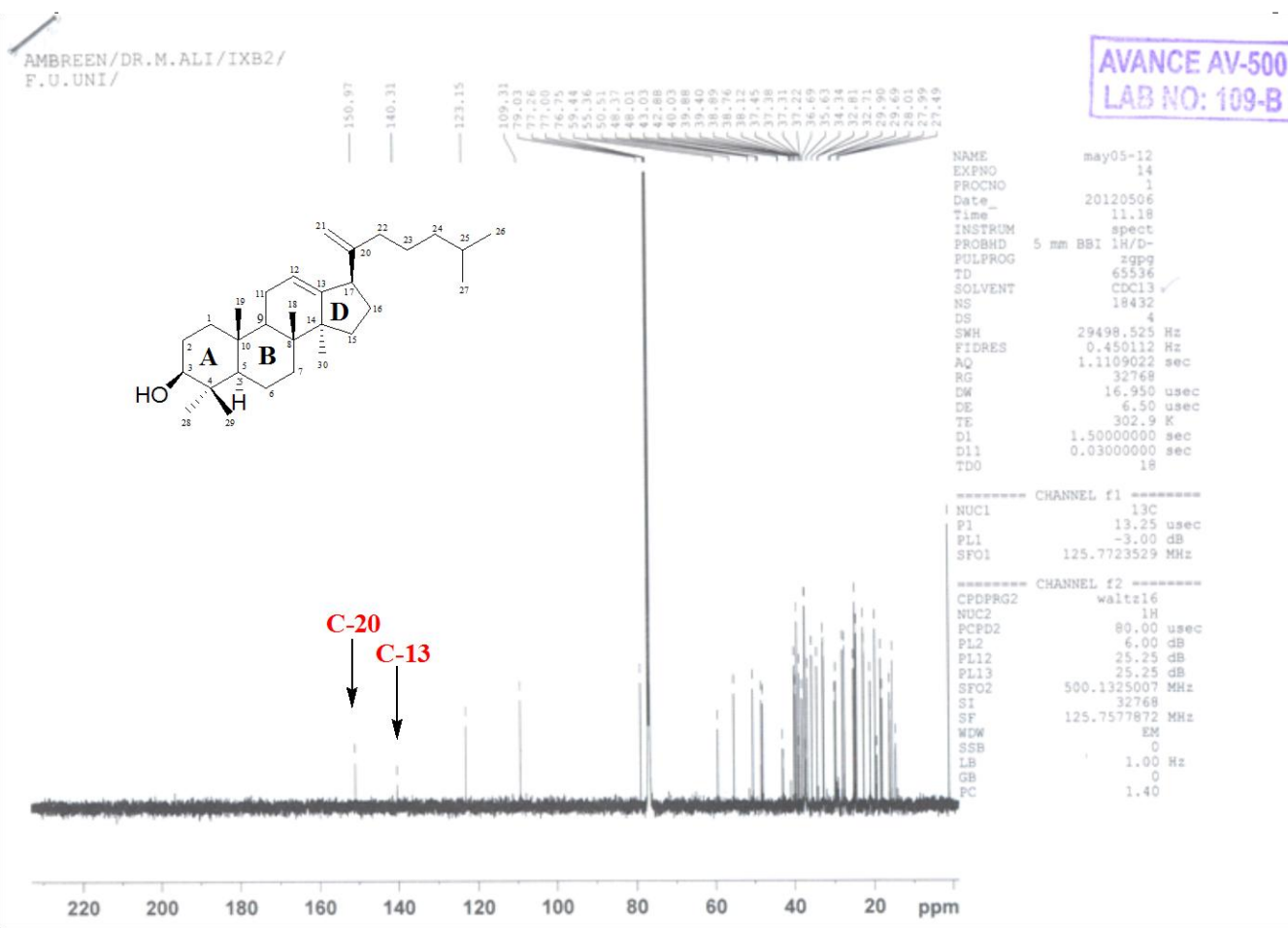


S4: Expansion of ¹H-NMR Spectrum of Compound 1 (ixorene) (From 4.5 to 5.4 ppm)

3.183
3.173
3.160
3.150



S5: Expansion of ¹H-NMR Spectrum of Compound **1** (ixorene)



S6: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of Compound 1 (ixorene)

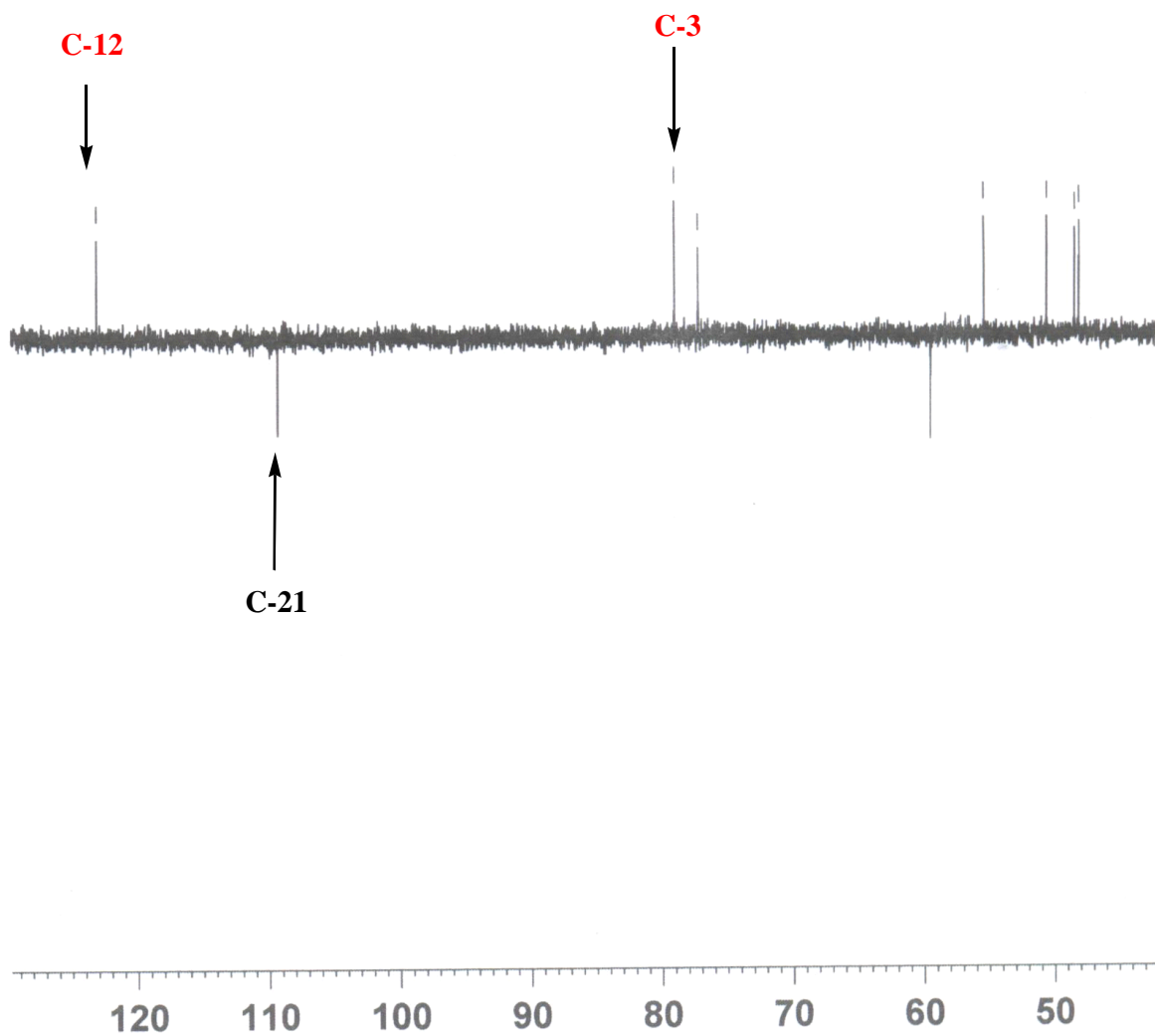
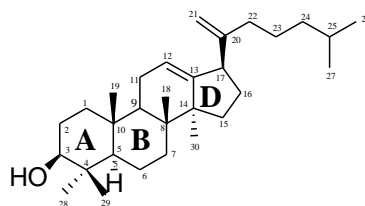
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DEPT135

123.13

109.33

79.03
77.22

59.45
55.35
50.49
48.36
48.02
40.03
39.89
39.40
38.75
38.11
37.45
37.38
37.31
36.69



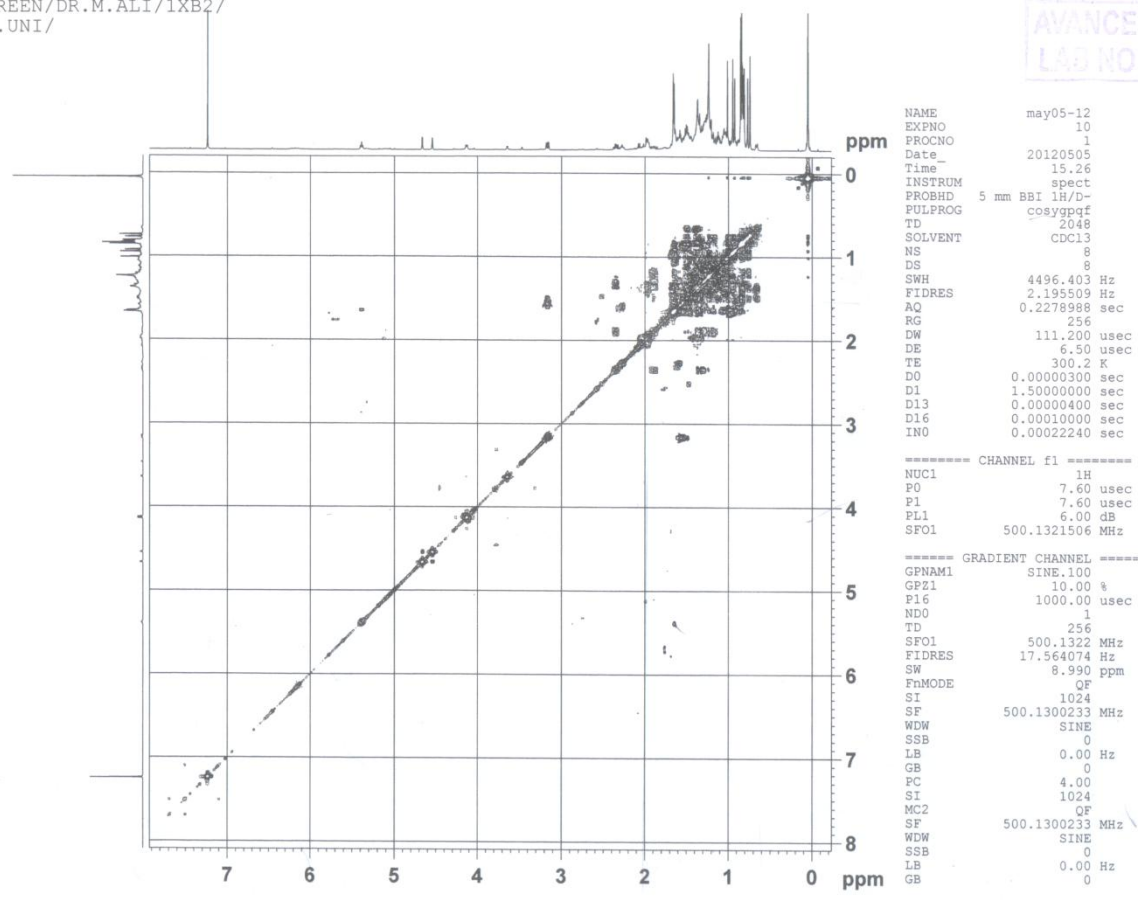
S7: DEPT -135 Spectrum of Compound 1 (ixorene) (From 50 to 120 ppm)



S8: DEPT -90 Spectrum of Compound **1** (ixorene) (From 50 to 120 ppm)

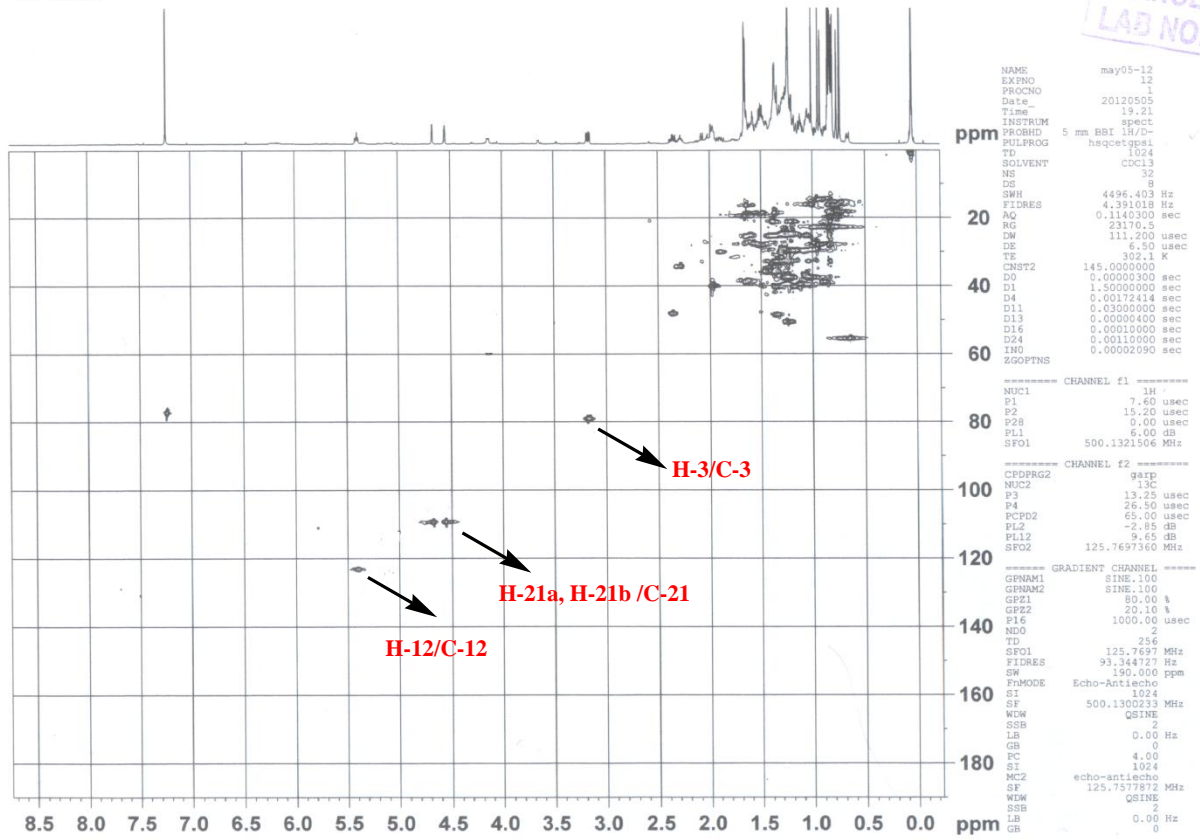
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F.U.UNI/

AVANCE
LAB NO



S9: COSY Spectrum of Compound 1 (ixorene)

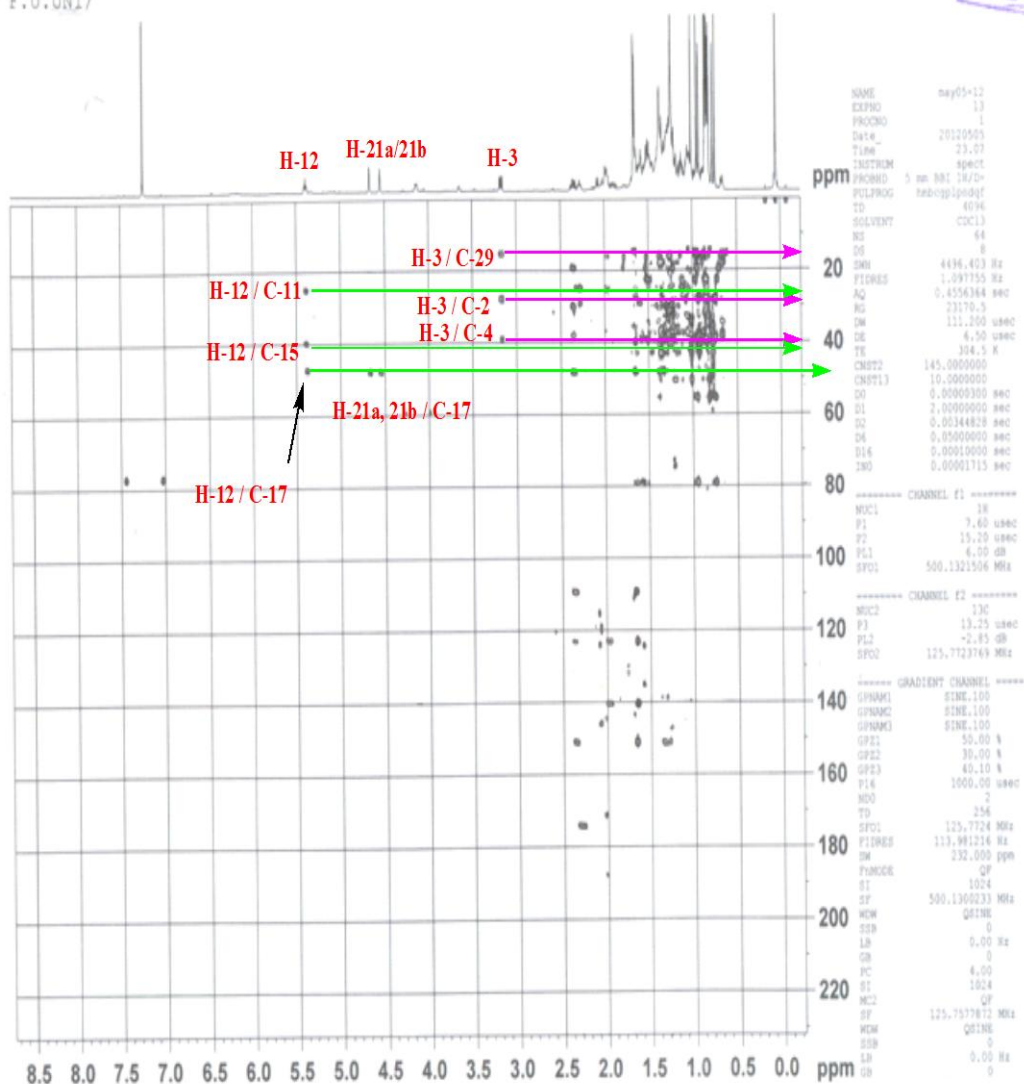
AVANCE A
LAB NO: 1



S10: HSQC (500 MHz) Spectrum of Compound 1 (ixorene) (From 50 to 125 ppm)

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F.U.UNI/

AVANCE AV-500
LAB NO: 109-B.



S11: HMBC Spectrum of Compound 1 (ixorene)