

# Metabolites Profiling and In Vitro Biological Characterization of Different Fractions of Cliona sp. Marine Sponge from the Red Sea Egypt

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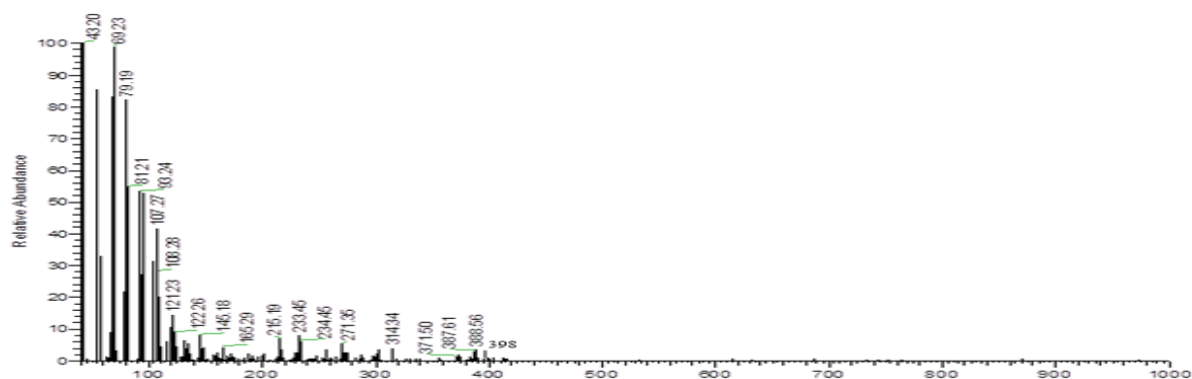
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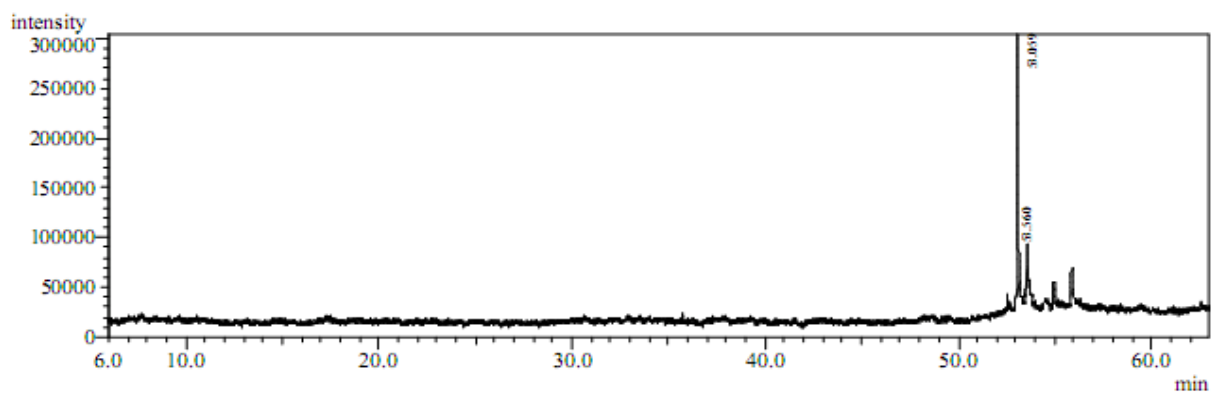
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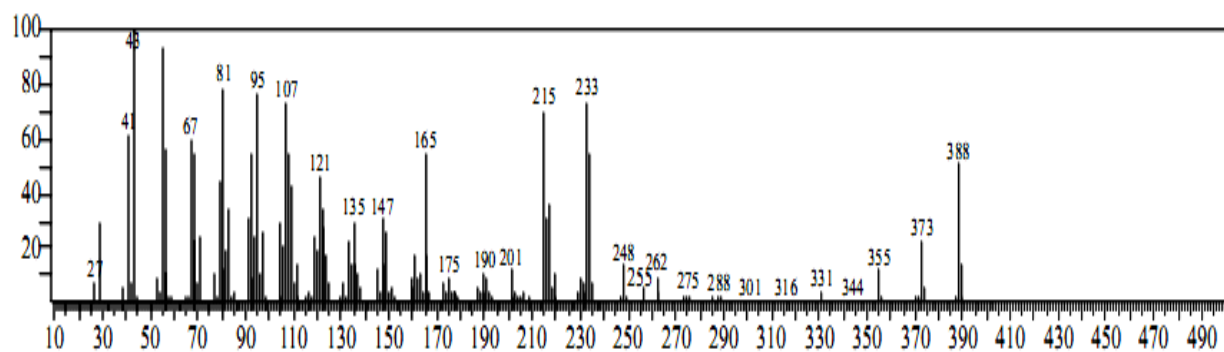
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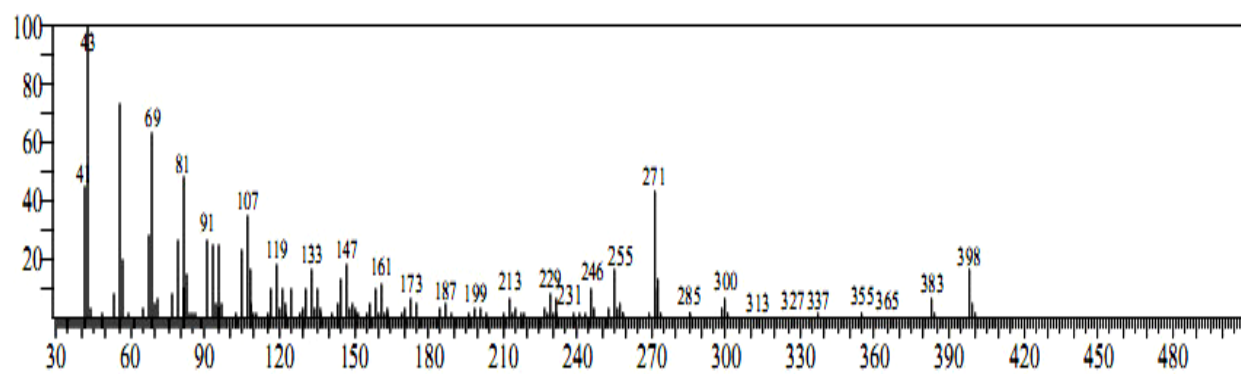
**Figure S1:** EI-MS spectrum of compounds 1 & 2 (Coprostanol & Brassicasterol)



**Figure S2:** GC-MS chromatogram of compounds 1 & 2 (Coprostanol 88.5% & Brassicasterol 11.5%)



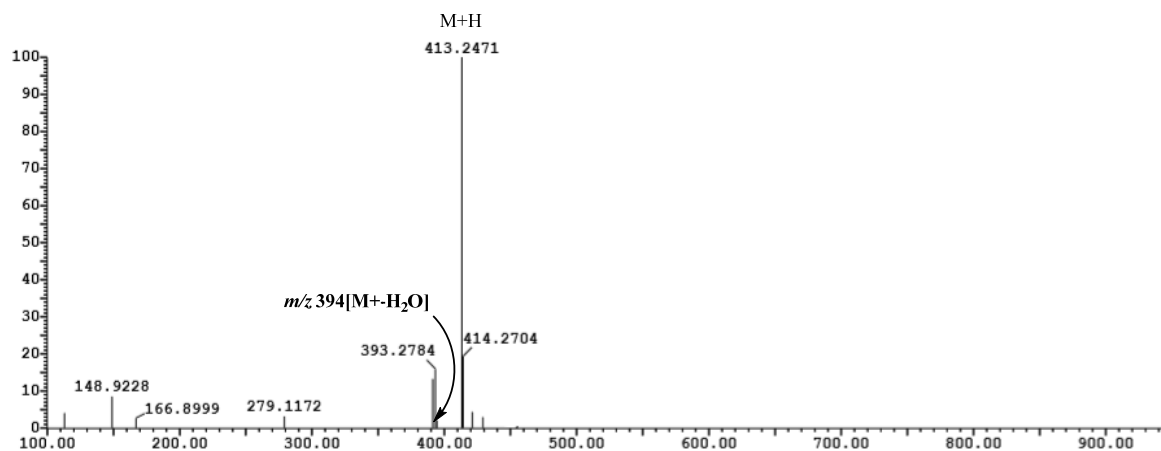
**Figure S3:** GC-MS spectrum of Coprostanol



**Figure S4:** GC-MS spectrum of Brassicasterol

**Table S1.**  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ )  $^{13}\text{C}$ -NMR-DEPT 135 (100 MHz,  $\text{CDCl}_3$ ) for compounds 1 (Coprostanol) and 2 (Ergosta-5,22-dien-3-ol (Brassicasterol)) in comparison with reference

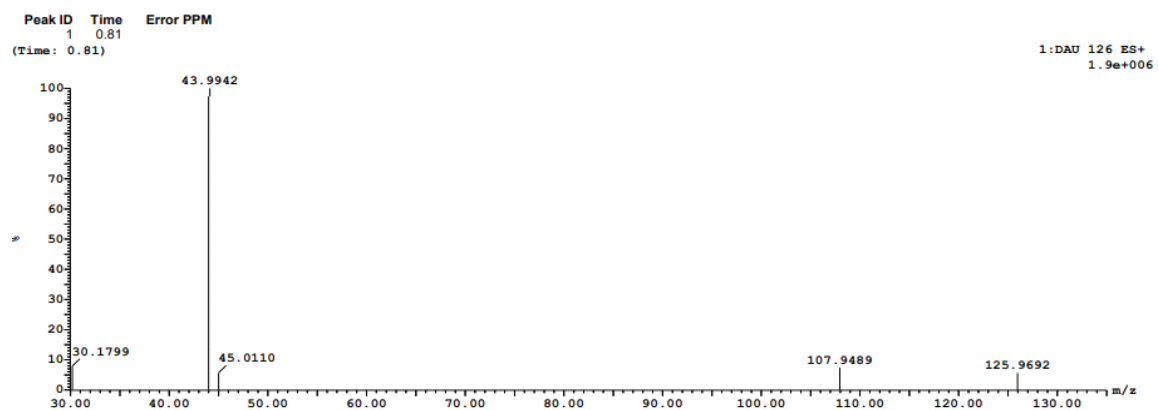
No.	Compound 1 (coprostanol)	Compound 2 Ergosta-5,22-dien-3-ol (brassicasterol)		
	$\delta_{\text{H}}$ , ppm [mult., $J(\text{Hz})$ ]	$\delta_{\text{C}}$ , ppm (mult.)	$\delta_{\text{H}}$ , ppm [mult., $J(\text{Hz})$ ]	$\delta_{\text{C}}$ , ppm (mult.)
1	1.58	35.5, t	1.32	31.3, t
2	1.72	31.5, t	1.51	37.2, t
3	3.55, (m)	71.4, d	3.61, (m, 1H)	71.8, d
4	1.66	37.0, t	2.20	42.3, t
5	1.13	39.9, d	--	<b>141.5, s</b>
6	1.64	28.8, t	5.17 (t, $J = 8 \text{ Hz}$ )	121.7, d
7	1.66	31.9, t	2.20	31.9, t
8	1.13	35.5, d	1.27	32.1, d
9	1.00	54.8, d	1.17	50.2, d
10	--	35.5, s	--	37.3, s
11	1.65	21.0, t	1.64	21.5, t
12	1.56	40.3, t	1.56	40.2, t
13	--	42.3, s	--	43.1, s
14	1.00	56.5, d	1.03	56.9, d
15	1.94	24.3, t	1.94	28.8, t
16	1.97	28.3, t	1.94	25.4, t
17	1.10	56.3, d	1.23	56.5, d
18	0.66, (s)	12.5, q	0.85 (s)	12.3, q
19	0.94, (s)	12.4, q	1.01(s)	20.0, q
20	1.32	35.8, d	1.99	40.2, d
21	0.89, (s)	19.4, q	0.88 (s)	20.3, q
22	1.21	36.2, t	5.35 [ d, $J = 4\text{Hz}$ ]	131.8, d
23	1.26	25.4, t	5.36 [ d, $J = 4\text{Hz}$ ]	136.1, d
24	1.21	28.0, t	1.99	43.07, d
25	1.64	40.2, d	1.63	33.1, q
26	0.92, (s)	23.0, q	0.92 (s)	20.8, q
27	0.92, (s)	23.0, q	0.92 (s)	19.5, q
28			0.89 (s)	20.8, q



**Figure S5:** ESI-MS/MS spectrum of compound 3 (Stigmasterol)

**Table S2:**  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ )  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ ) for compound 3 (Stigmasterol)

No.	$\delta_{\text{C}}$ , ppm (mult.)	$\delta_{\text{H}}$ , ppm [mult., $J(\text{Hz})$ ]	No.	$\delta_{\text{C}}$ , ppm (mult.)	$\delta_{\text{H}}$ , ppm [mult., $J(\text{Hz})$ ]
1	37.4 (t)	1.32	16	28.83 (t)	1.95
2	31.75 (t)	1.51	17	56.45 (d)	1.11
3	71.79 (d)	3.53	18	12.51 (q)	1.29
4	42.69 (t)	2.33	19	19.23 (q)	1.14
5	141.1 (s)	---	20	40.13 (d)	1.12
6	121.28 (d)	5.53 (t, $J = 4$ Hz)	21	20.42 (q)	1.10
7	32.18 (t)	2.15	22	137.5 (d)	5.40 (d, $J = 4$ Hz)
8	31.99 (d)	1.27	23	129.28 (d)	5.40 (d, $J = 4$ Hz)
9	50.22 (d)	1.23	24	50.22 (d)	1.55
10	37.09 (s)	---	25	35.5 (d)	0.99
11	22.9 (t)	1.63	26	19.4 (q)	0.84
12	40.13 (t)	1.55	27	21.1 (q)	0.88
13	42.93 (s)	---	28	24.31 (t)	1.08
14	56.59 (d)	---	29	12.2 (q)	0.85
15	24.31 (t)	1.95			



**Figure S6:** ESI-MS/MS Spectrum of compound 4 (Taurine)