



In-silico molecular studies of the phytochemicals in ethanolic extract of *Chromolaena Odorata* against H^+/K^+ -ATPase enzyme for Proton Pump inhibitor

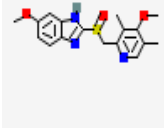
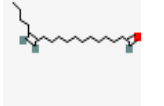
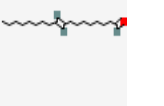
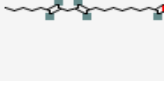
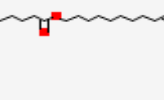
Chinyere B.C. Ikpa,^{1*} Oluwatosin Maduka Tochukwu²

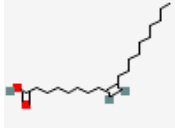
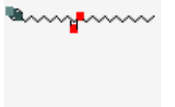
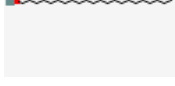
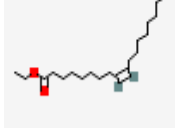
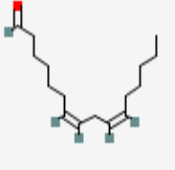
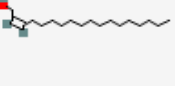
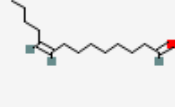
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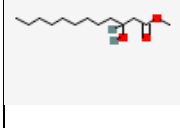
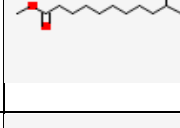
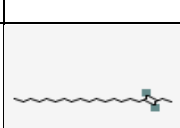
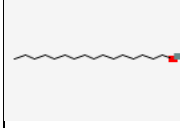
Supporting information file

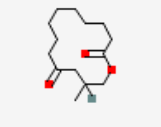
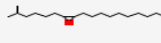
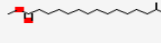
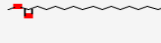
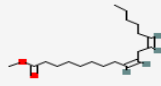
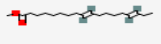
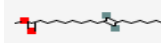
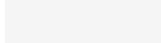
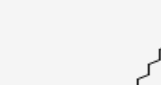
Table 1S: GC-MS result of ethanolic extract of *chromolaena odorata* leaves extract

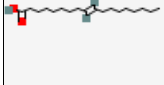
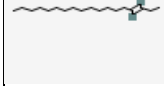
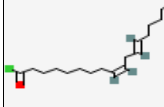
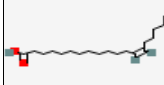
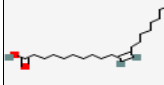
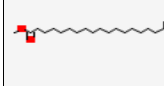
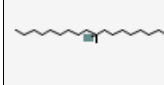
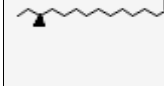
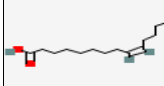
The compounds presented on the table below showing all the possible compounds present in the ethanolic extract of *C. odorata* as identified by the GCMS.

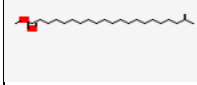
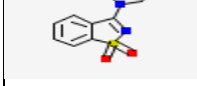
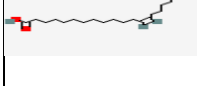
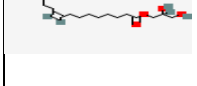
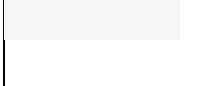
s/n	PK	Compounds Name	RT	% AREA	MW g/mol	MF	Pubchem id	COMPDS STRUCTURE
Cnt	-	Omeprazole	-	-	345.4	<u>C₁₇H₁₉N₃O₃</u> <u>S</u>	4594	
1	1a	9,17-Octadecadienal, (Z)-	8.987	0.35	264.4	<u>C₁₈H₃₂O</u>	5365667	
2	1b	13-Octadecenal, (Z)-	8.987	0.35	266.5	<u>C₁₈H₃₄O</u>	5364497	
3	1c	9-Octadecenal	8.987	0.35	266.5	<u>C₁₈H₃₄O</u>	<u>5283381</u>	
4	2a	9,12-Octadecadienal	10.329	2.21	264.4	<u>C₁₈H₃₂O</u>	5283383	
5	2b	Pentanoic acid, 10-undecenyl ester	10.329	2.21	254.41	<u>C₁₆H₃₀O₂</u>	543363	

6	3a	9-Eicosenoic acid, (Z)-	10.676	0.60	310.5	C₂₀H₃₈O₂	5282767	
7	3b	Undec-10-ynoic acid, dodecyl ester	10.676	0.60	350.6	C₂₃H₄₂O₂	91692432	
8	3c	Behenic alcohol	10.676	0.60	326.6	C₂₂H₄₆O	12620	
9	4a	Ethyl Oleate	10.895	0.53	310.5	C₂₀H₃₈O₂	5363269	
10	4b	(S)(+)-Z-13-Methyl-11-pentadecen-1-ol acetate	10.895	0.53	282.5	C₁₈H₃₄O₂	91691416	
11	5b	cis,cis-7,10,-Hexadecadienal	11.158	0.61	236.39	C₁₆H₂₈O	5365665	
12	6a	Z-2-Octadecen-1-ol	11.284	0.35	268.5	C₁₈H₃₆O	5365011	
13	7a	9-Tetradecenal, (Z)-	11.413	0.43	210.36	C₁₄H₂₆O	5364471	

14	7b	Undec-10-ynoic acid, nonyl ester	11.413	0.43	308.5	C₂₀H₃₆O₂	91692547	
15	8a	Dodecanoic acid, methyl ester	11.581	1.27	230.34	C₁₃H₂₆O₂	155752	
16	8a	Undecanoic acid, 10-methyl-, methyl ester	11.581	1.27	214.34	C₁₃H₂₆O₂	554144	
17	9a	3-Chloropropionic acid, heptadecyl ester	13.367	0.10	347.0	C₂₀H₃₉ClO₂	545757	
18	9b	9-Eicosene, (E)-	13.367	0.10	280.5	C₂₀H₄₀	5365037	
19	9c	3-Eicosene, (E)-	13.367	0.10	280.5	C₂₀H₄₀	5365051	
20	10a	1-Hexadecanol	17.773	0.07	242.44	C₁₆H₃₄O	2682	
21	10b	Cetene	17.773	0.07	224.42	C₁₆H₃₂	12395	
22	10c	2-Dodecanol	17.773	0.07	186.33	C₁₂H₂₆O	25045	

23	11a	Oxacyclotetradecane-2,11-dione, -methyl-	19.762	0.13	240.34	C₁₄H₂₄O₃	543408	
24	11b	Disparlure	19.762	0.13	282.5	C₁₉H₃₈O	205983	
25	12a	Pentadecanoic acid, 14-methyl-, methyl ester	20.309	2.20	270.5	C₁₇H₃₄O₂	21205	
26	12b	Hexadecanoic acid, methyl ester	20.309	2.20	270.5	C₁₇H₃₄O₂	8181	
27	13a	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	23.378	0.27	294.5	C₁₉H₃₄O₂	5284421	
28	13b	9,15-Octadecadienoic acid, methyl ester, (Z,Z)-	23.378	0.27	294.5	C₁₉H₃₄O₂	5362738	
29	14a	10-Octadecenoic acid, methyl ester	23.580	6.01	296.5	C₁₉H₃₆O₂	5364425	
30	14b	trans-13-Octadecenoic acid, methyl ester	23.580	6.01	296.5	C₁₉H₃₆O₂	5364506	
31	15a	Methyl stearate	24.159	1.15	298.5	C₁₉H₃₈O₂	8201	
32	16a	cis-Vaccenic acid	24.886	0.23	282.5	C₁₈H₃₄O₂	5282761	

33	16b	9-Octadecenoic acid	24.886	0.23	282.5	C₁₈H₃₄O₂	637517	
34	16c	3-Octadecene, (E)-	24.886	0.23	252.5	C₁₈H₃₆	5365984	
35	17a	9,12-Octadecadienoyl chloride, (Z, Z)-	25.152	0.13	298.9	C₁₈H₃₁ClO	86740353	
36	18a	cis-13-Eicosenoic acid	27.130	0.47	310.5	C₂₀H₃₈O₂	5312518	
37	18b	cis-11-Eicosenoic acid	27.130	0.47	310.5	C₂₀H₃₈O₂	5282768	
38	19a	Methyl 18-methylnonadecanoate	27.693	0.53	326.6	C₂₁H₄₂O₂	530340	
39	19b	Nonadecanoic acid, 10-methyl-, methyl ester	27.693	0.53	326.6	C₂₁H₄₂O₂	554154	
40	19c	Tetradecanoic acid, 12-methyl-, methyl ester, (S)-	27.693	0.53	256.42	C₁₆H₃₂O₂	23618376	
41	20a	Oleic Acid	29.109	0.51	282.5	C₁₈H₃₄O₂	445639	

42	20c	trans-13-Octadecenoic acid	29.109	0.51	282.5	<u>C₁₈H₃₄O₂</u>	6161490	
43	21a	(Z)-Decyl icos-9-enoate	29.993	0.69	450.8	<u>C₃₀H₅₈O₂</u>	<u>76964864</u>	
44	22a	Methyl 20-methyl-heneicosanoate	30.963	2.90	354.6	<u>C₂₃H₄₆O₂</u>	15089804	
45	23a	9-Octadecenoic acid (Z)-, 2-hydroxyethyl ester	32.061	2.86	326.5	C ₂₀ H ₃₈ O ₃	<u>5364420</u>	
46	24a	cis-13-Octadecenoic acid	34.013	25.45	282.5	<u>C₁₈H₃₄O₂</u>	<u>5312441</u>	
47	25a	3-(Azepan-1-yl)-1,2-benzothiazole 1,1-dioxide	34.475	11.05	264.35	<u>C₁₃H₁₆N₂O₂</u> <u>S</u>	535203	
48	25b	Erucic acid	34.475	11.05	338.6	C ₂₂ H ₄₂ O ₂	5281116	
49	27a	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	34.777	6.74	356.5	<u>C₂₁H₄₀O₄</u>	<u>5283468</u>	
50	30a	Glycerol 1-palmitate	38.298	1.00	330.5	<u>C₁₉H₃₈O₄</u>	14900	
51	30c	Oleic acid, eicosyl ester	38.298	1.00	563.0	<u>C₃₈H₇₄O₂</u>	6436542	