

Supporting Information

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Chemical Investigation and Bioactivity Screening of *Salvia cassia* Extracts

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Table of Contents	Page
Figure S1: ¹ H-NMR Spectrum 1 of Compound 1.	2
Figure S2: Expansion of ¹ H-NMR Spectrum of Compound 1. H-12 and H-3 peaks.	3
Figure S3: Expansion of ¹ H-NMR Spectrum of Compound 1. Methyl group peaks.	4
Figure S4: ¹³ C-NMR DEPT Spectrum 1 of Compound 1. All protonated carbons.	5
Figure S5: ¹³ C-NMR DEPT Spectrum of Compound 1.	6
Figure S6: ¹³ C-NMR APT Spectrum of Compound 1. All carbons including quaternary carbons. Methylene carbons and quaternary carbons positive phase and methyl and methine carbons negative phase.	7
Figure S7: Expansion of ¹³ C-NMR APT Spectrum of Compound 1. All carbons including quaternary carbons. Methylene carbons and quaternary carbons negative phase and methyl and methine carbons positive phase.	8
Table S1: Table for comparison of C-13 data of some pentacyclic triterpene skeletons with the assigned carbons of Compound 1.	9
Figure S8: APCI-MS spectrum of Compound 1 and fragmentation patterns	10
Figure S9: GC-MS analysis of <i>Salvia cassia</i> dichloromethane extract	11

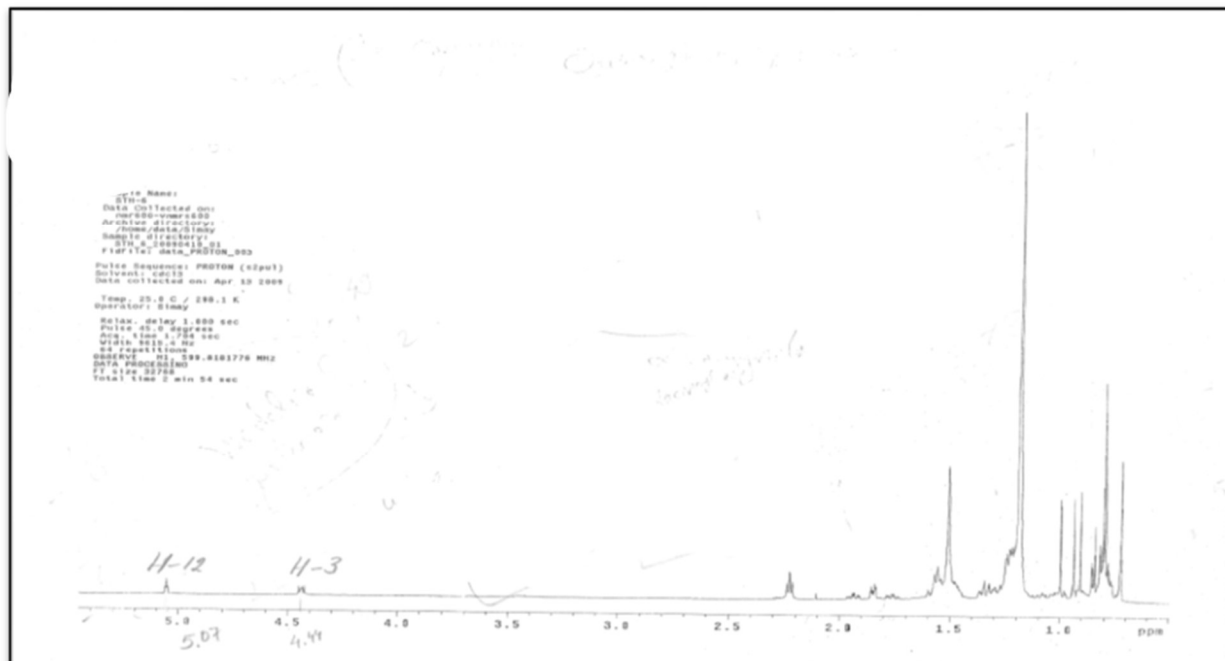


Figure S1. ¹H-NMR Spectrum 1 of Compound 1.

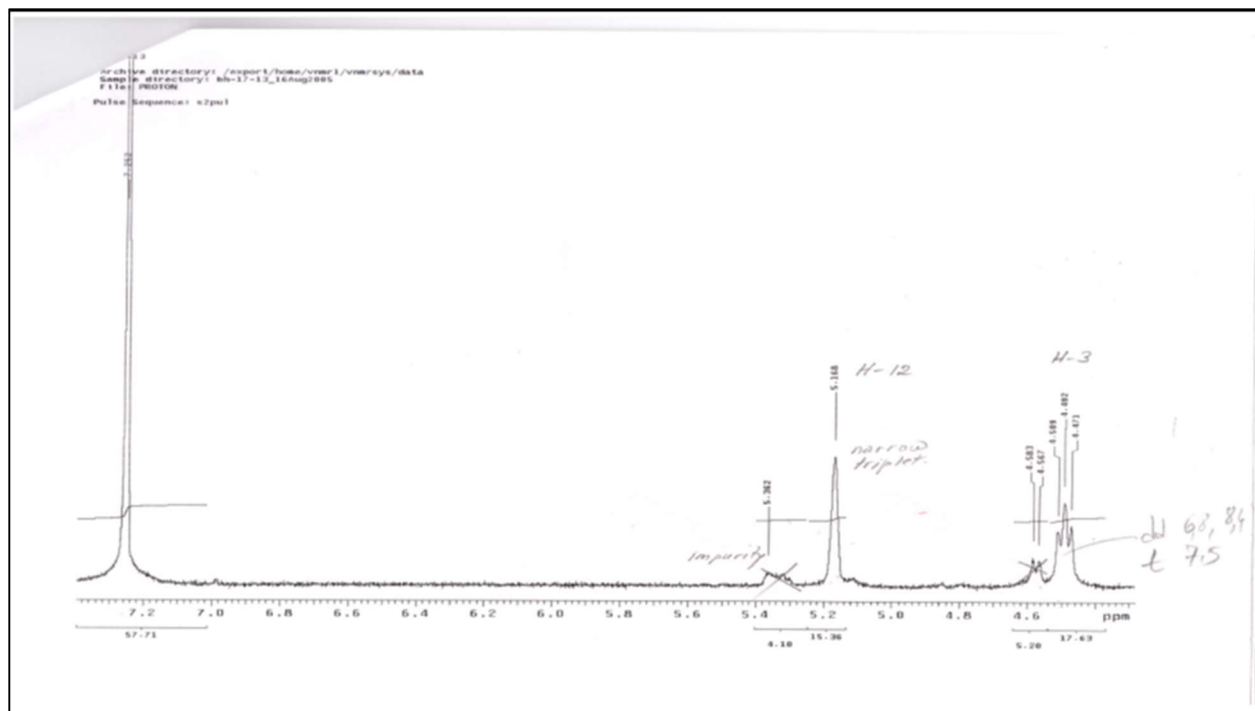


Figure S2. Expansion of $^1\text{H-NMR}$ Spectrum of Compound 1. H-12 and H-3 peaks.

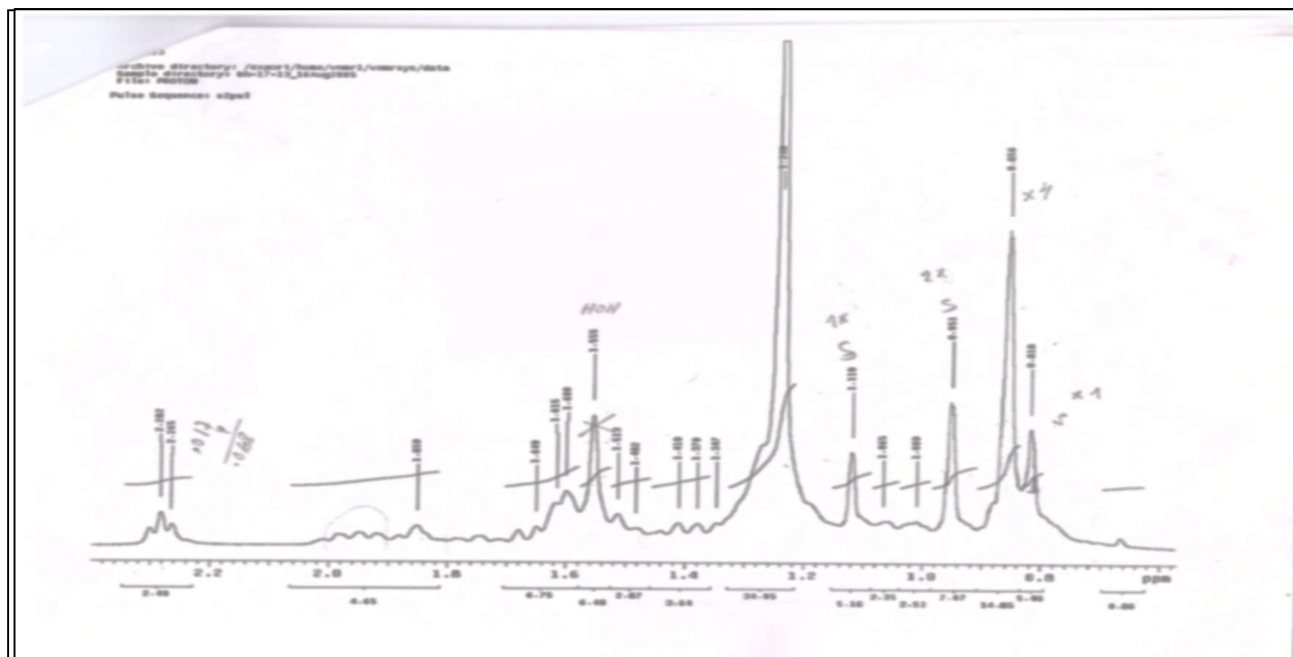


Figure S3. Expansion of $^1\text{H-NMR}$ Spectrum of Compound 1. Methyl group peaks.

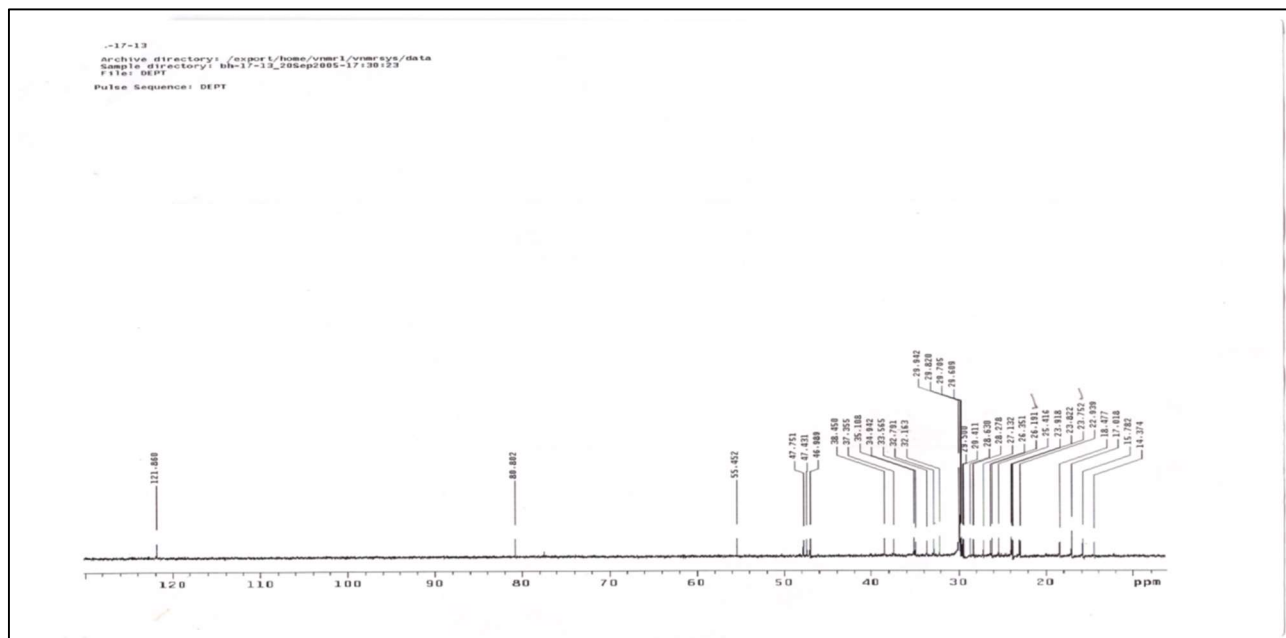


Figure S4. ^{13}C -NMR DEPT Spectrum 1 of Compound **1**. All protonated carbons.

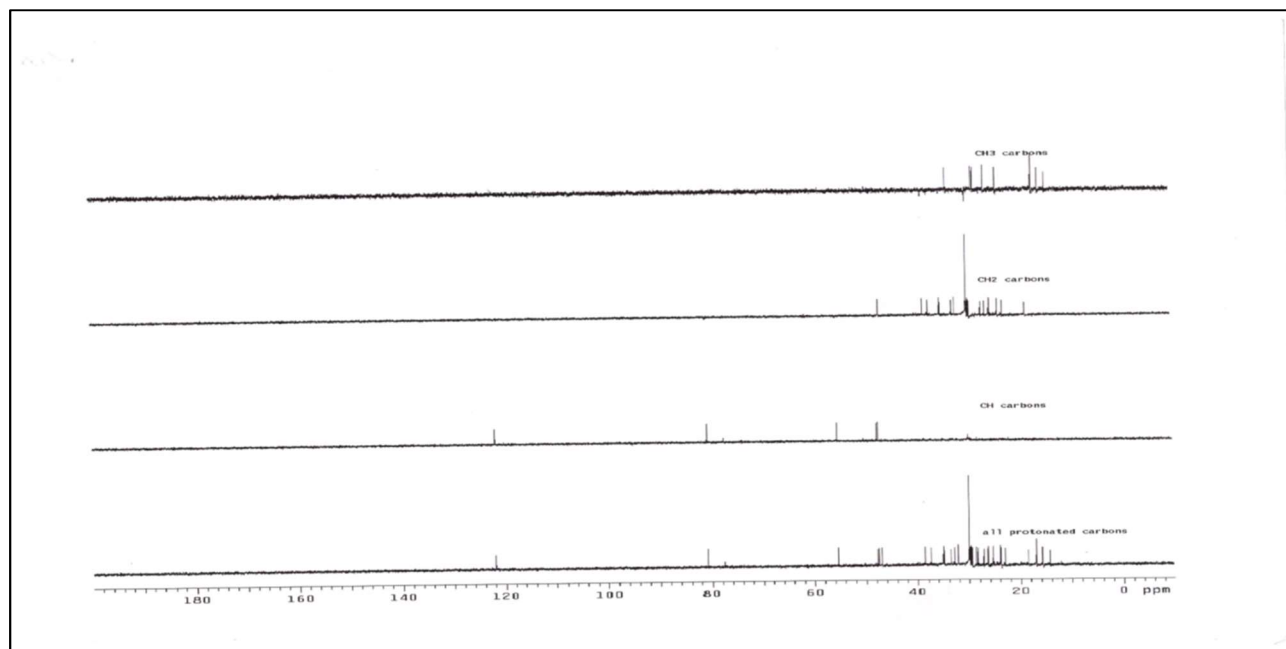


Figure S5. ^{13}C -NMR DEPT Spectrum of Compound 1.

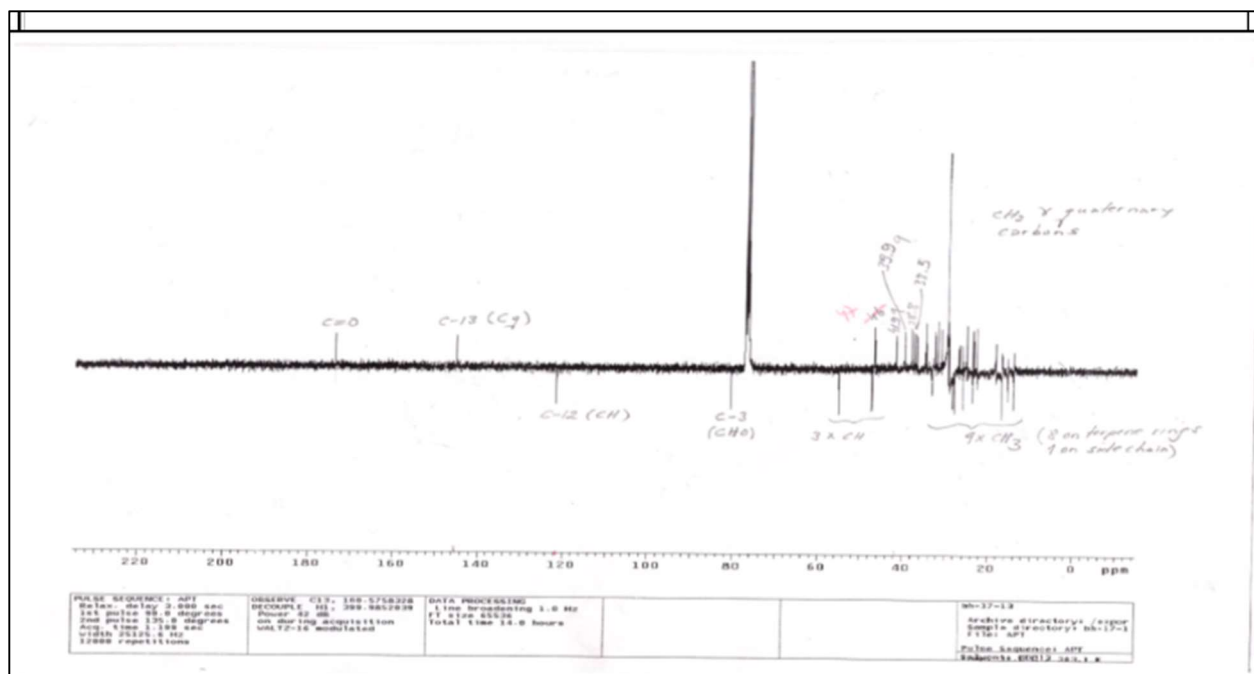
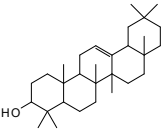
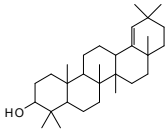
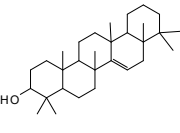
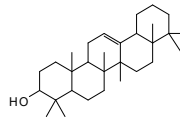


Figure S 6. ^{13}C -NMR APT Spectrum of Compound **1**. All carbons including quaternary carbons; methylene carbons and quaternary carbons positive phase and methyl and methine carbons negative phase.

Table S1. Comparison of C-13 data of some pentacyclic triterpene skeletons with the assigned carbons of Compound 1 [28].

Carbon	<i>Compound 1</i>	<i>Oleonane</i> 	<i>Germanicol</i> 	<i>Taraxerol</i> 	<i>Kairatenol</i> 
1	38.5	38.7	38.5	38.1	37.9
2	27.1	27.3	27.4	27.3	27.2
3	80.8	79.0	79.0	79.2	79.1
4	39.9	38.8	39.0	39.1	38.8
5	55.5	55.3	55.7	55.7	55.7
6	18.5	18.5	18.3	19.0	18.7
7	32.8	32.8	34.7	35.3	32.4
8	37.4	38.8	40.8	38.9	39.4
9	47.8	47.7	51.3	48.9	48.4
10	37.2	37.6	37.3	37.9	36.6
11	23.7	23.6	21.2	17.7	23.2
12	122.0	121.8	26.2	35.9	117.5
13	145.2	145.1	39.0	37.9	146.7
14	41.9	41.8	43.4	158.1	41.8
15	26.2	26.2	27.6	117.0	24.6
16	26.4	27.0	37.7	36.9	29.2
17	32.7	32.5	34.4	38.1	37.4
18	47.7	47.4	142.8	49.4	41.7
19	47.1	46.9	129.8	41.4	23.9
20	31.3	31.1	32.3	29.0	21.9
21	34.9	34.8	33.4	33.9	36.2
22	38.0	37.2	37.4	33.2	37.7
23	28.6	28.2	28.0	28.1	28.0
24	14.4	15.5	15.4	15.6	15.3
25	15.8	15.6	16.1	15.6	15.4
26	17.0	16.9	16.7	30.1	16.3
27	26.2	26.0	14.6	26.0	21.5
28	28.3	28.4	25.3	30.1	21.3
29	33.6	33.3	31.3	33.5	25.5
30	23.9	23.7	29.2	21.5	22.2

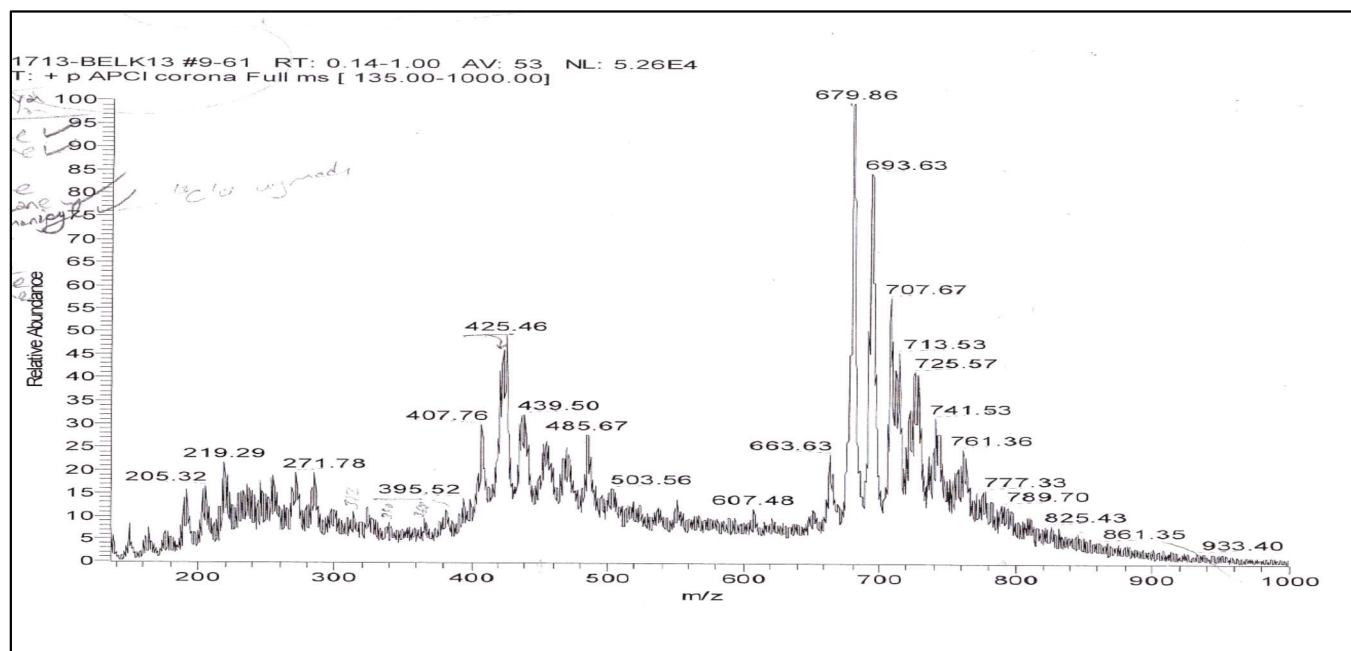


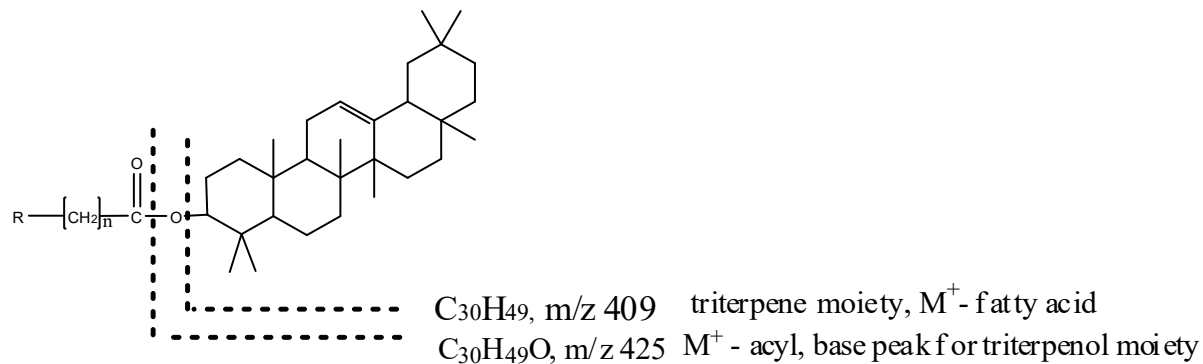
Figure S8. APCI-MS spectrum of Compound **1** (**1a**, **1b**, **1c**, **1d**).

1a. $C_{46}H_{81}O_2^+$: m/z 665 ; $[M+H]^+$ 425 (M^+ - long chain acyl group) 407 (M^+ - fatty acid - $2H^+$)

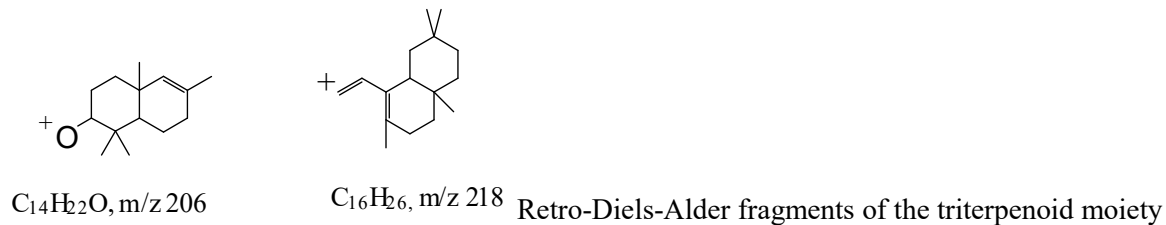
1b. $C_{47}H_{83}O_2^+$: m/z 679; $[M+H]^+$ 425 (M^+ - long chain acyl group) 407 (M^+ - fatty acid - $2H^+$)

1c. $C_{48}H_{85}O_2^+$: m/z 693; $[M+H]^+$ 425 (M^+ - long chain acyl group) 407 (M^+ - fatty acid - $2H^+$)

1d. $C_{49}H_{87}O_2^+$: m/z 707; $[M+H]^+$ 425 (M^+ - long chain acyl group) 407 (M^+ - fatty acid - $2H$)



Fragmentation pattern of Compound **1**.



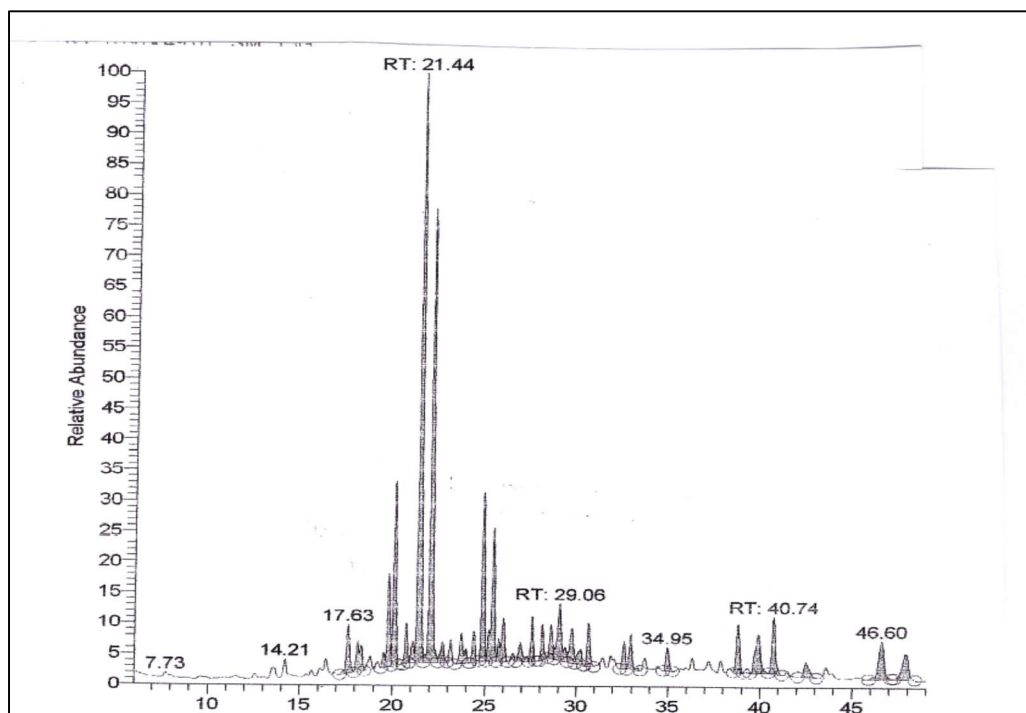


Figure S9. GC-MS analysis of *Salvia cassia* dichloromethane extract