Quim. Nova, Vol. 48, No. 6, 2025

Supplementary Material

COMPARATIVE STUDY OF THE CHEMICAL COMPOSITION OF AMAPA LATEX FROM *Parahancornia amapa* AND *Brosimum parinarioides* BY HPLC-UV-DAD

Rita Cynara de Oliveira Salles[a,b,*], Sergio Massayoshi Nunomura[b], Norberto Peporine Lopes[c] and Rita de Cássia Saraiva Nunomura[a,*]

[a]Departamento de Química, Instituto de Ciências Exatas, Universidade Federal do Amazonas, 69077-000 Manaus – AM, Brasil

[b]Coordenação de Pesquisa de Tecnologia e Inovação, Instituto Nacional de Pesquisas da Amazônia, 69067-375 Manaus – AM, Brasil

[c]Departamento de Física e Química, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, 14040-903 Ribeirão Preto – SP, Brasil

Received: 02/27/2025; accepted: 07/08/2025; published online: 07/29/2025

*e-mail: ritacynara@gmail.com; ritasnunomura@gmail.com

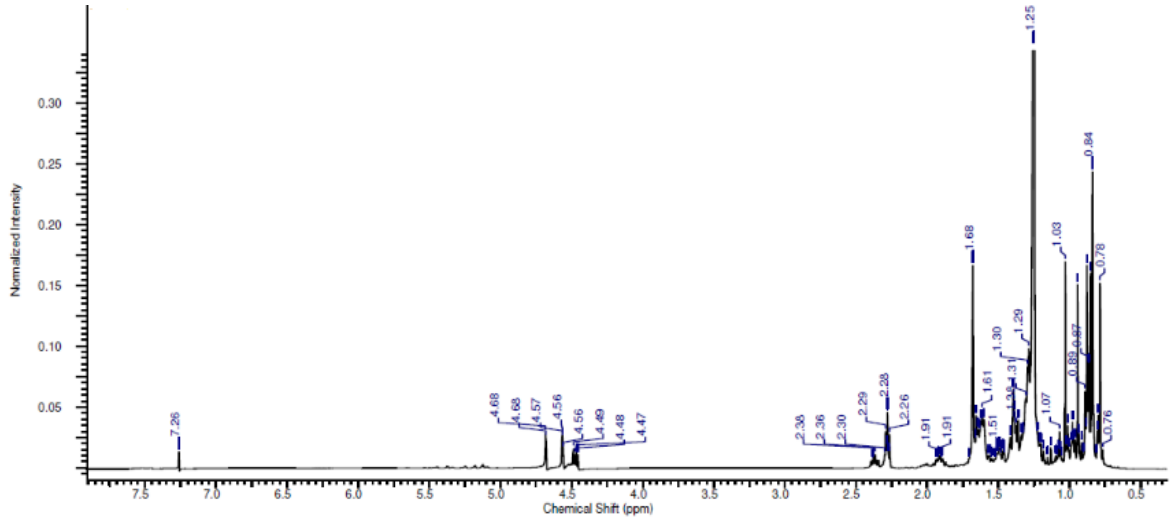

Figure 1S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of* ***MIST-1*** *(mixture of non-hydroxylated lupeol esters)*

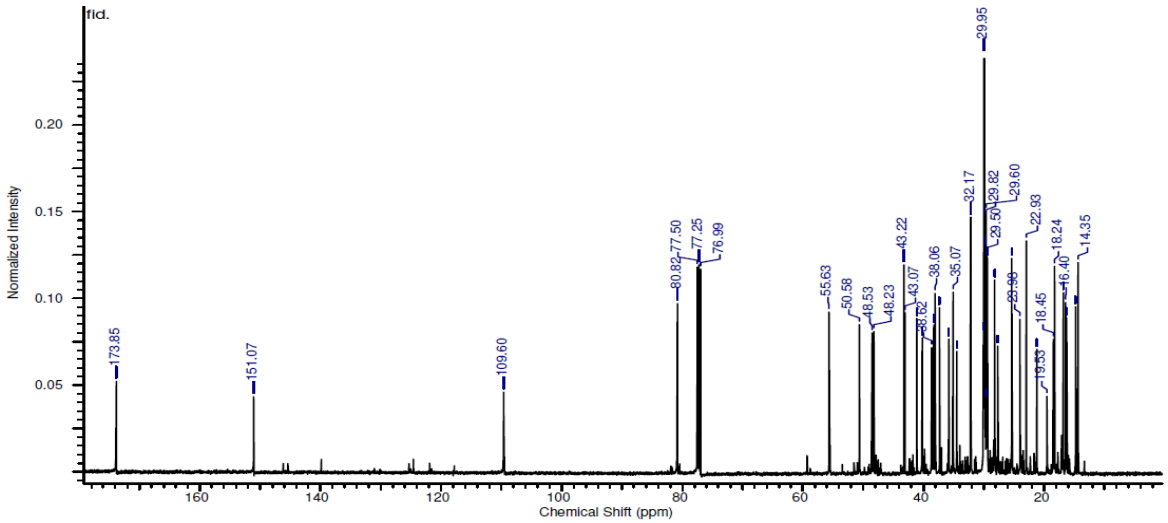

Figure 2S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of* ***MIST-1*** *(mixture of lupeol esters non-hydroxylated)*

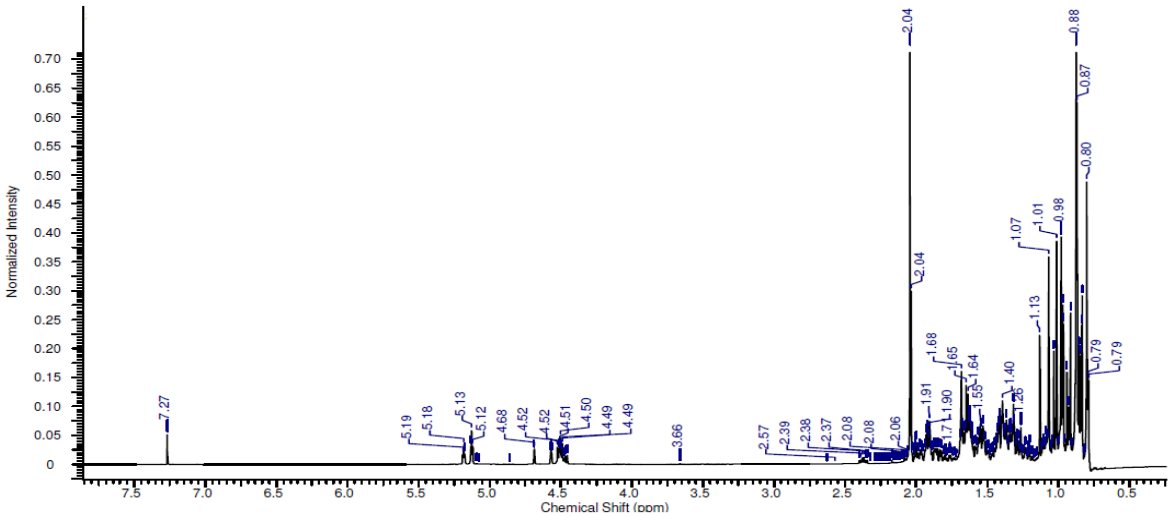

Figure 3S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of* ***MIST-2*** *(mixture of acetylated triterpenes- α-amyrin acetate, β-amyrin acetate and lupeol acetate)*

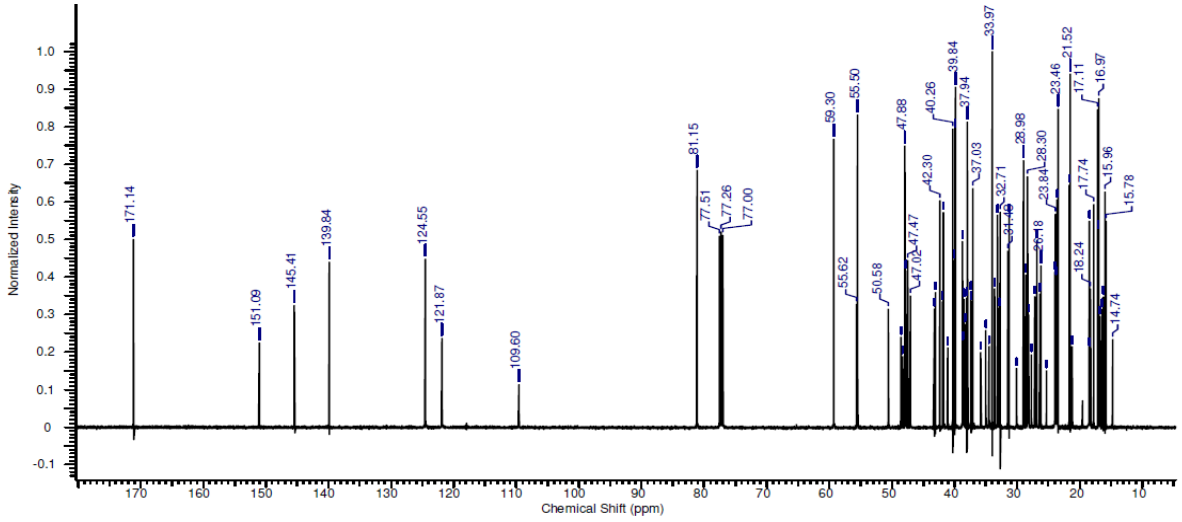

Figure 4S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of* ***MIST-2*** *mixture of acetylated triterpenes-(mixture of acetylated triterpenes- α-amyrin acetate, β-amyrin acetate and lupeol acetate)*

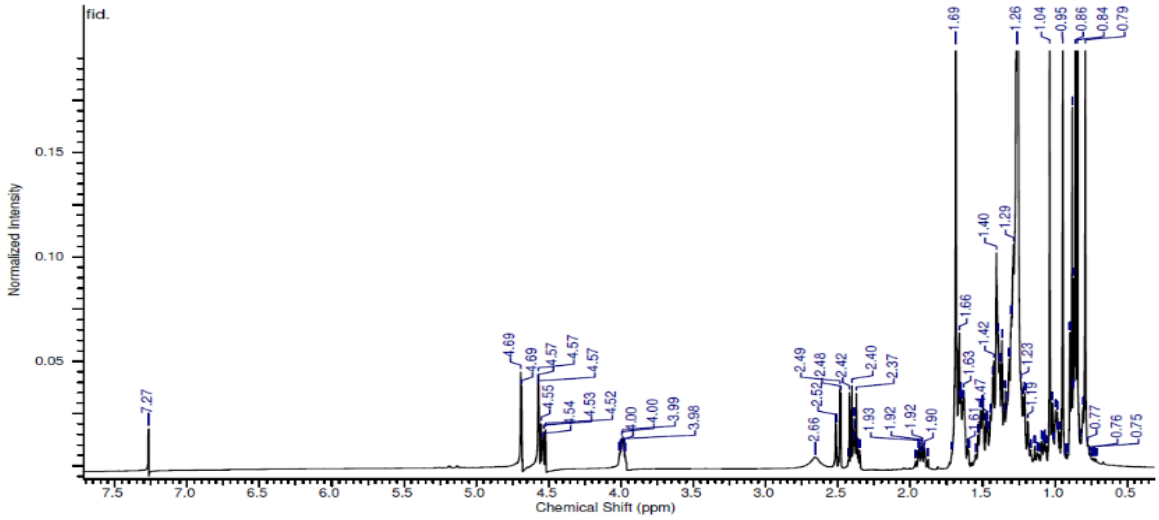

Figure 5S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of* ***MIST-3*** *(mixture of hhydroxylated esters lupeol)*

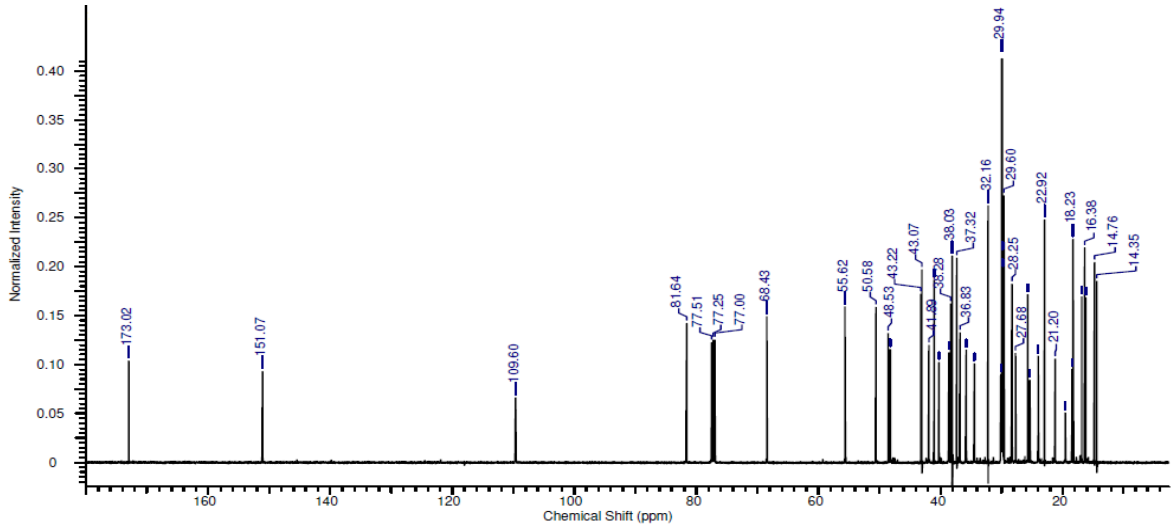

Figure 6S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of* ***MIST-3*** *(mixture of hydroxylated esters of lupeol)*

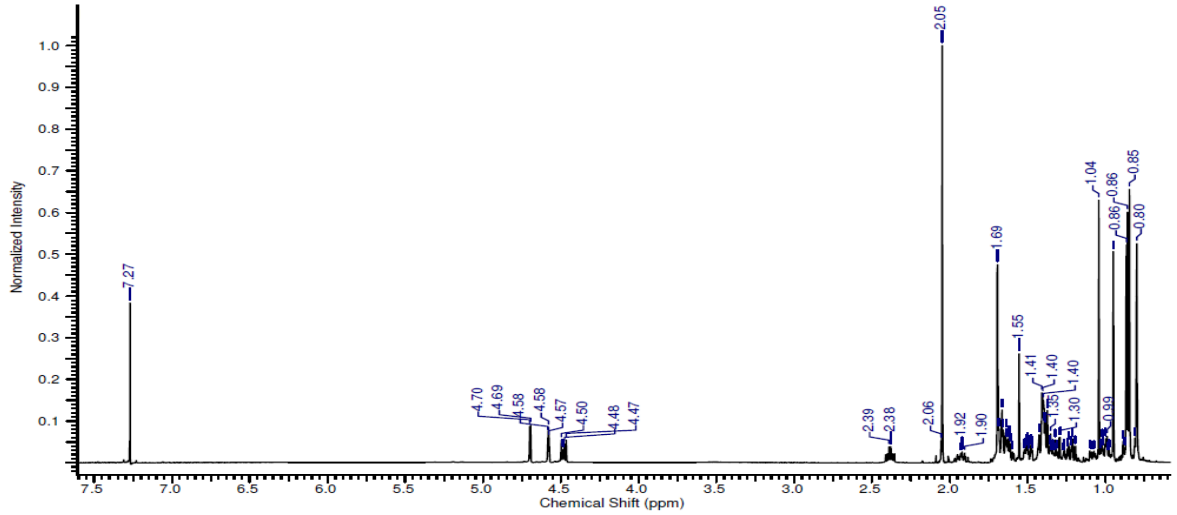

Figure 7S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of lupeol acetate (**1**) from P. amapa esters hydroxylated)*

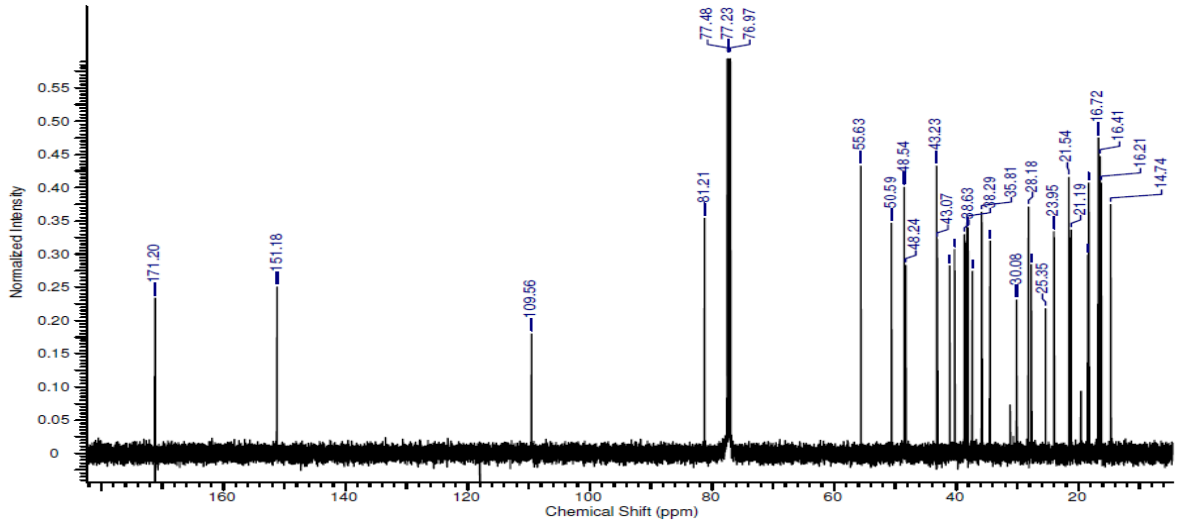

Figure 8S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of lupeol acetate (**1**) from P. amapa*

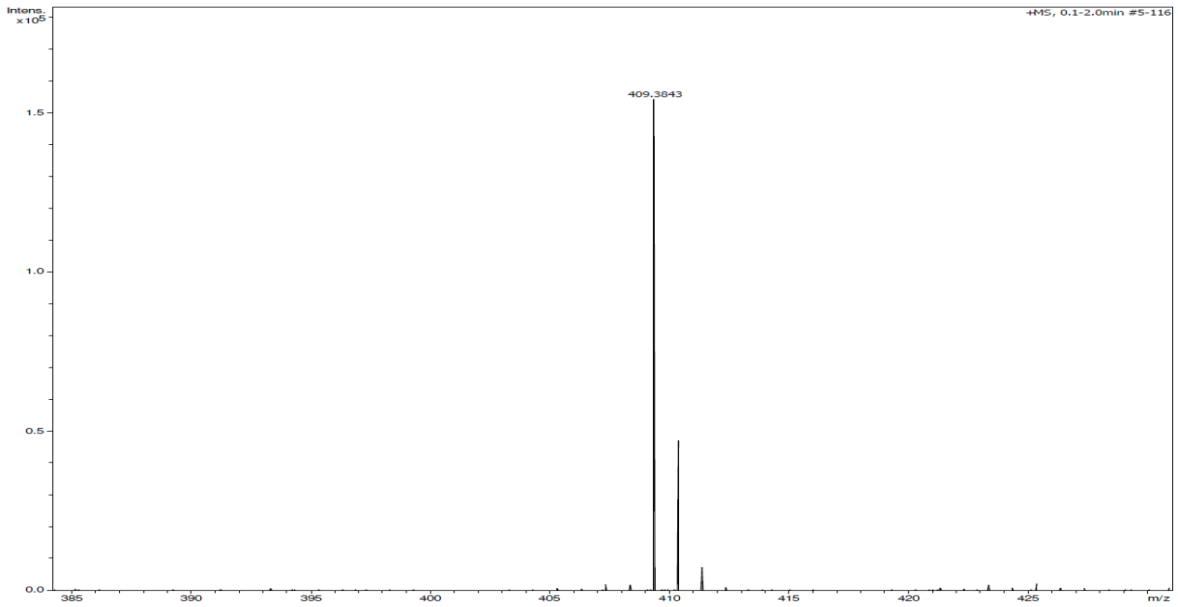

Figure 9S. *HR-APCI-MS (positive mode) spectrum of lupeol acetate (**1**) (P. amapa)*

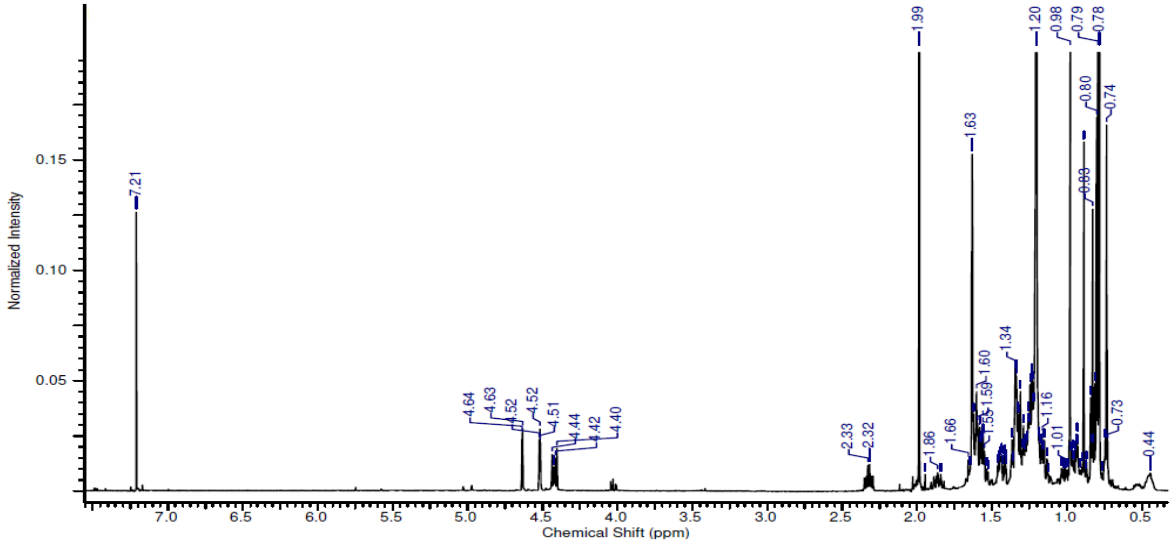

Figure 10S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of lupeol acetate (**1**) from B. parinarioides*

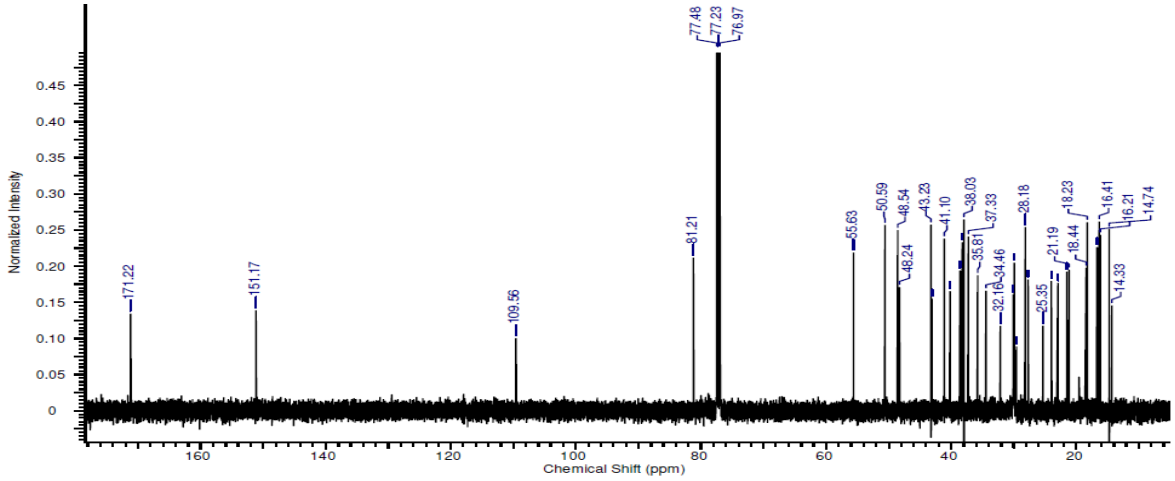

Figure 11S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of lupeol acetate (**1**) from B. parinarioides*

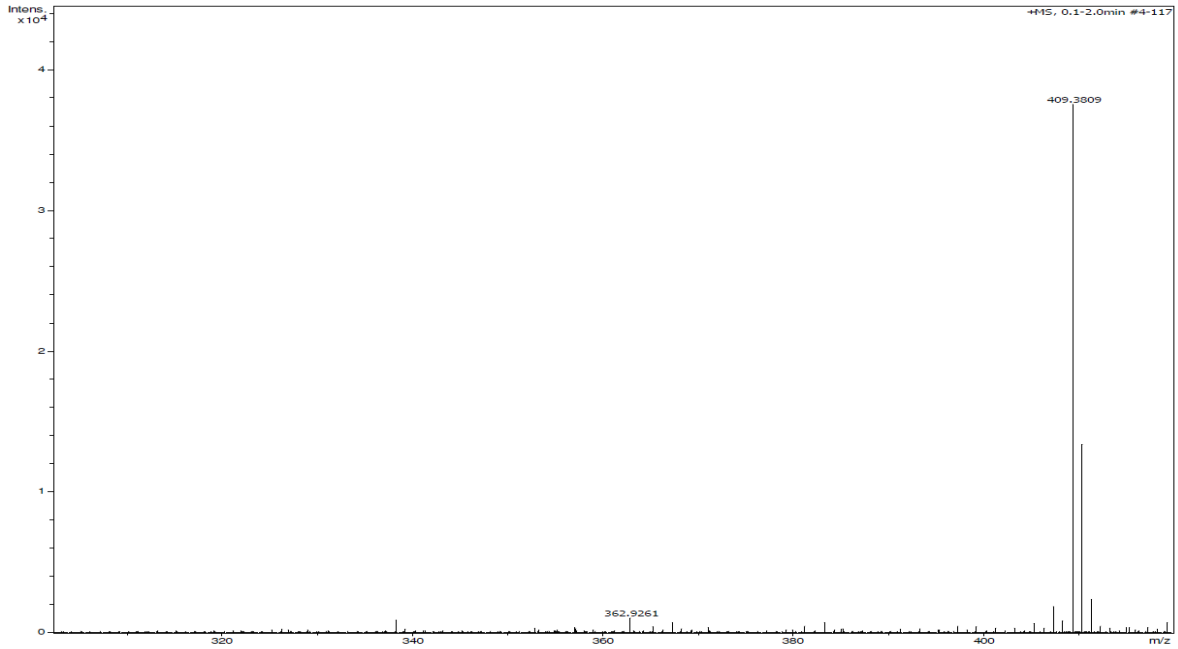

Figure 12S. *HR-APCI-MS (positive mode) spectrum of lupeol acetate (**1**) (B. parinarioides)*

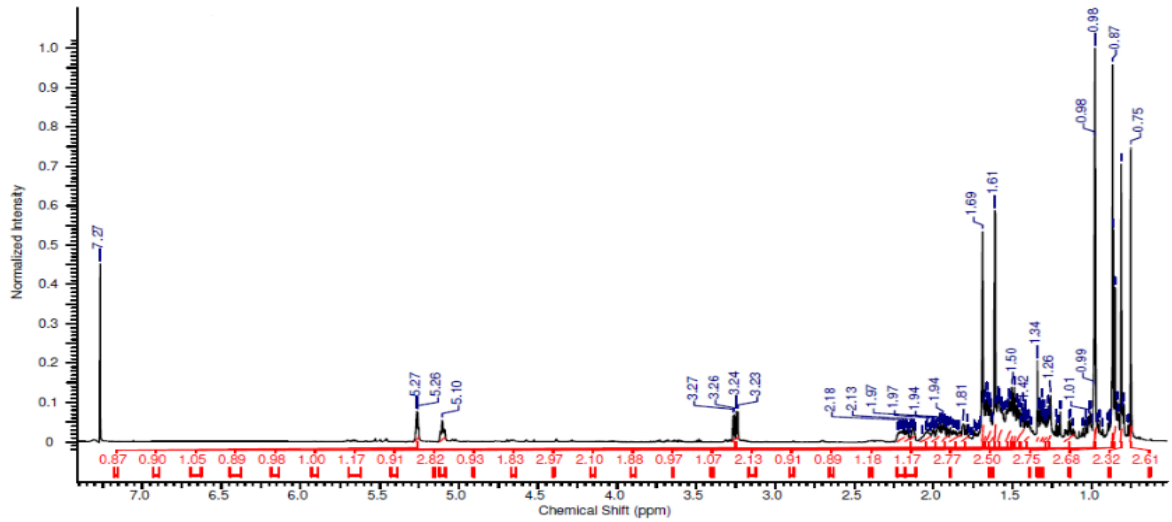

Figure 13S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of butyrospermol (**2**)*

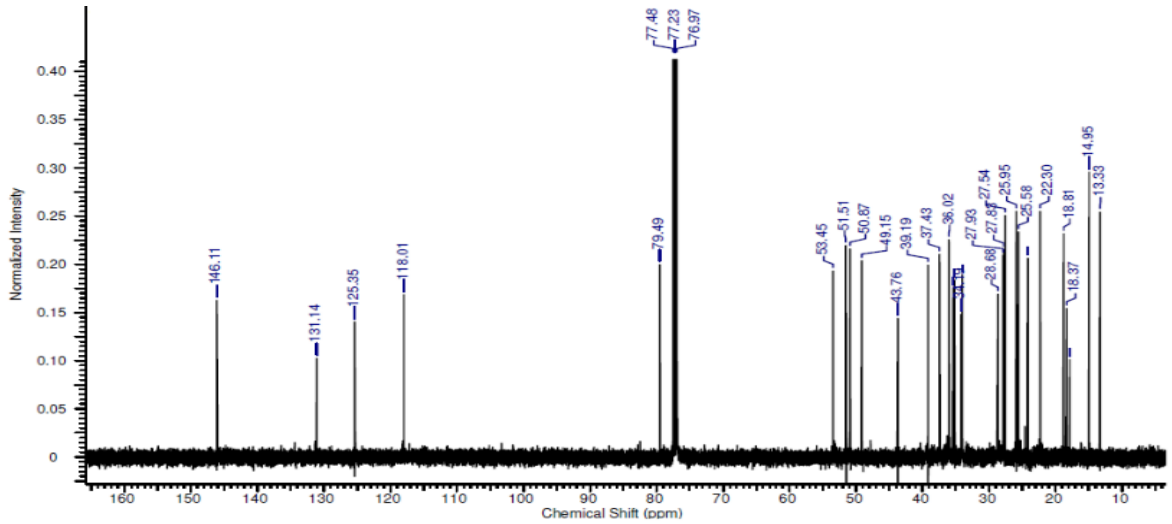

Figure 14S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of butyrospermol (**2**)*

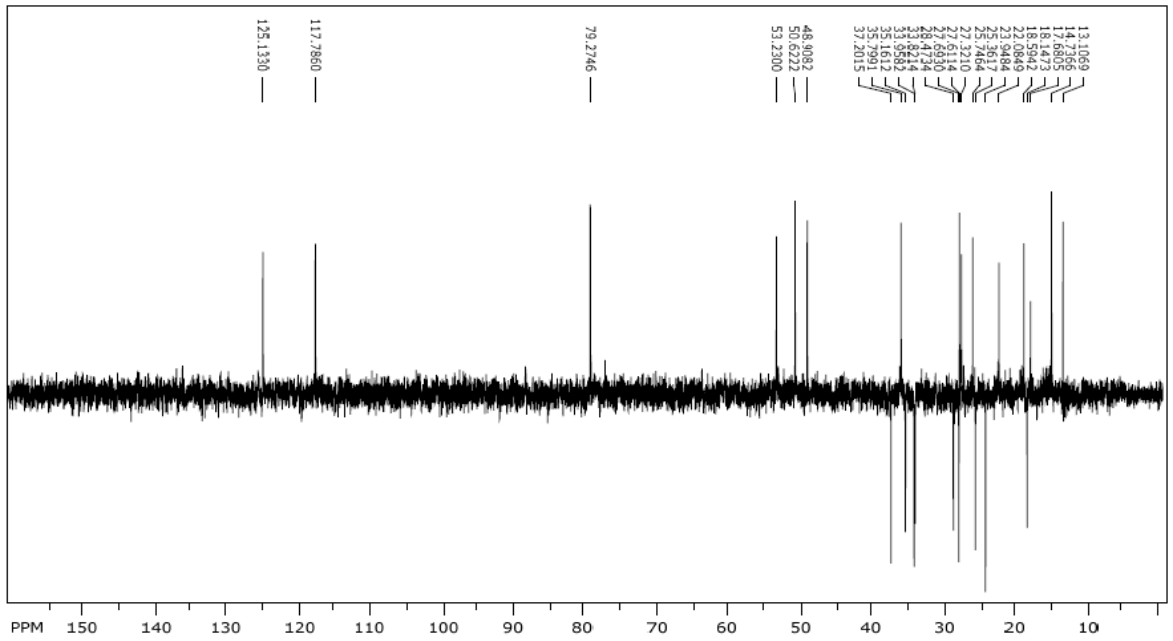

Figure 15S. *DEPT-135 spectrum ($CDCl_3$, 75 MHz) of butyrospermol (**2**)*

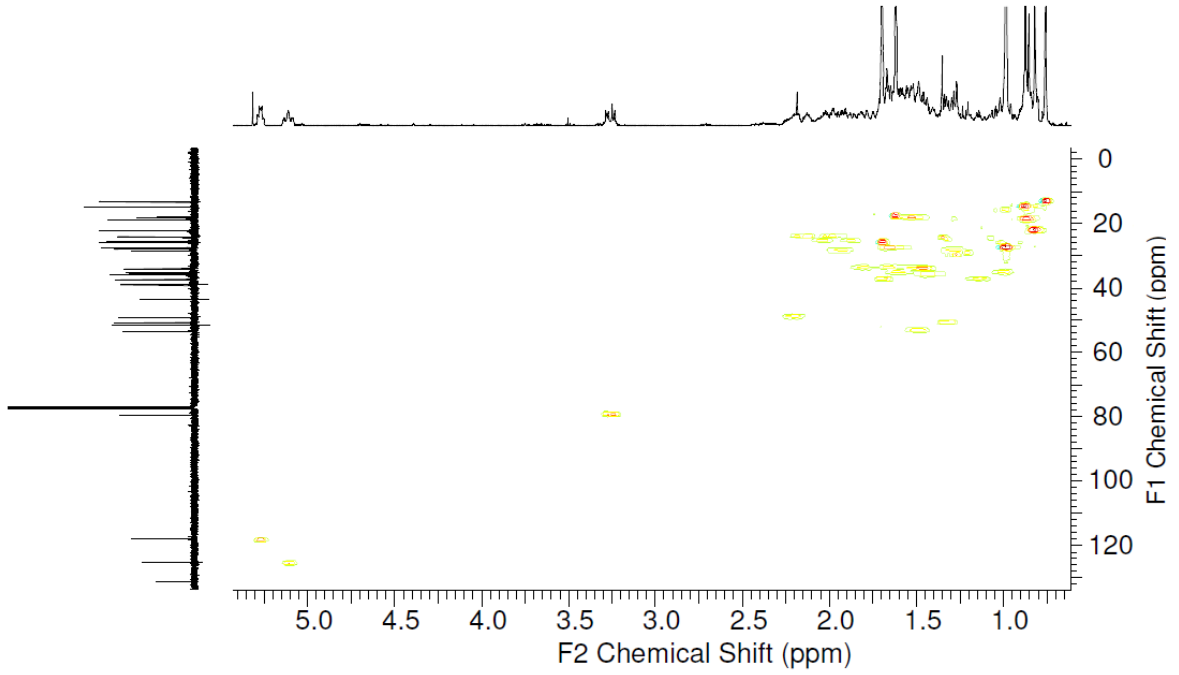

Figure 16S. *HSQC spectrum of butyrospermol (**2**)*

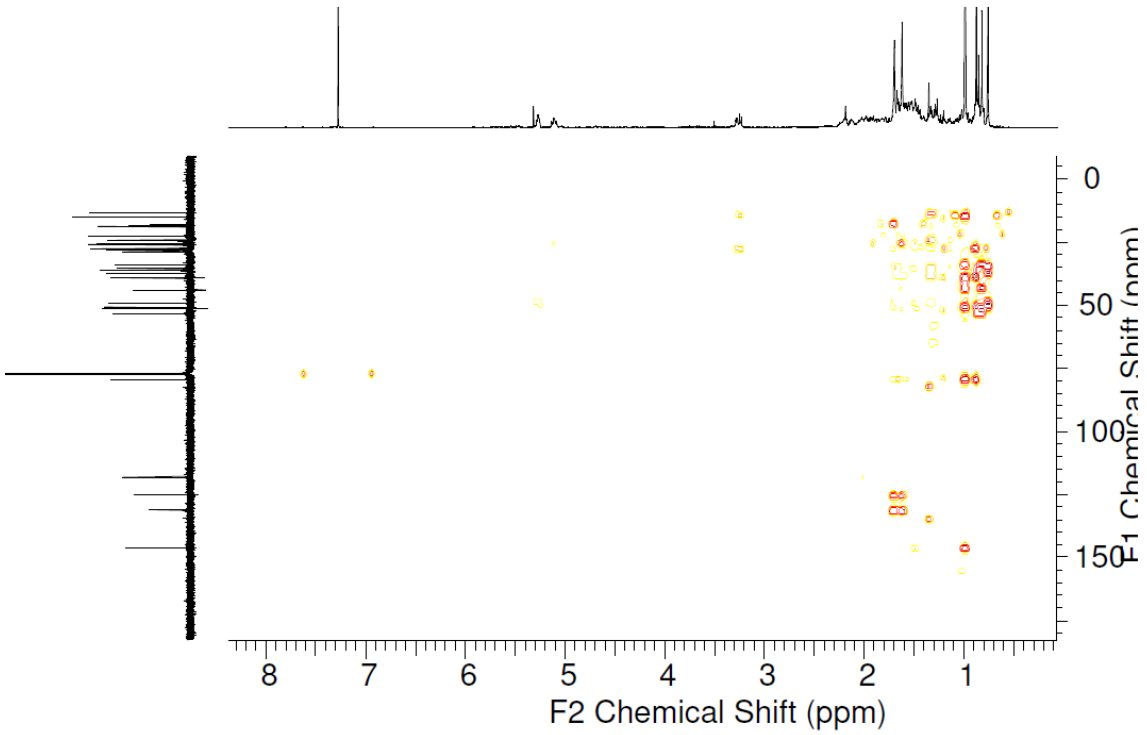

Figure 17S. *HMBC spectrum of butyrospermol (**2**)*

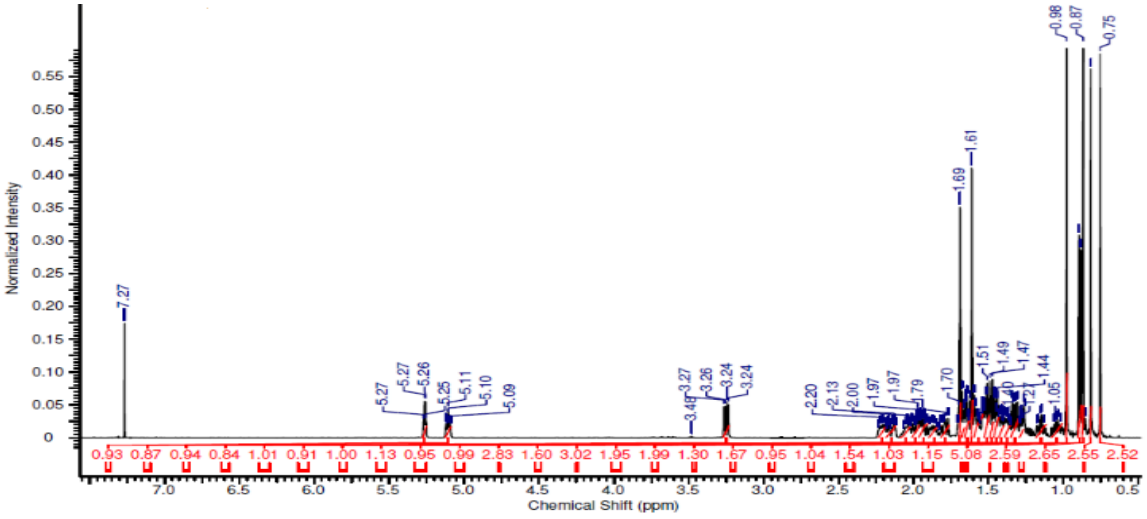

Figure 18S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of tirucalla-7,24-dien-3β-ol (**3**)*

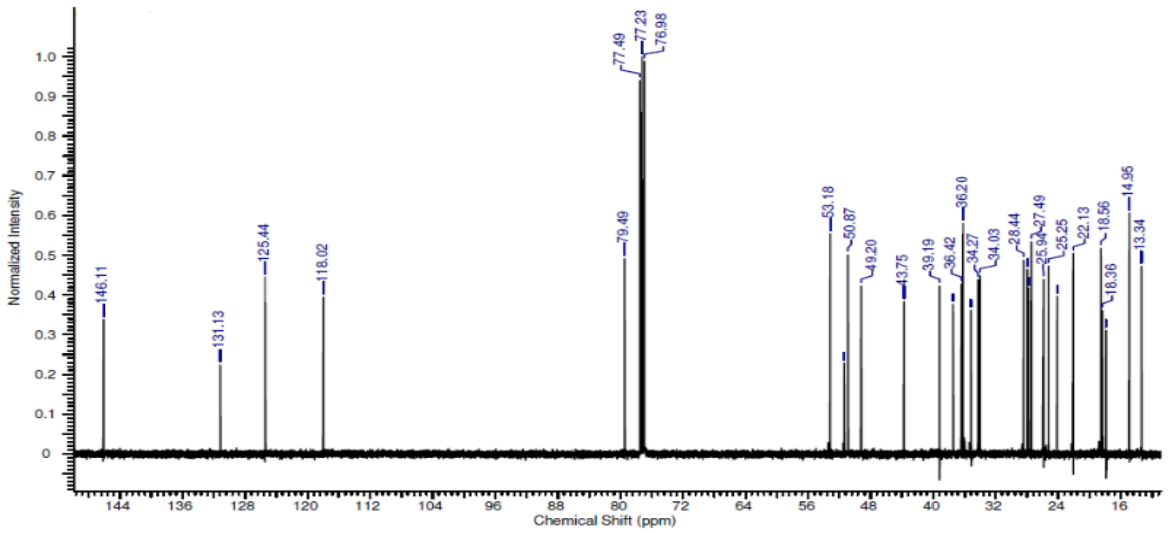

Figure 19S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of tirucalla-7,24-dien-3β-ol (**3**)*

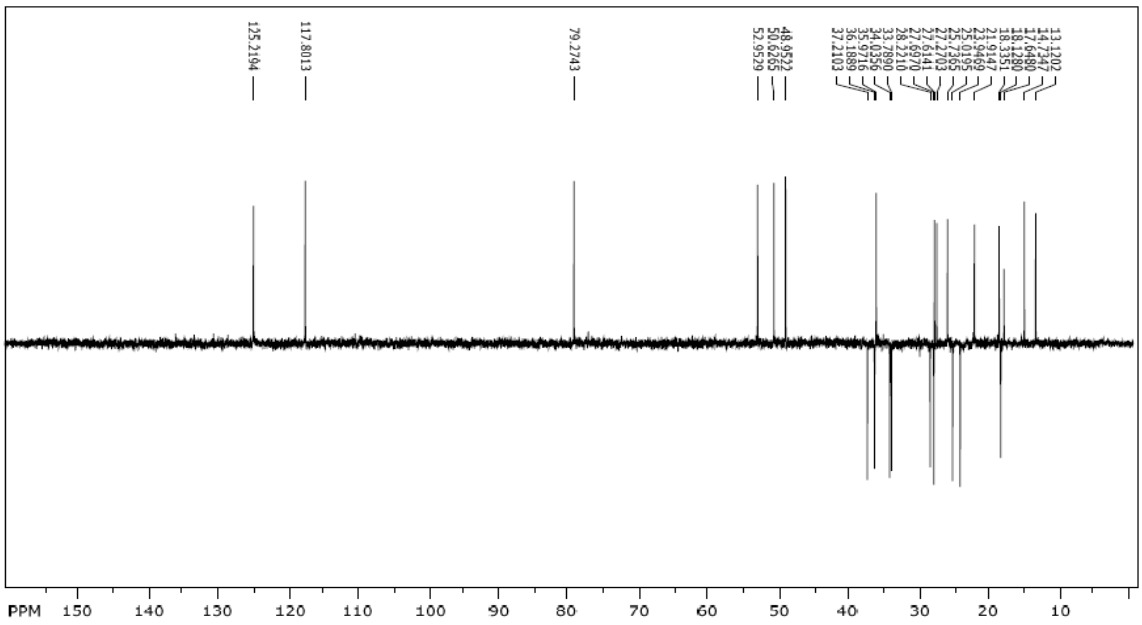

Figure 20S. *DEPT-135 spectrum ($CDCl_3$, 75 MHz) of tirucalla-7,24-dien-3β-ol (**3**)*

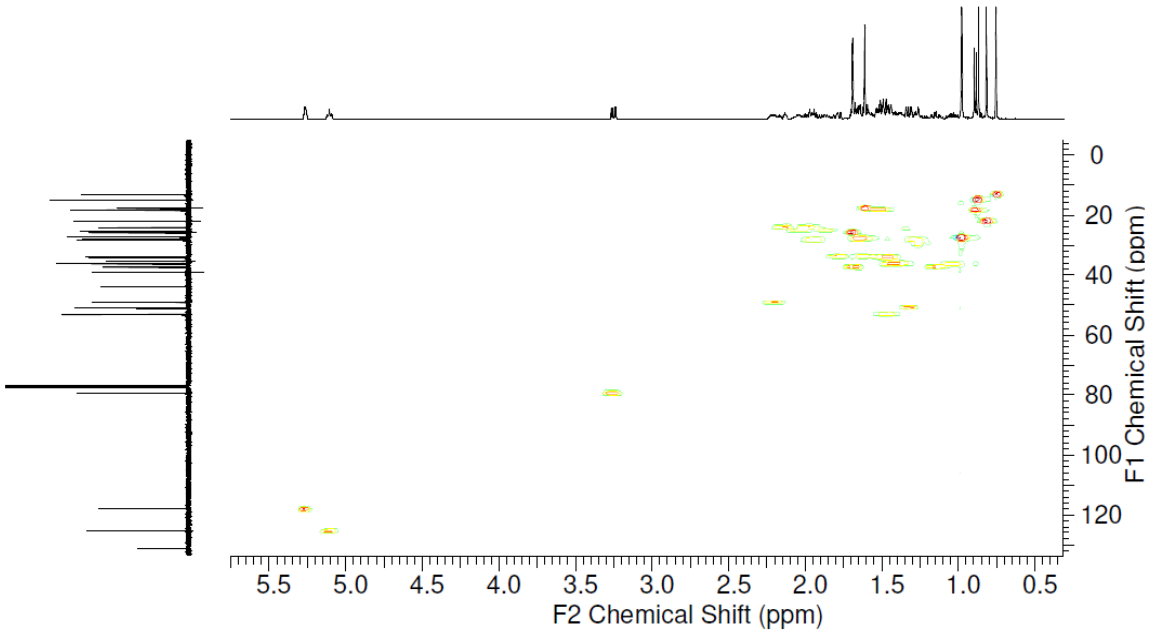

Figure 21S. *HSQC spectrum of tirucalla-7,24-dien-3β-ol (**3**)*

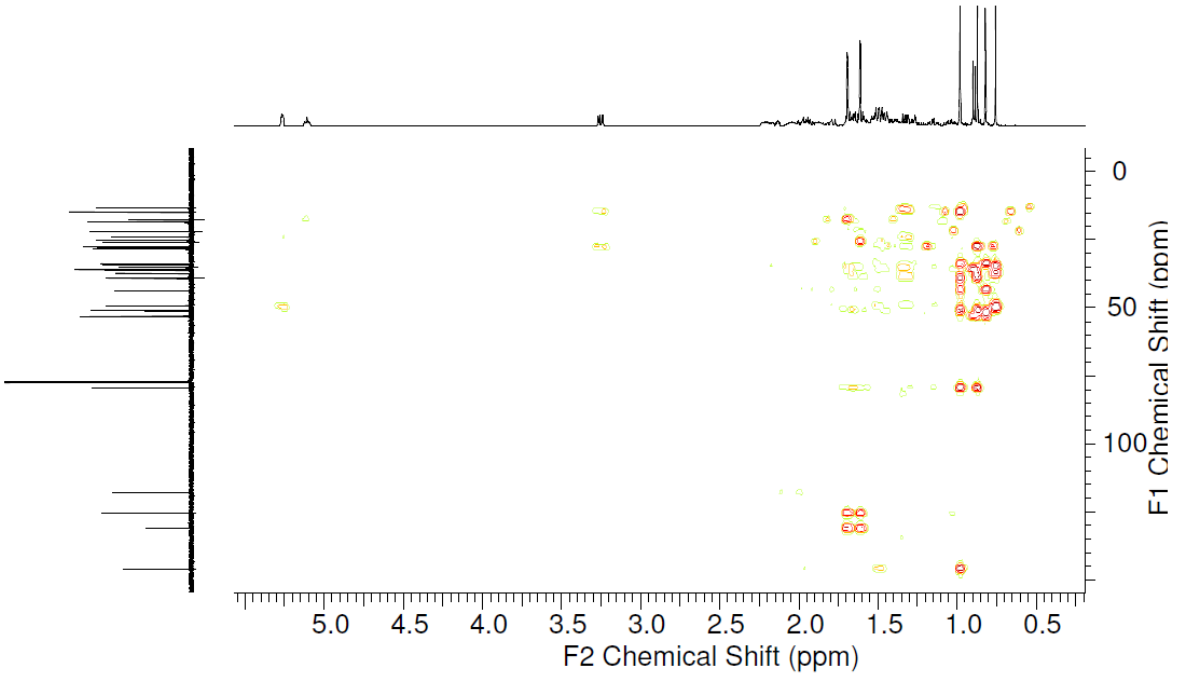

Figure 22S. *HMBC spectrum of tirucalla-7,24-dien-3β-ol (**3**)*

LC-HR-APCI-MS analysis for (2) and (3)

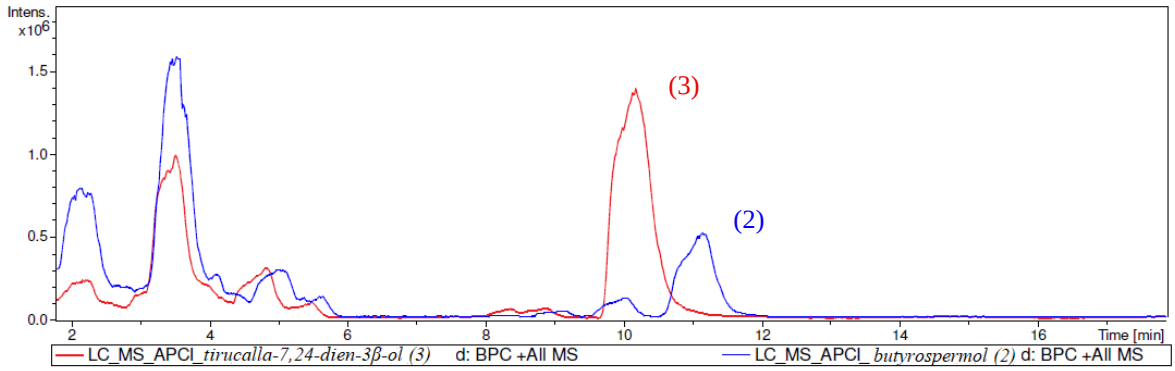

Figure 23S. *Analysis LC-HR-APCI-MS for substances butyrospermol (**2**) and tirucalla-7,24-dien-3β-ol (**3**). Full LC-APCI-QTOF-MS base peak chromatogram (BPC) (positive mode) of tirucalla-7,24-dien-3β-ol (**3**) (red color) and butyrospermol (**2**) (blue color)*

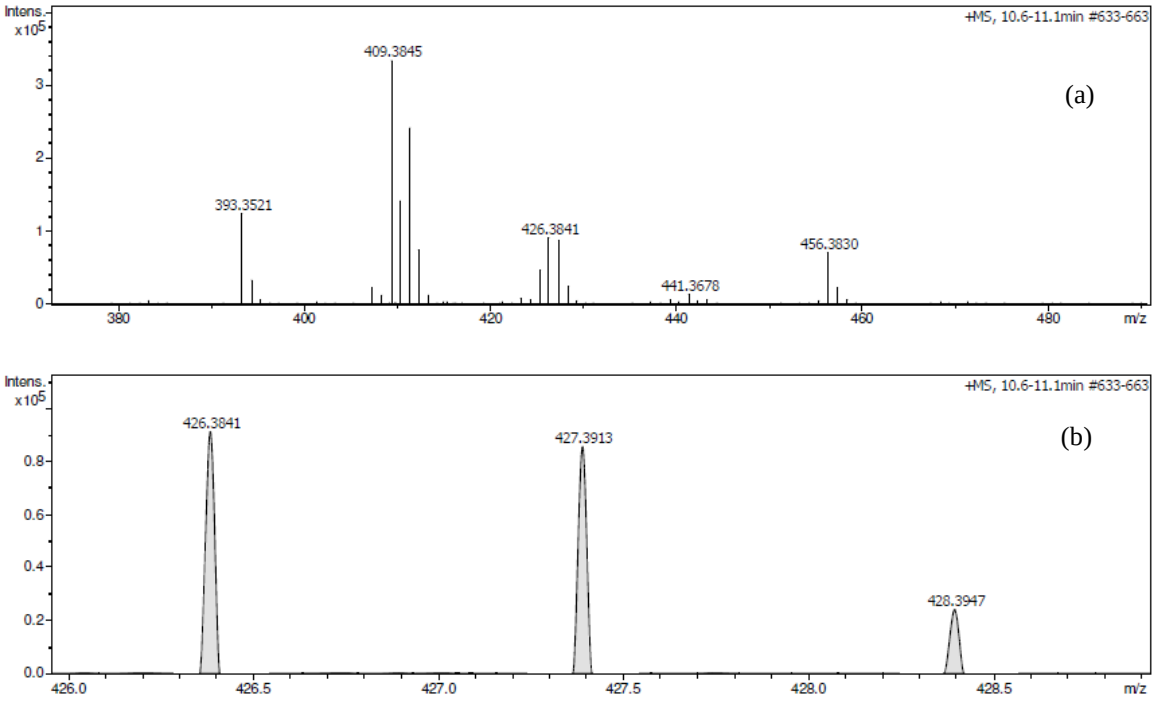

Figure 24S. *(a) Full HR-APCI-MS (positive mode) spectrum of butyrospermol (**2**); (b) HR-APCI-MS (positive mode) spectrum of butyrospermol (**2**) in the m/z 427 region*

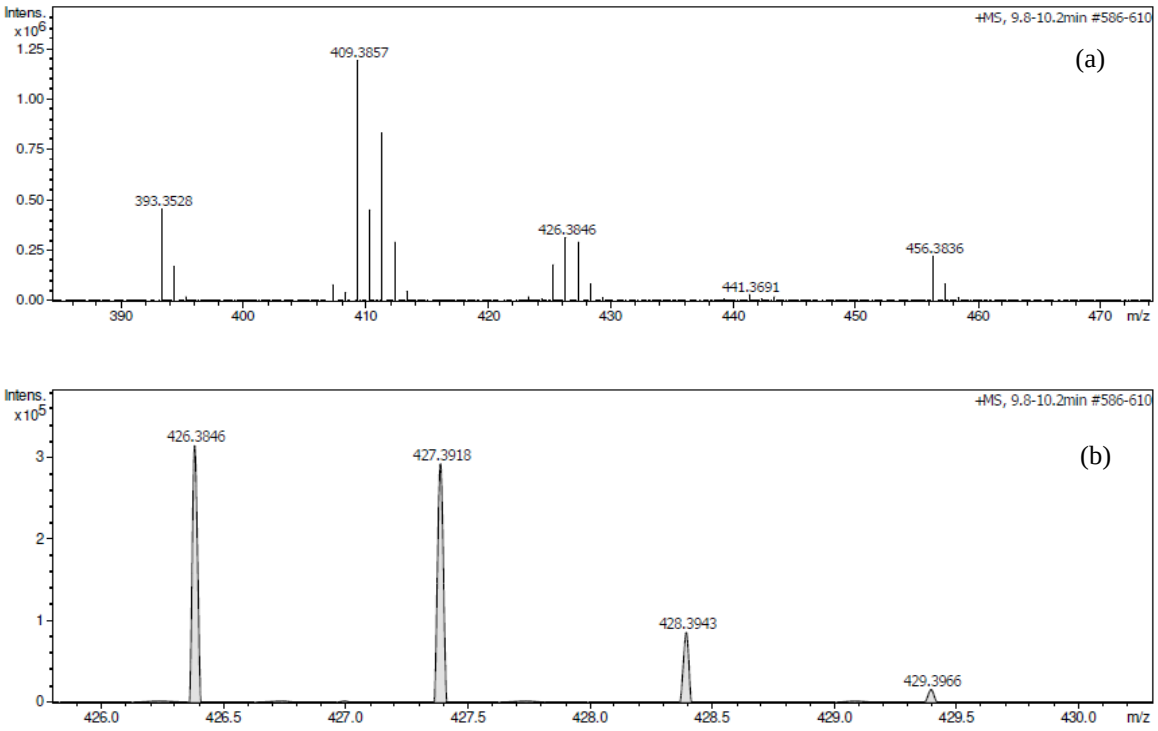

Figure 25S. *(a) Full HR-APCI-MS (positive mode) spectrum of tirucalla-7,24-dien-3β-ol (**3**); (b) HR-APCI-MS (positive mode) spectrum of tirucalla-7,24-dien-3β-ol (**3**) in the m/z 427 region*

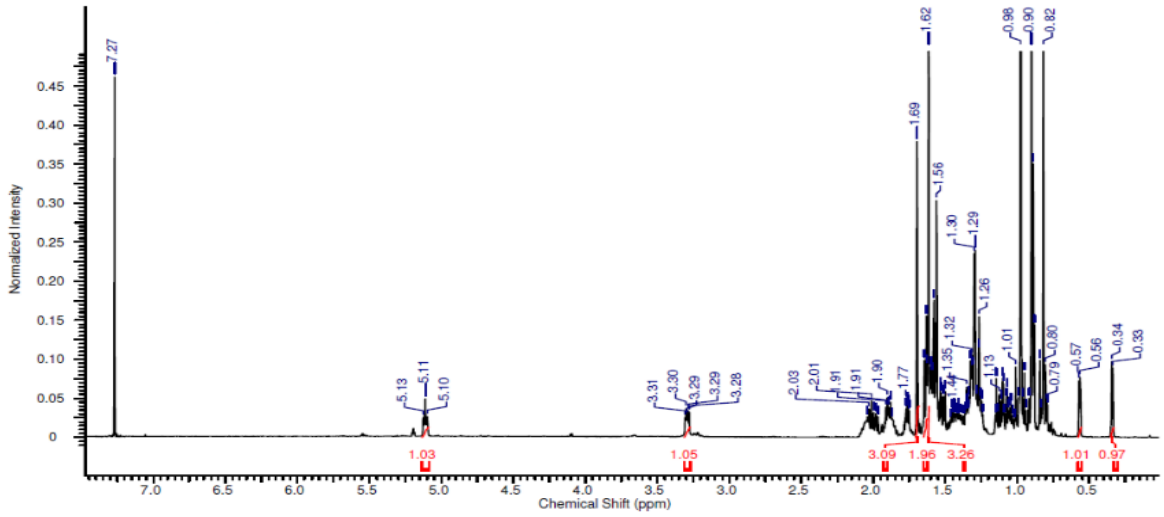

Figure 26S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of cicloartenol (**4**)*

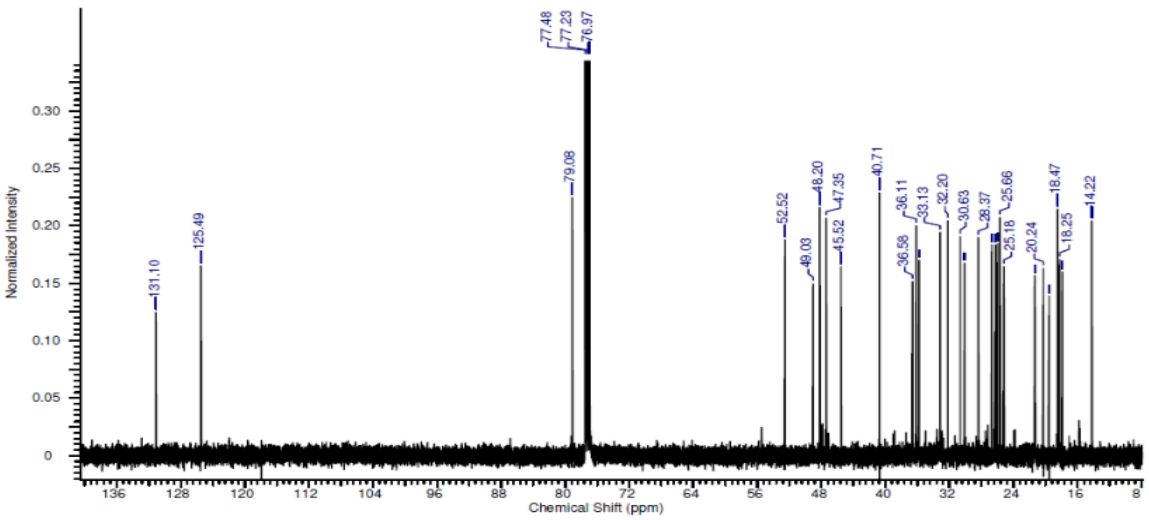

Figure 27S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of cycloartenol (**4**)*

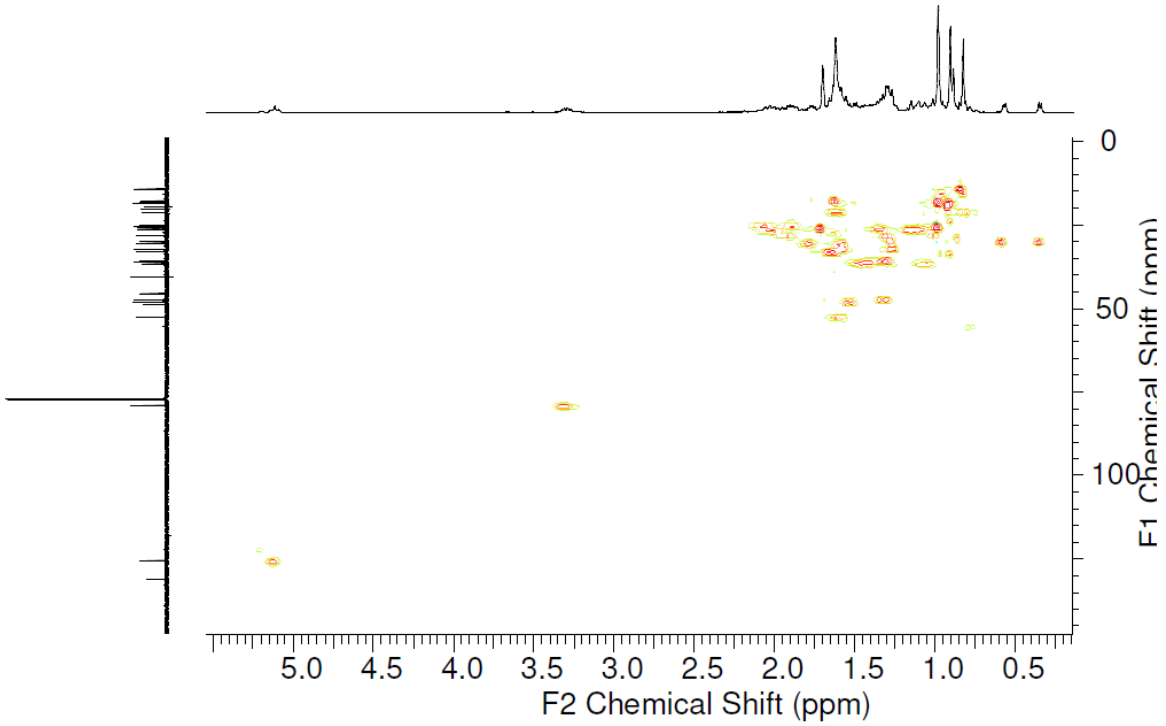

Figure 28S. *HSQC spectrum of cycloartenol (**4**)*

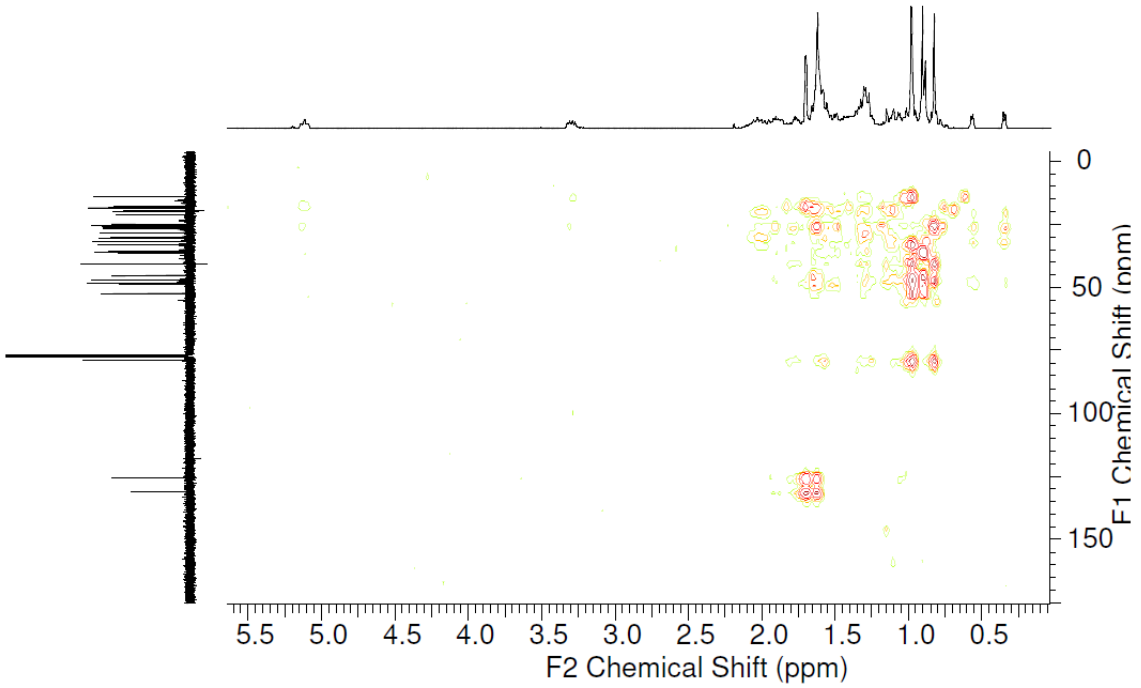

Figure 29S. *HMBC spectrum of cycloartenol* ***(4)***

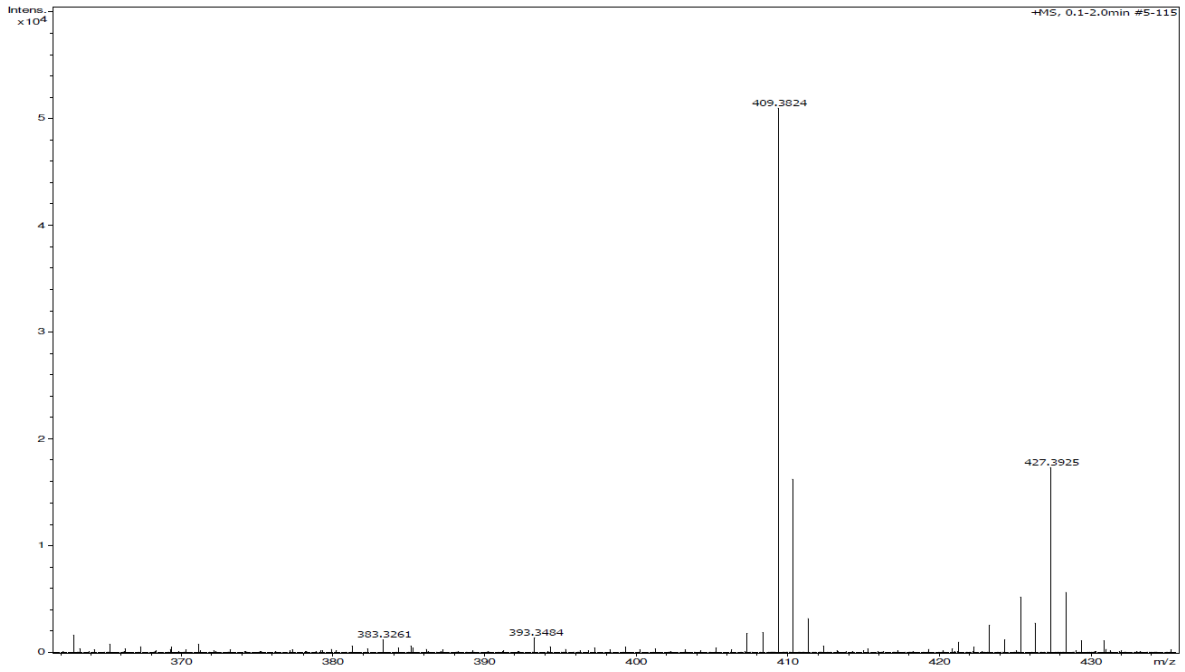

Figure 30S. *HR-APCI-MS (positive mode) spectrum of cycloartenol* ***(4)***

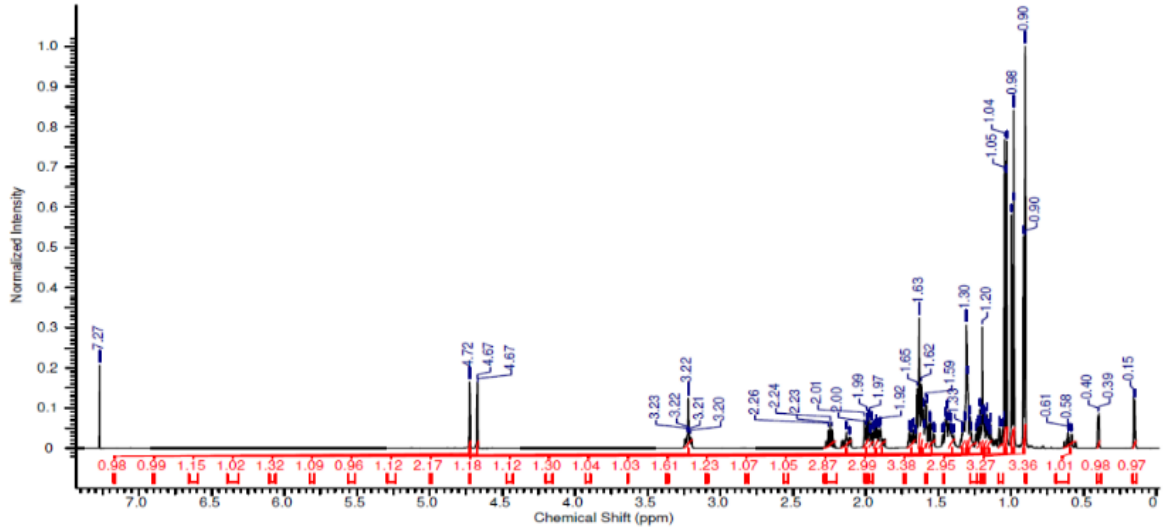

Figure 31S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of cicloeucalenol (**5**)*

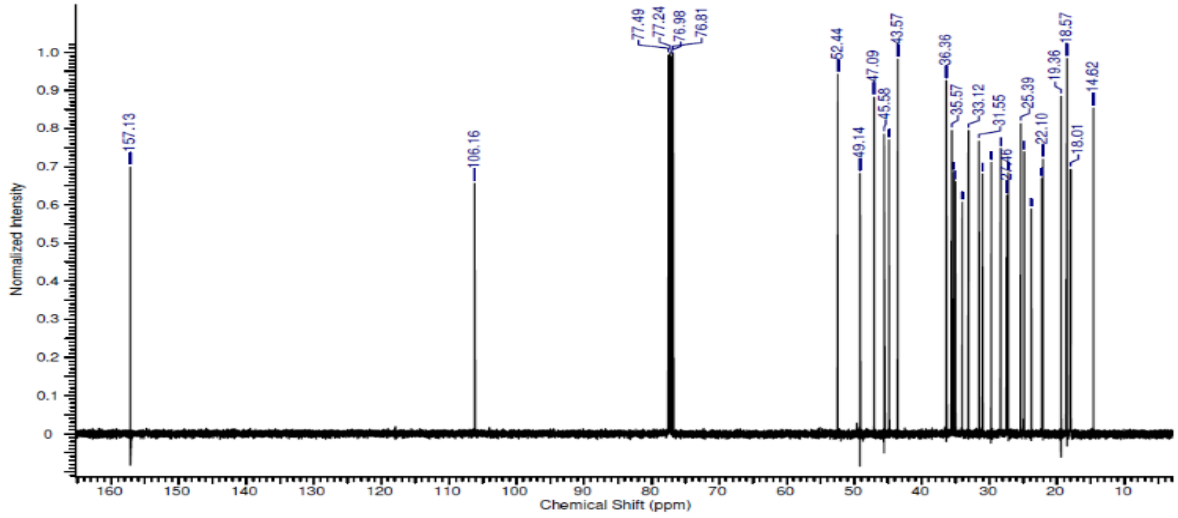

Figure 32S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of cycloeucalenol (**5**)*

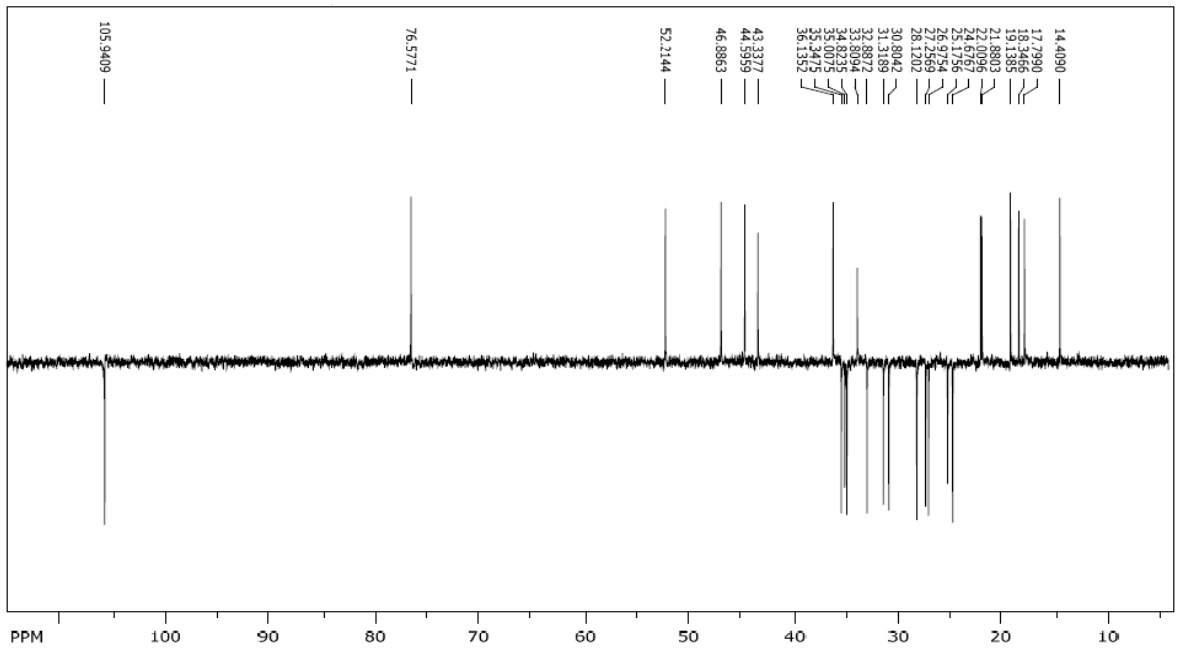

Figure 33S. *DEPT-135 spectrum ($CDCl_3$,75 MHz) of cycloeucalenol (**5**)*

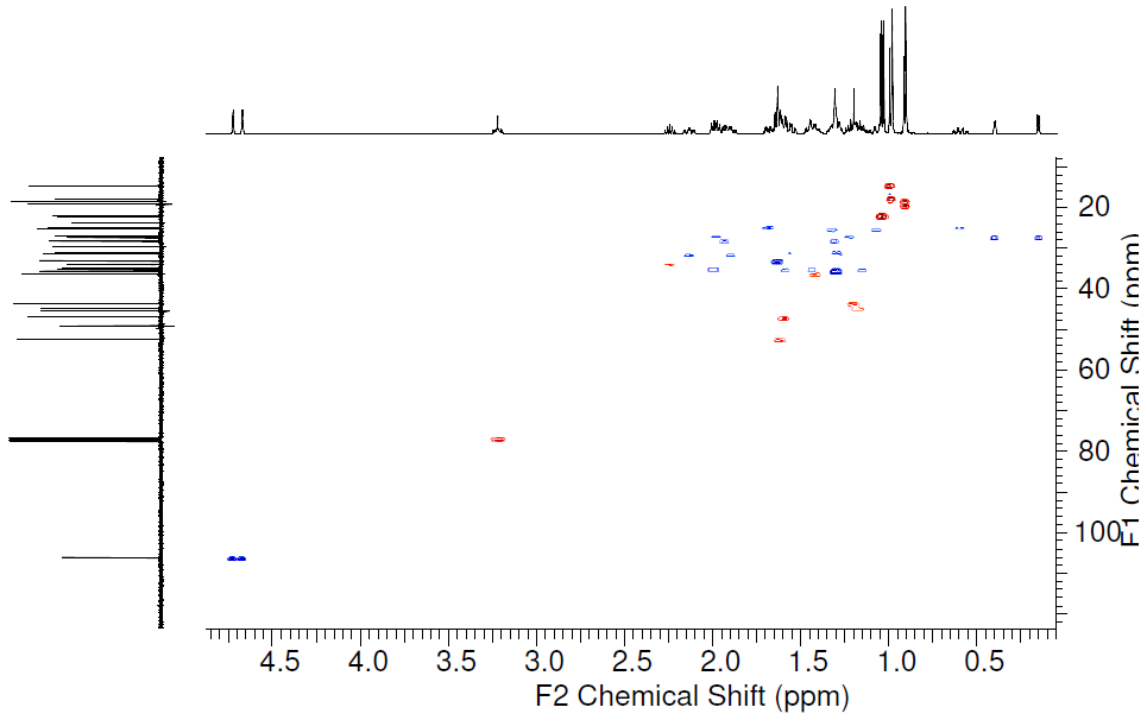

Figure 34S. *HSQC spectrum of cycloeucalenol (**5**)*

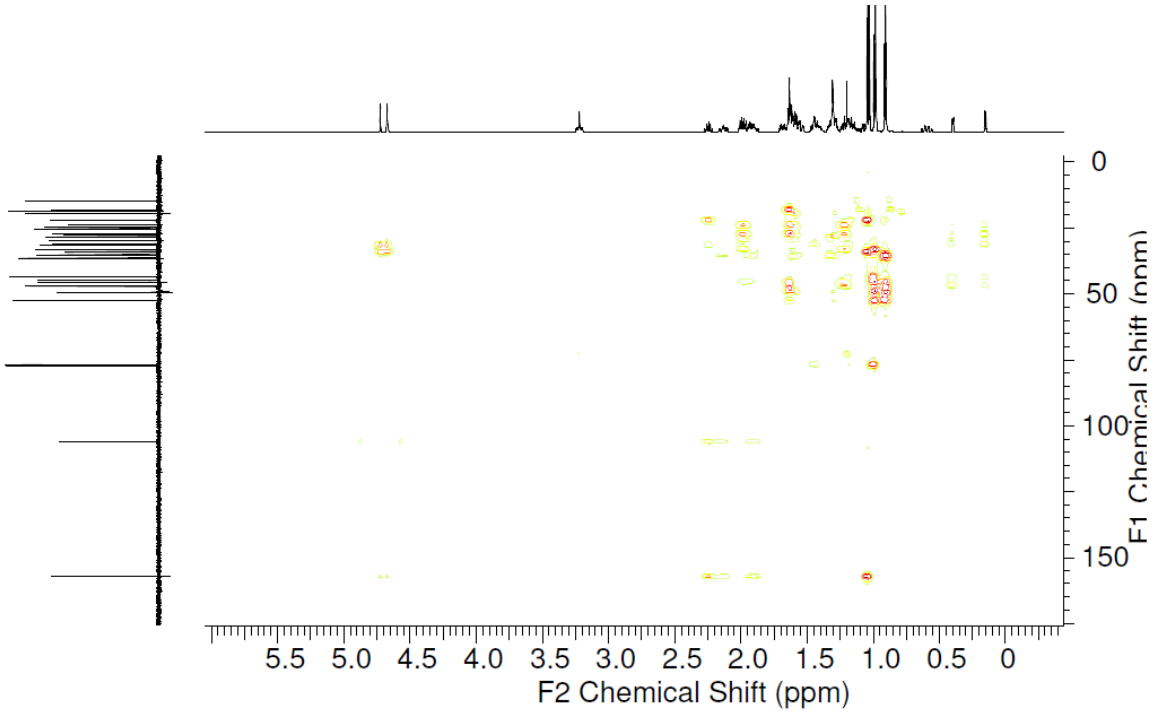

Figure 35S. *HMBC spectrum of cycloeucalenol (**5**)*

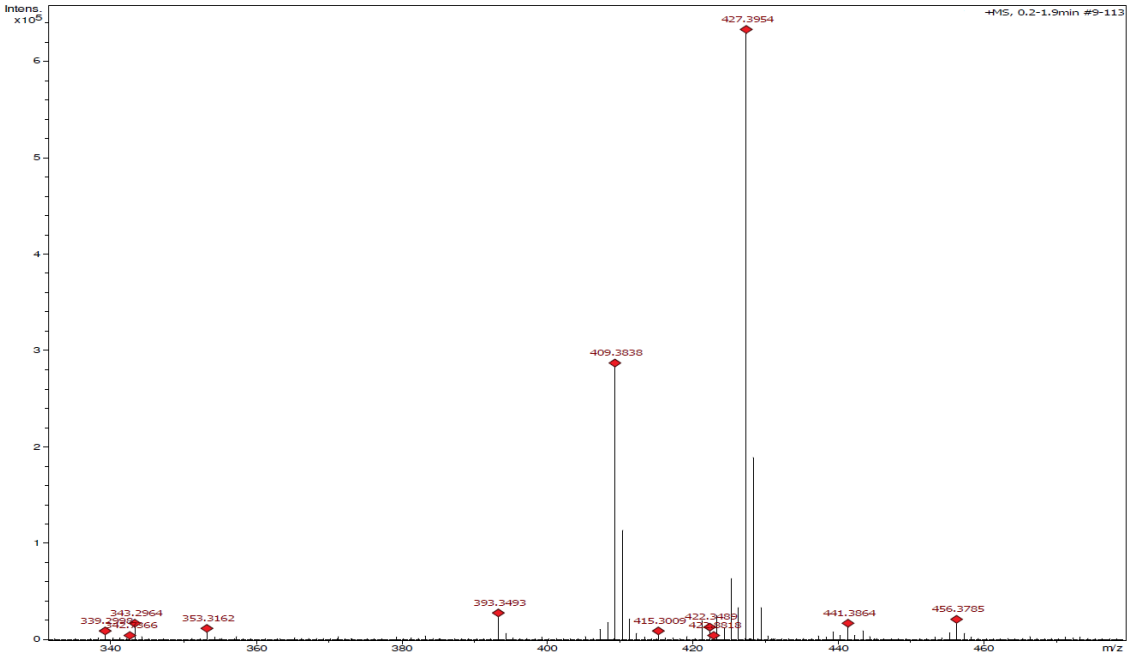

Figure 36S. *HR-APCI-MS (positive mode) spectrum of cycloeucalenol (**5**)*

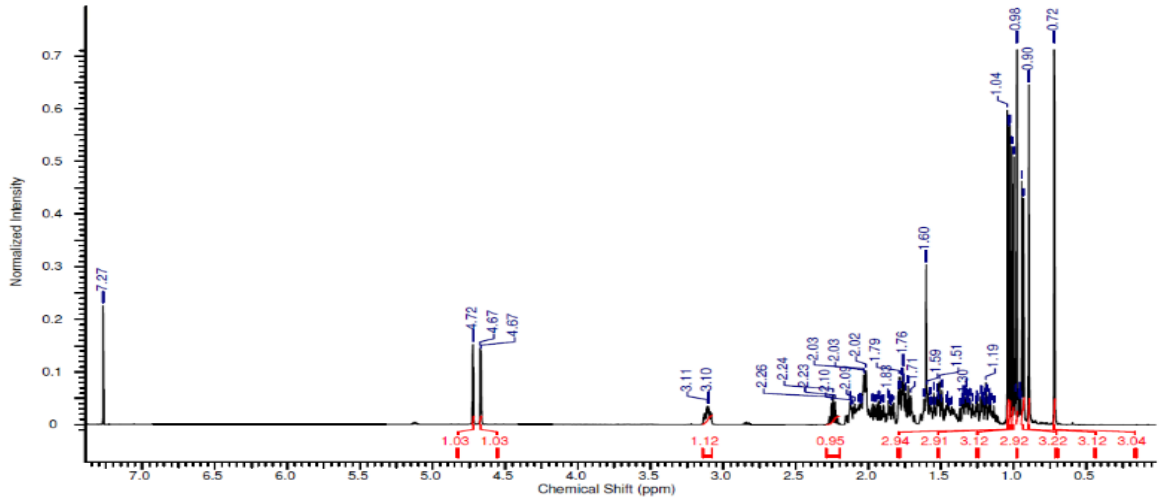

Figure 37S. *^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of obtusifoliol (**6**)*

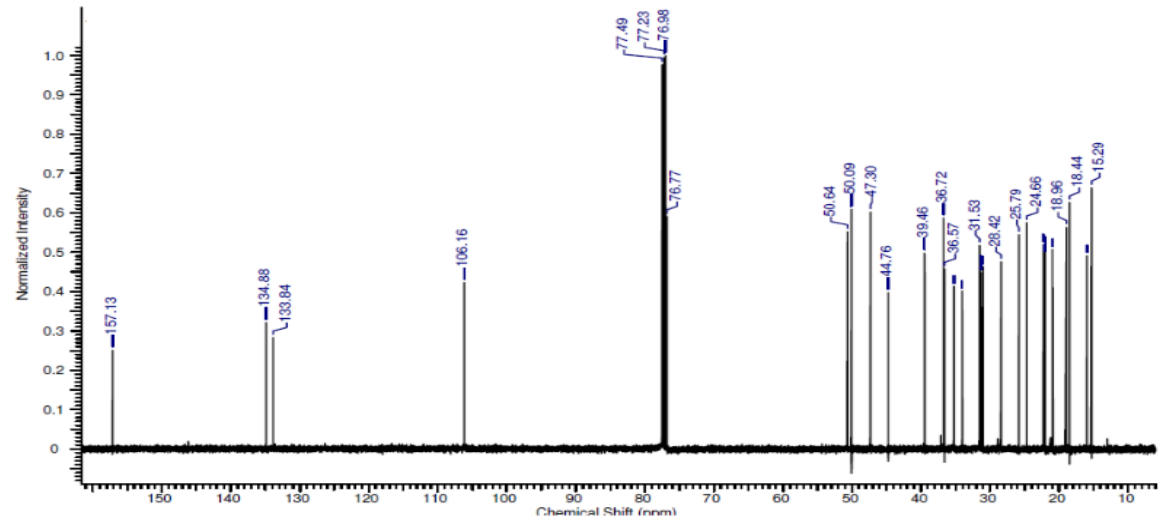

Figure 38S. *^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of obtusifoliol (**6**)*

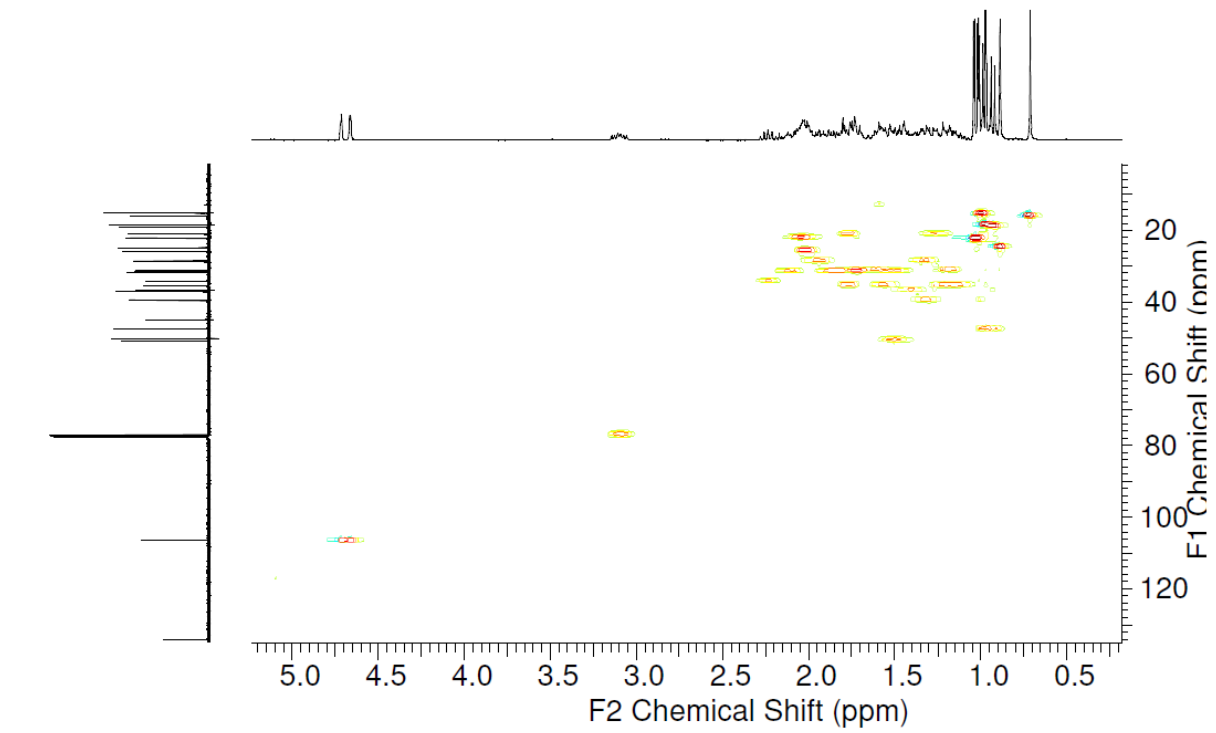

Figure 39S. *HSQC spectrum of obtusifoliol (**6**)*

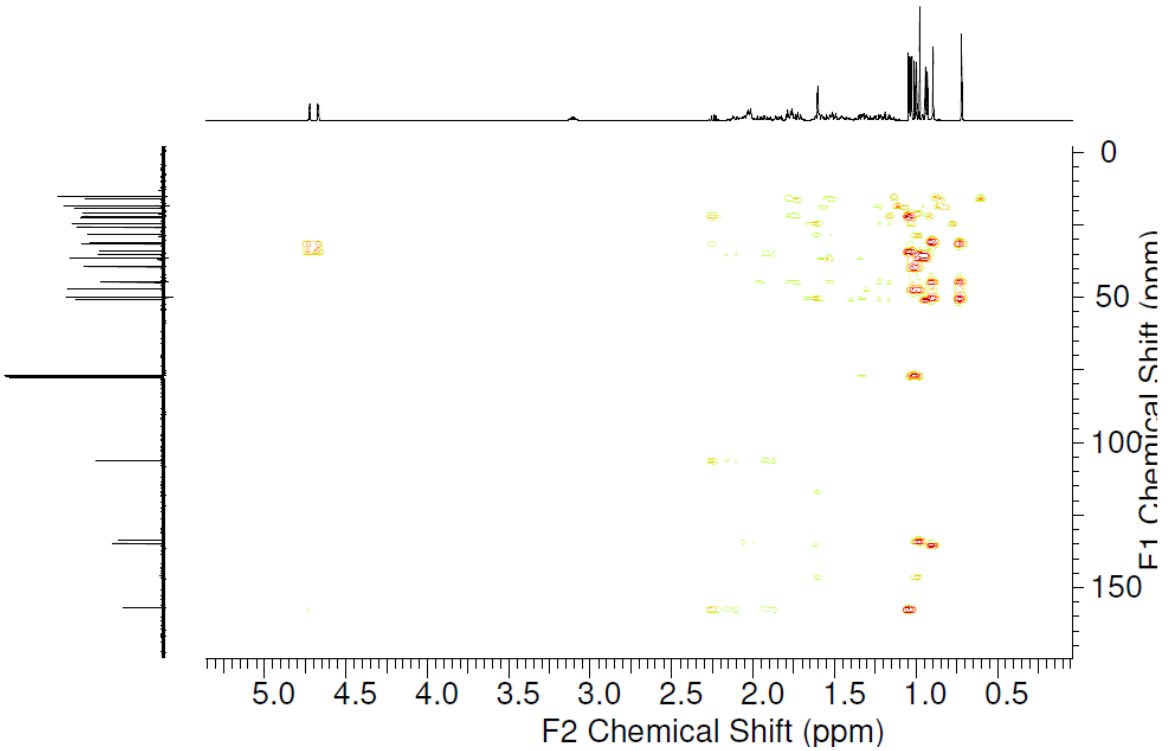

Figure 40S. *HMBC spectrum of obtusifoliol (**6**)*

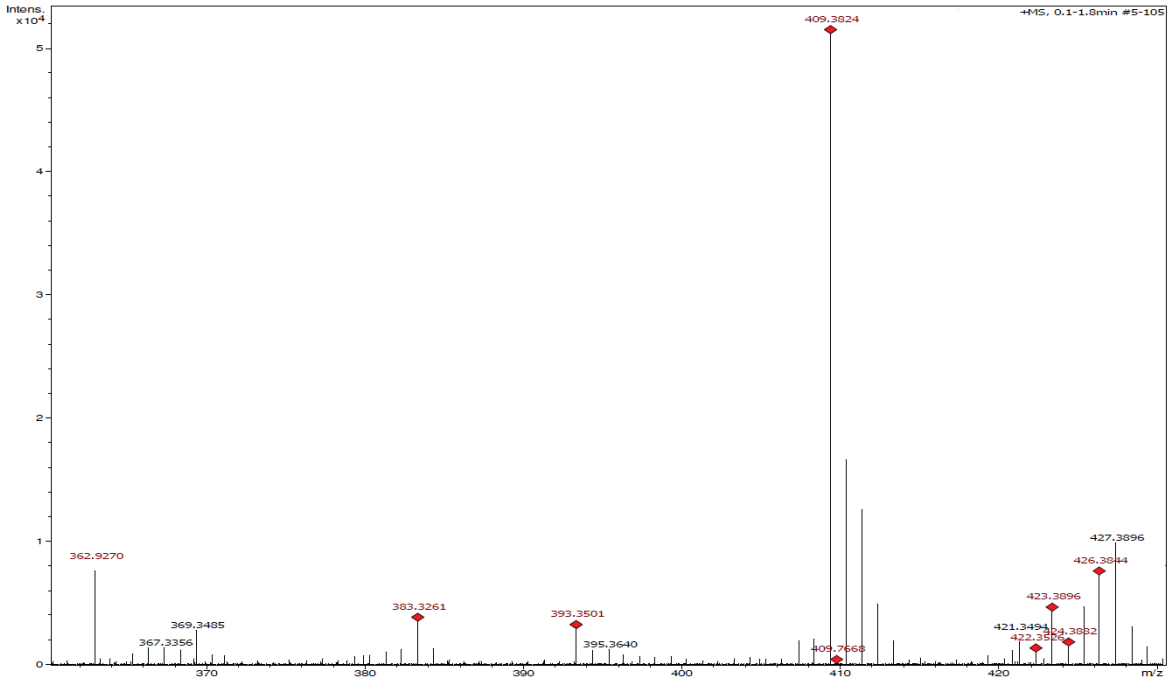

Figure 41S. *HR-APCI-MS (positive mode) spectrum of obtusifoliol (**6**)*

Analysis of methyl ester mixture (MIST-1 and MIST-3) and lupeol by GC-MS after transesterification

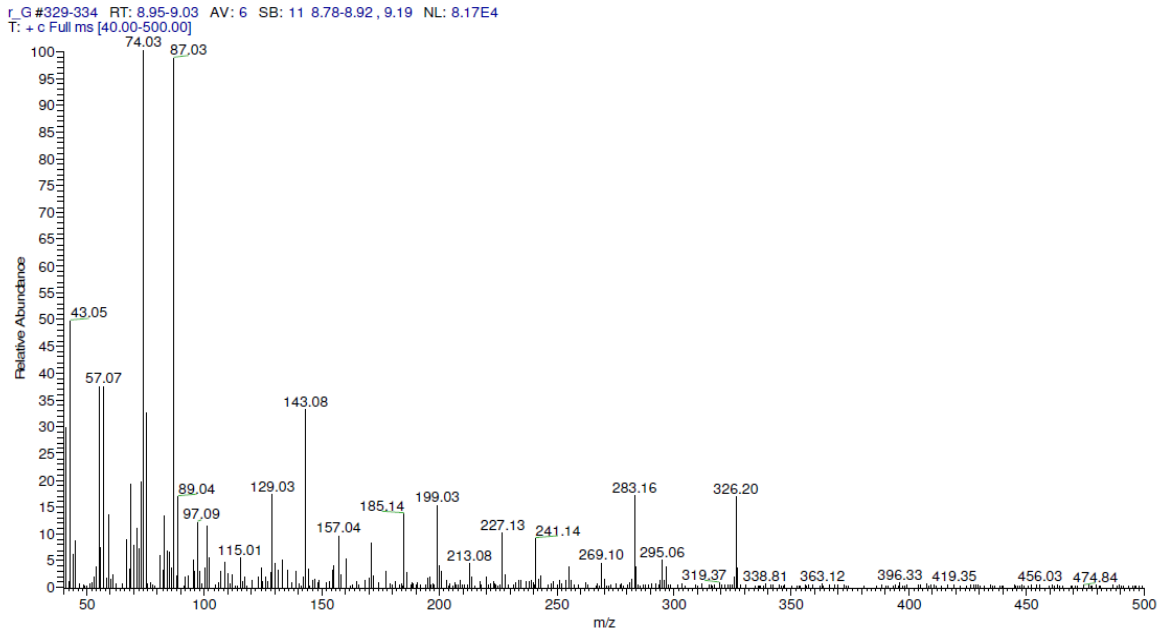

Figure 42S. *GC-MS spectrum of **MIST-1a'***

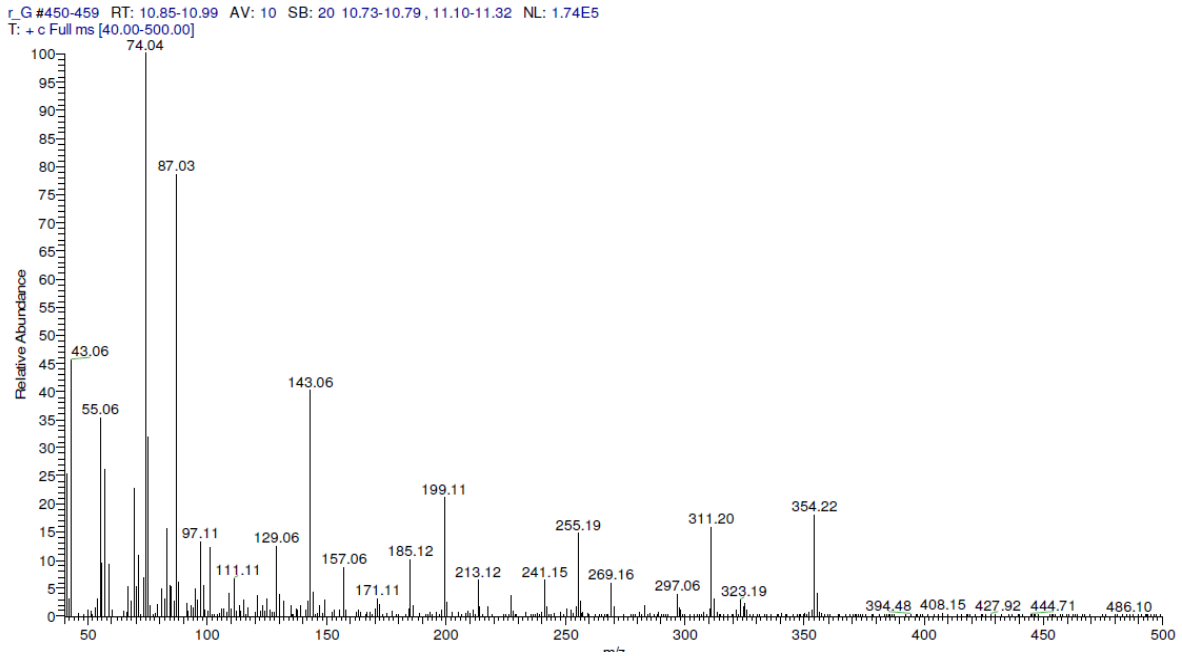

Figure 43S. *GC-MS spectrum of* ***MIST-1b'***

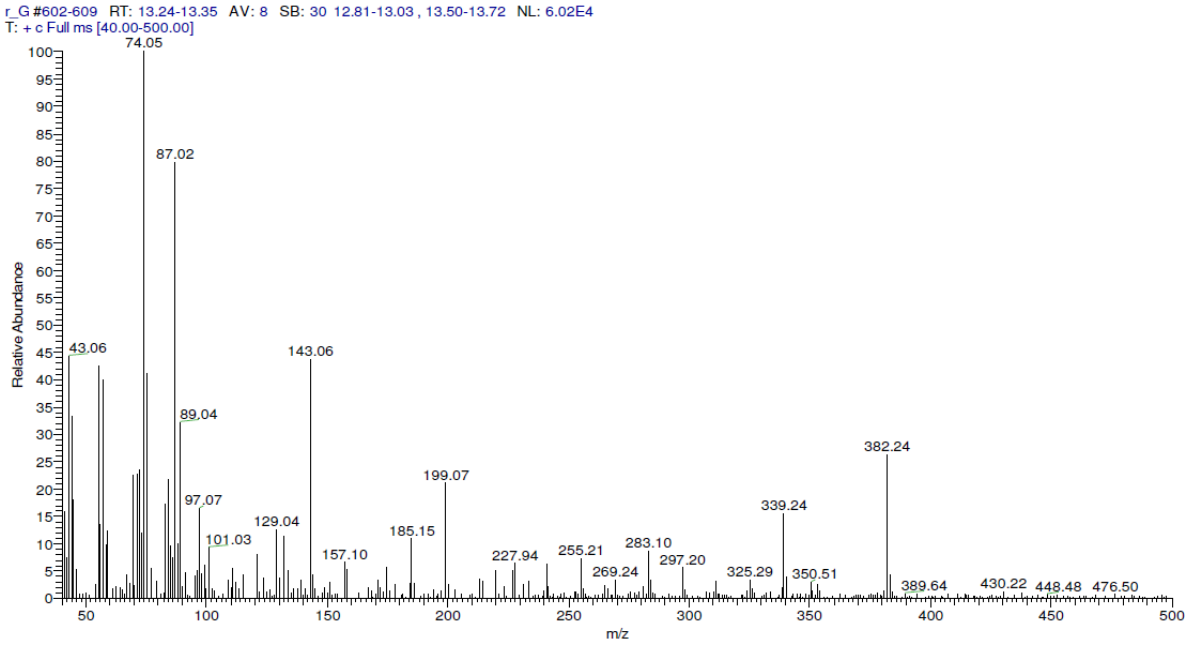

Figure 44S. *GC-MS spectrum of* ***MIST-1c'***

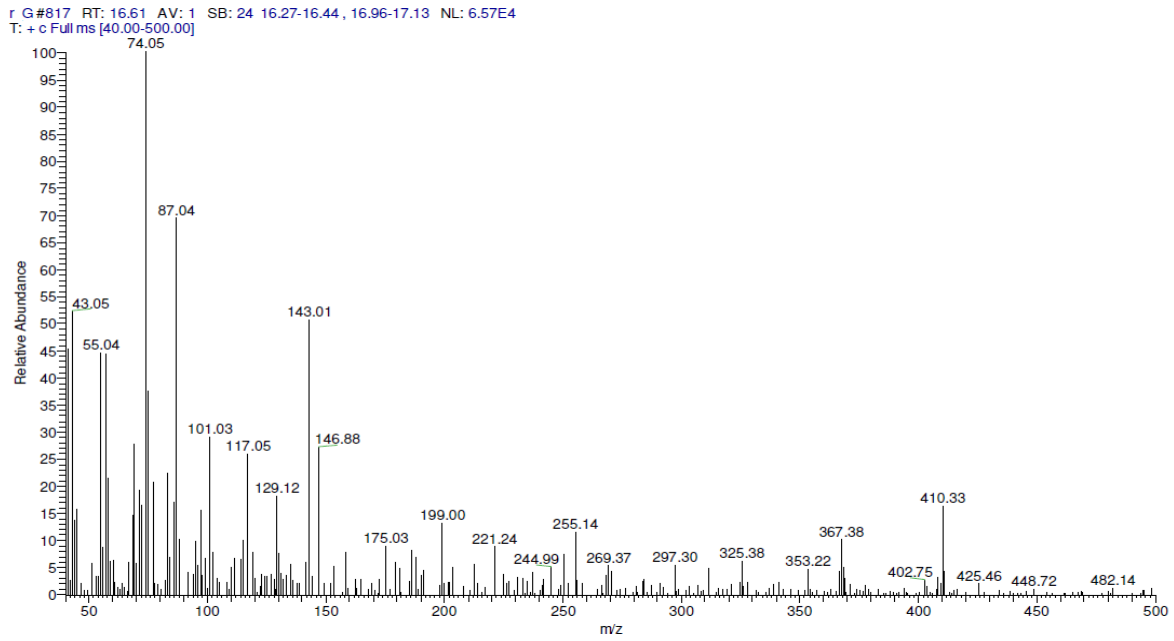

Figure 45S. *GC-MS spectrum of* ***MIST-1d'***

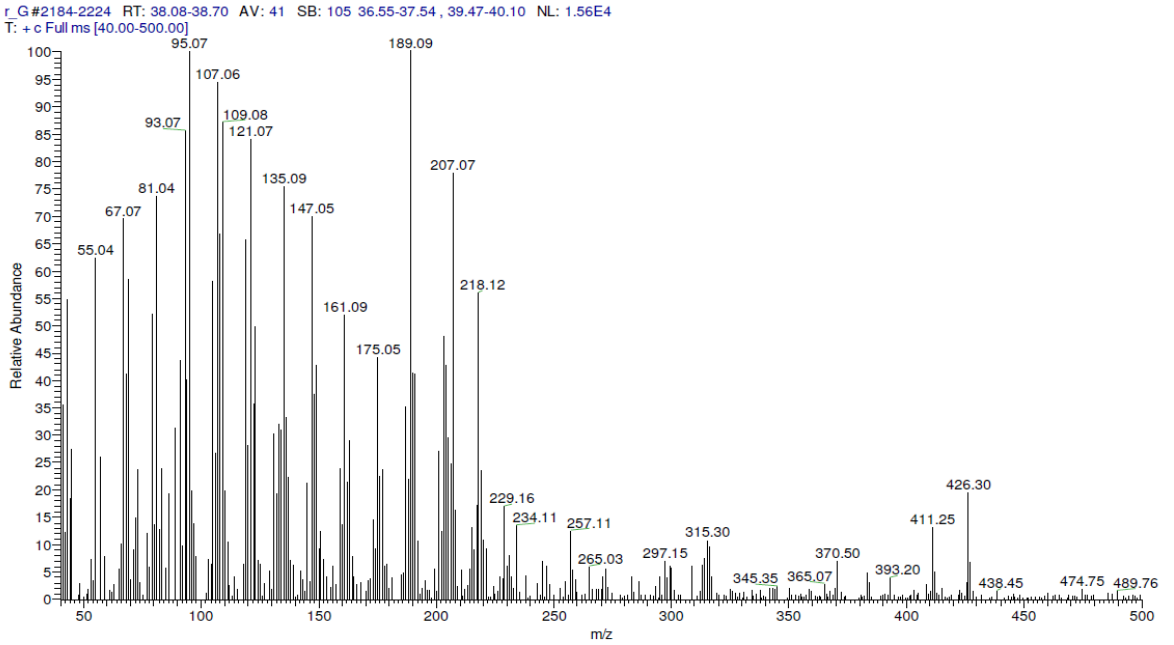

Figure 46S. *GC-MS spectrum of lupeol obtained after transesterification of* ***MIST-1***

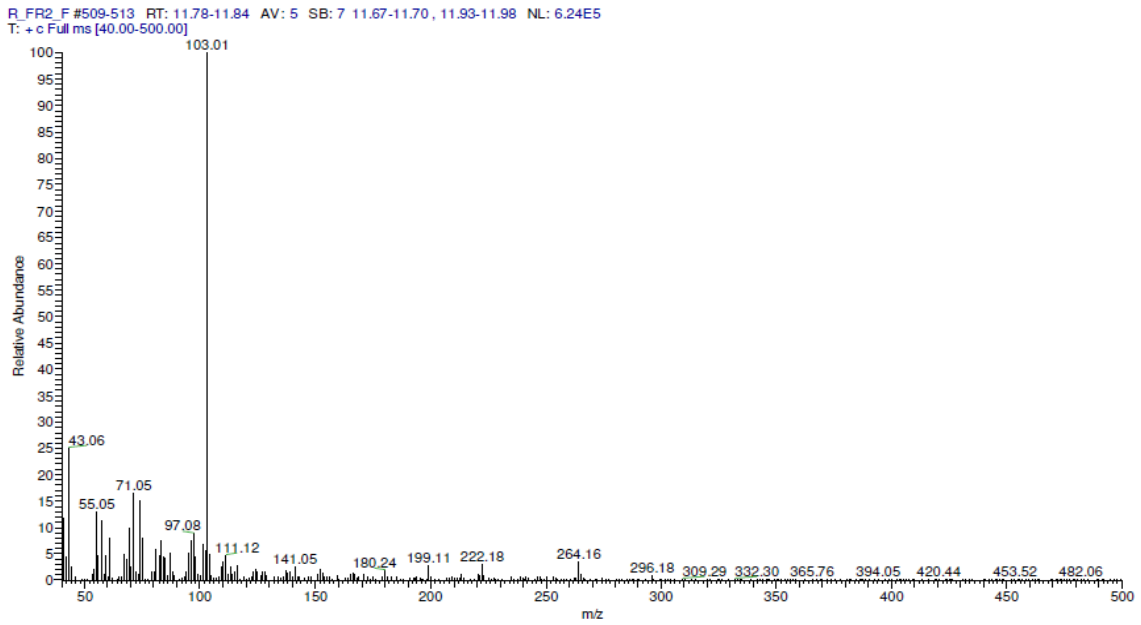

Figure 47S. *GC-MS spectrum of* ***MIST-3a'***

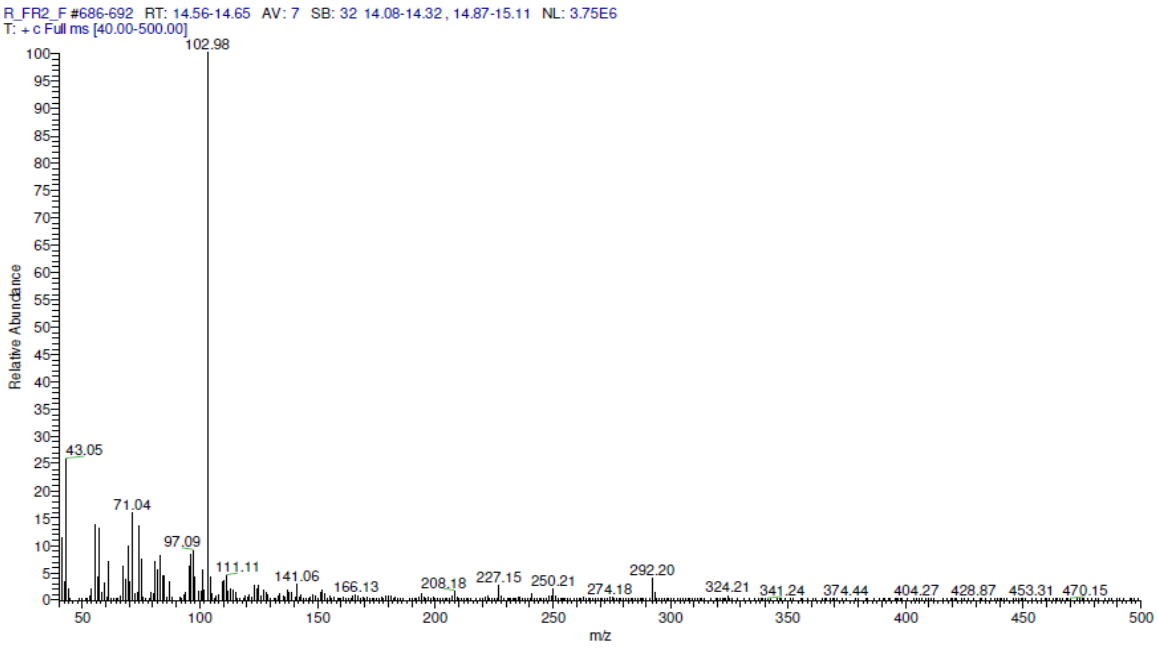

Figure 48S. *GC-MS spectrum of* ***MIST-3b'***

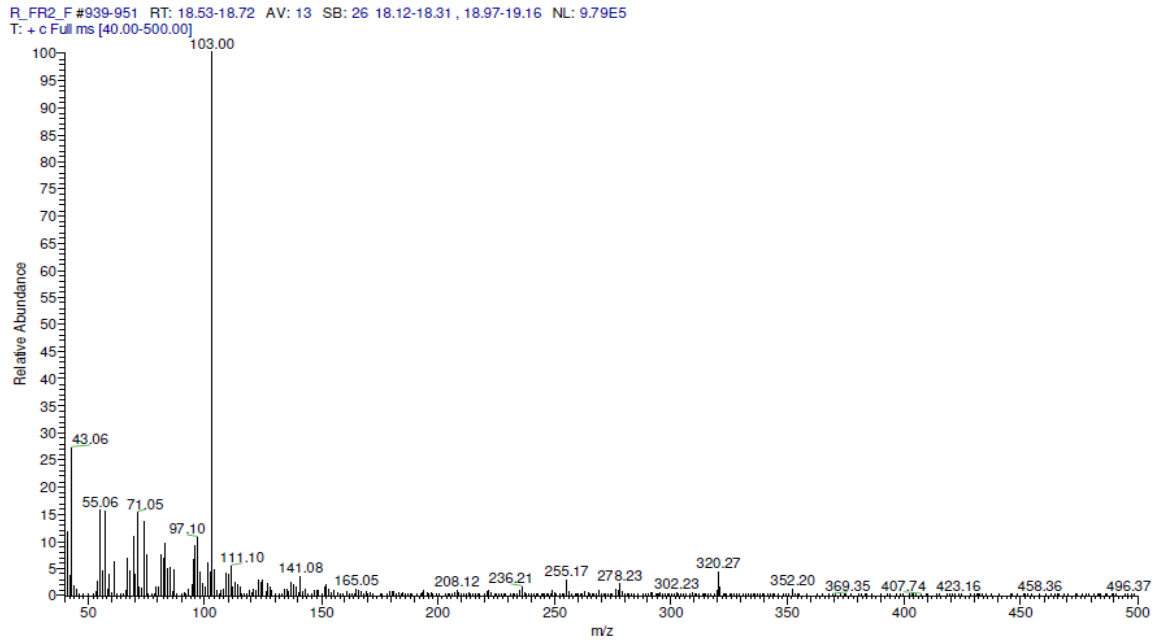

Figure 49S. *GC-MS spectrum of* ***MIST-3c'***

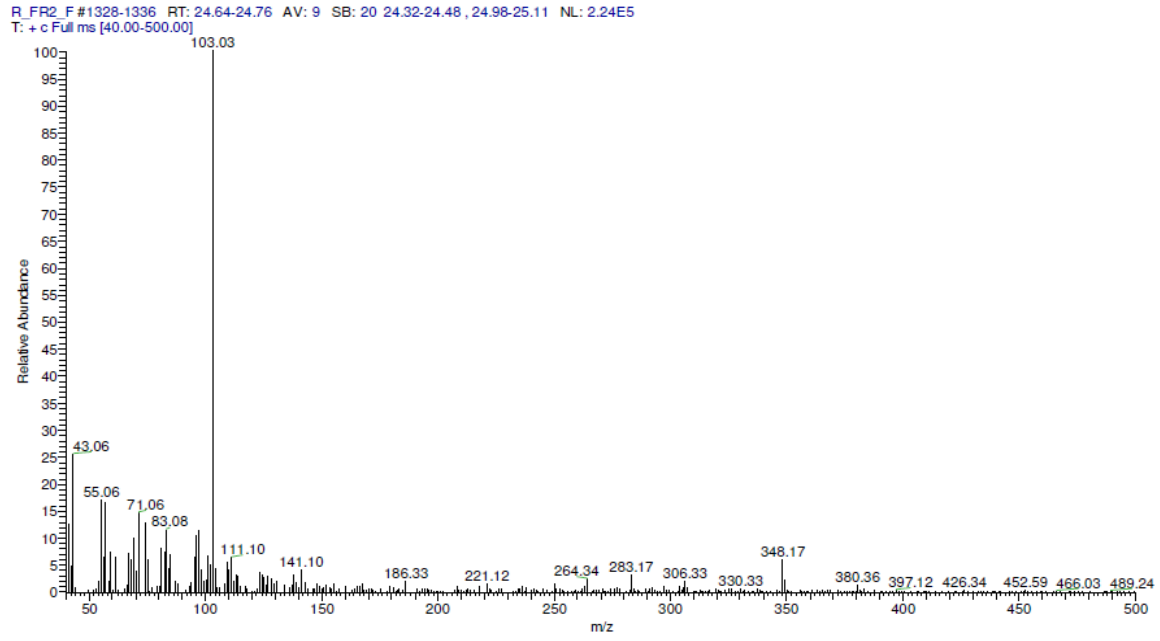

Figure 50S. *GC-MS spectrum of* ***MIST-3d'***

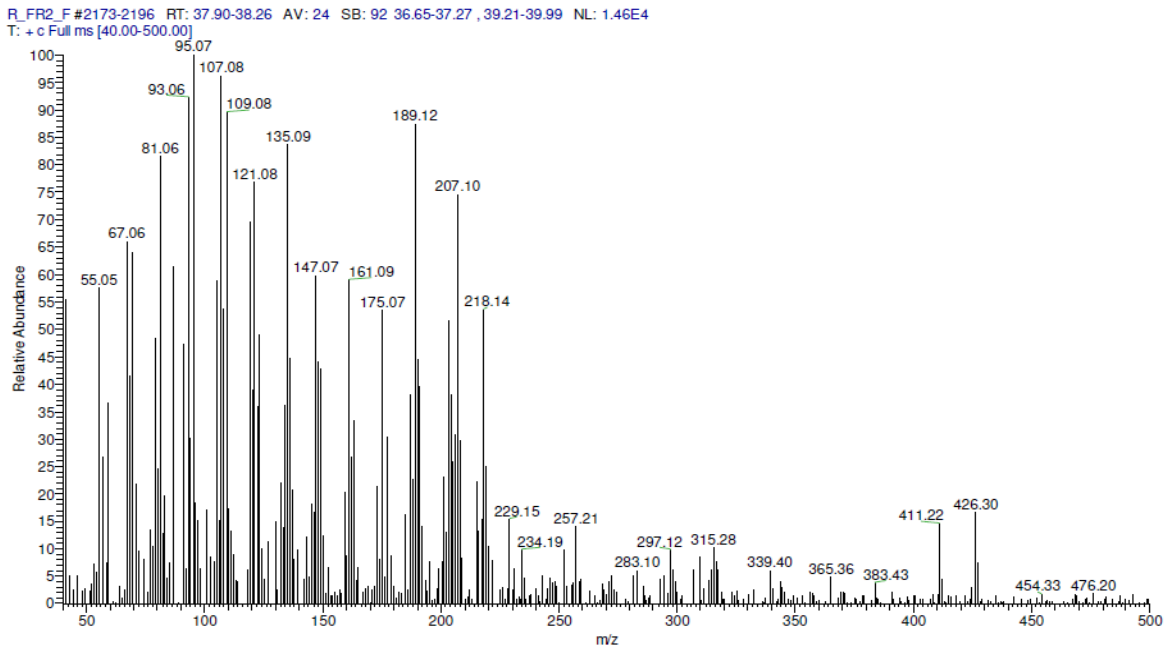

Figure 51S. *GC-MS spectrum of lupeol obtained after transesterification of* ***MIST-3***

Analysis by GC-MS for mixture of acetylated triterpenes (MIST-2)

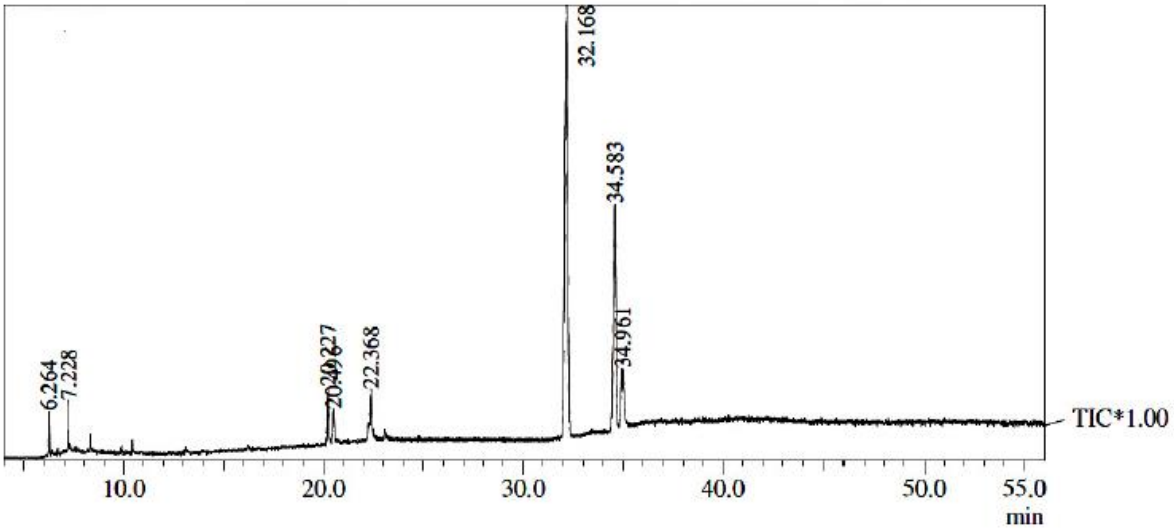

Figure 52S. *GC-MS Chromatogram of* ***MIST-2*** *(mixture of acetylated triterpenes- α-amyrin acetate, β-amyrin acetate and lupeol acetate) isolated from P. amapa*

Table 1S. Analysis by GC-MS of **MIST-2**

Compound	Retention time / min	% Area	*m/z*
β-Amyrin acetate	32.168	54.60	218; 203; 189
α-Amyrin acetate	34.583	27.21	218; 203; 189
Lupeol acetate	34.961	5.98	189

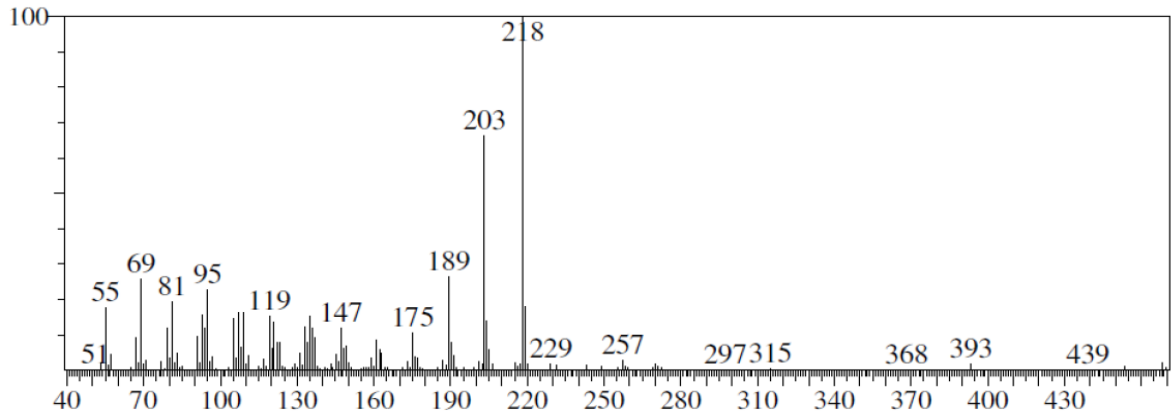

Figure 53S. *GC-MS spectrum of β-amyrin acetate obtained of* ***MIST-2*** *(t_R 32.168 min)*

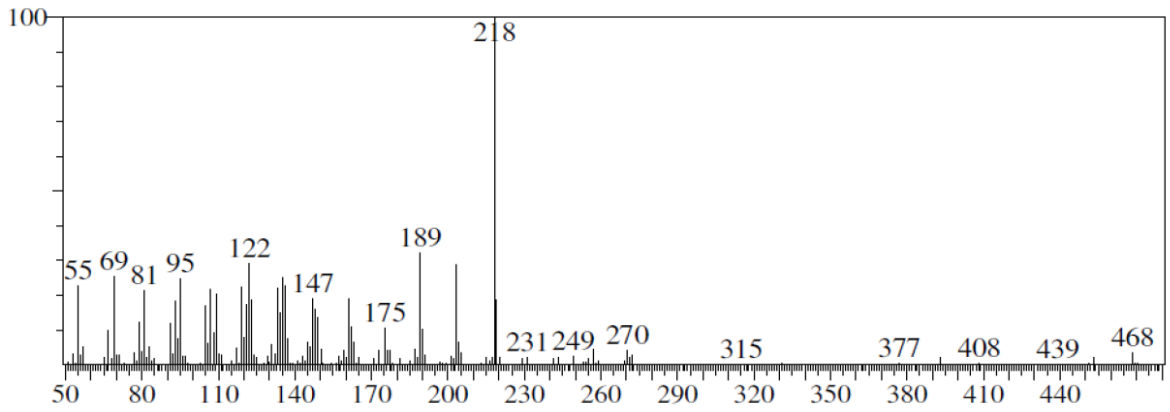

Figure 54S. *GC-MS spectrum of α-amyrin acetate obtained of* ***MIST-2*** *(t_R 34.583 min)*

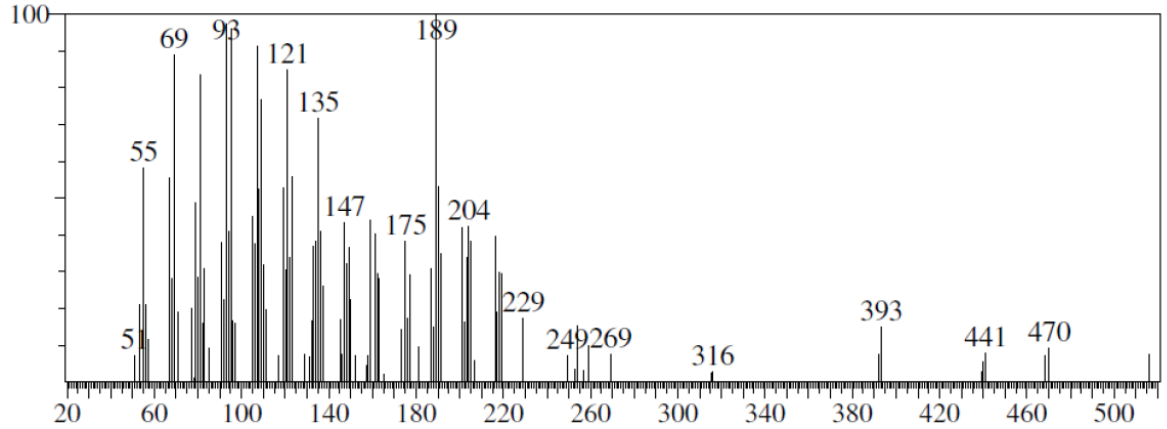

Figure 55S. *GC-MS spectrum of lupeol acetate obtained of* ***MIST-2*** *(t_R 34.958 min)*