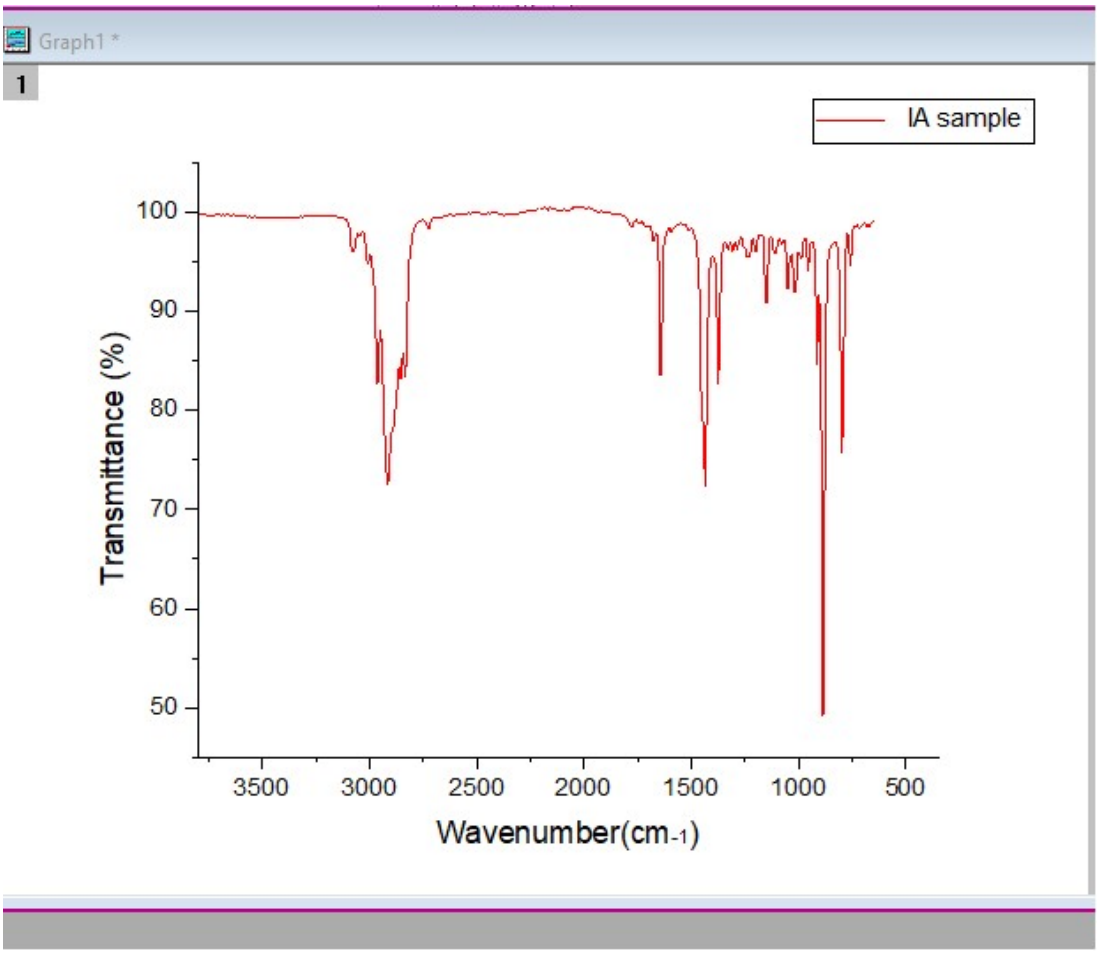
Supporting supplementary data

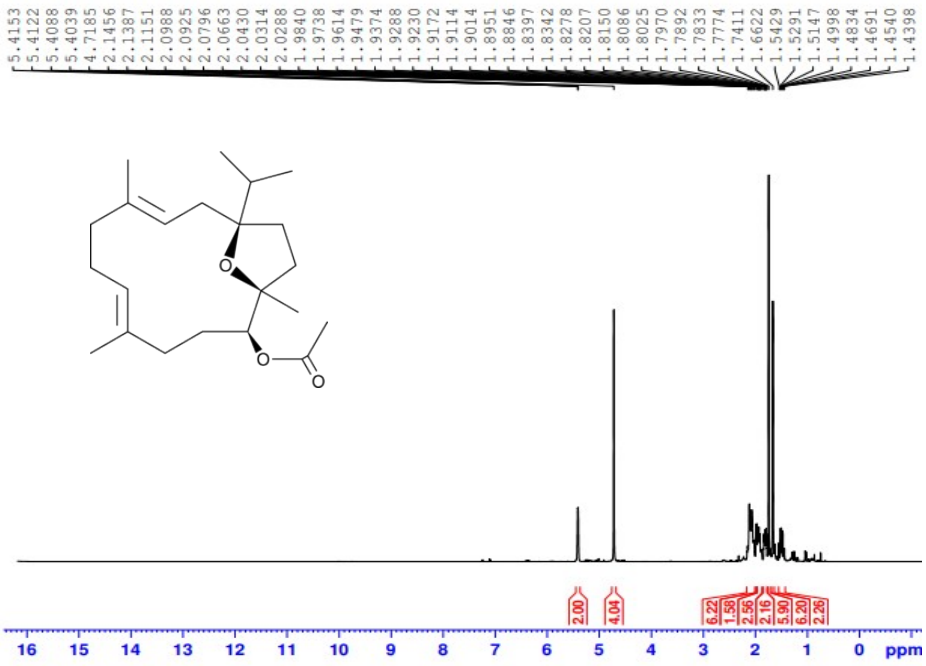
Supplementary Table T1; Chemical composition and percentage of phytochemicals identified by GC-MS analysis of *C. roseus* essential oil

SR. No	Area %	RT (minutes)	Compound Name	Mol. wt. (g/mol)	Mol. formula
1	0.14	4.178	1,2,4,4-Tetramethylcyclopentene	124.22	C_9H_{16}
2	0.40	6.577	beta-Pinene	136.23	$C_{10}H_{16}$
3	1.19	6.660	Gamma terpinene	136	$C_{10}H_{18}O$
4	36.03	6.898	alpha-Pinene	136.23	$C_{10}H_{16}$
5	2.16	7.299	Camphene	136.23	$C_{10}H_{16}$
6	1.53	7.363	Terpinolene	136.23	$C_{10}H_{16}$
7	0.09	7.683	Cyclopropane	42.08	C_3H_6
8	0.09	7.691	2-Aminoresorcinol	125.13	$C_6H_7NO_2$
9	0.13	8.08	beta-Myrcene	136.23	$C_{10}H_{16}$
10	0.04	8.293	3,5-Octadiene	110.2	C_8H_{14}
11	0.28	8.561	o-Isopropenyltoluene	132.2	$C_{10}H_{12}$
12	0.09	8.805	p-Cymene	134.22	$C_{10}H_{14}$
13	1.85	8.948	o-Cymene	134.22	$C_{10}H_{14}$
14	1.47	9.049	D-Limonene	136.23	$C_{10}H_{16}$
15	1.47	9.051	Limonene	136.24	$C_{10}H_{16}$
16	0.81	9.141	Eucalyptol	154.25	$C_{10}H_{16}O$
17	0.11	9.730	Pinocarvone	150.22	$C_{10}H_{14}O$
18	0.04	9.995	Cyclohexanol	100.15	$C_6H_{12}O$
19	0.26	10.333	Methoxy(methyl)chlorosilane	324.9	$C_{19}H_{17}ClOSi$
20	0.33	10.371	Cyclopentanol	86.13	$C_5H_{10}O$
21	0.39	10.374	Artemiseole	152.23	$C_{10}H_{16}O$
22	0.17	10.980	1-Phenylpropanol	136.19	$C_9H_{12}O$

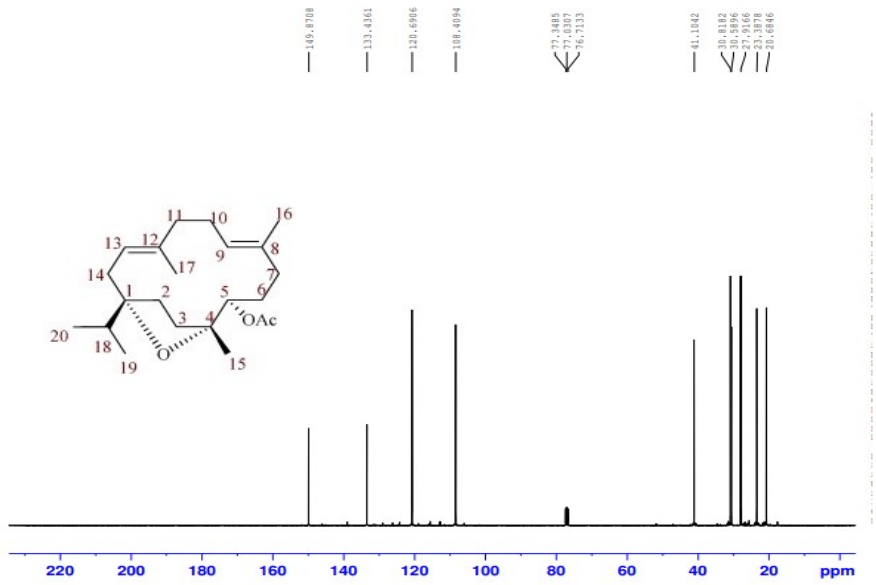
23	0.19	11.065	Thujone	152.23	$C_{10}H_{16}O$
24	0.36	11.135	Camphene	136.23	$C_{12}H_{16}$
25	2.93	11.300	alpha- Campholenal	152.23	$C_{10}H_{16}O$
26	2.93	11.311	Fumaric acid	116.07	$C_4H_4O_4$
27	3.37	11.660	1,4,9-Decatriene	136.23	$C_{10}H_{16}$
28	5.66	11.816	Trans-verbenol	152.237	$C_{10}H_{16}O$
29	0.24	12.455	Terpinen-4-ol	154.25	$C_{10}H_{16}O$
30	0.09	12.547	Ethanone	43.04	C_2H_3O
31	0.65	12.630	m-Cymen-8-ol	192.25	$C_{12}H_{16}O_2$
32	0.17	12.981	Acetic acid	60.052	CH_3COOH
33	0.63	13.276	trans-Carveol	152.23	$C_{10}H_{16}O$
34	0.21	13.777	Carvone	150.22	$C_{10}H_{14}O$
35	0.38	13.891	Isobutyric acid	136.23	$C_{10}H_{16}$
36	2.96	14.966	Camphenone	150.22	$C_{10}H_{14}O$
37	0.22	15.579	alpha-Campholenal	152.23	$C_{10}H_{16}O$
38	1.18	15.772	2-Carene	136.23	$C_{10}H_{16}$
39	0.17	16.364	Copaene	204.35	$C_{15}H_{24}$
40	0.49	16.863	Octanoic acid	144.21	$C_8H_{16}O_2$
41	0.12	17.354	alpha-Campholenal	152.23	$C_{10}H_{16}O$
42	0.20	19.651	Nerolidol	222	$C_{15}H_{26}O$
43	0.11	25.832	n-Hexadecanoic acid	256.42	$C_{16}H_{32}O$
44	1.12	28.693	Incensole, acetate	334.49	$C_{21}H_{34}O$
45	0.19	36.284	Hexasiloxane	248.51	O_5Si_6



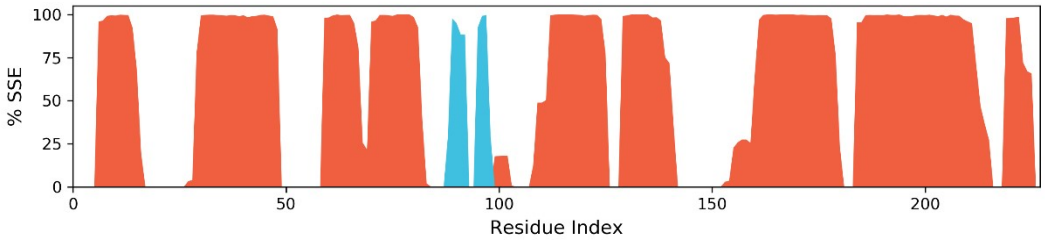
Supplementary figure S1; IR spectrum of incensole acetate.



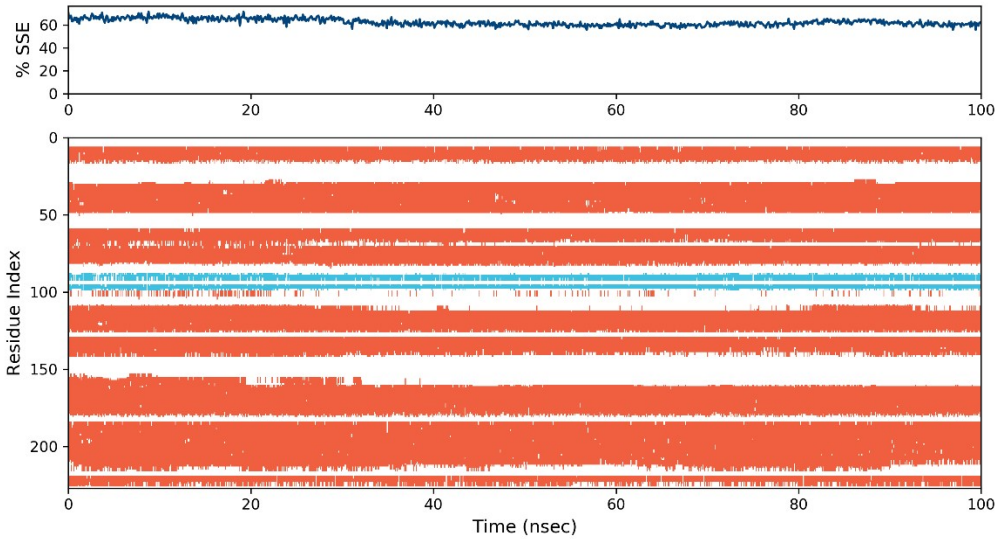
Supplementary figure S2; [1]H-NMR of incensole acetate



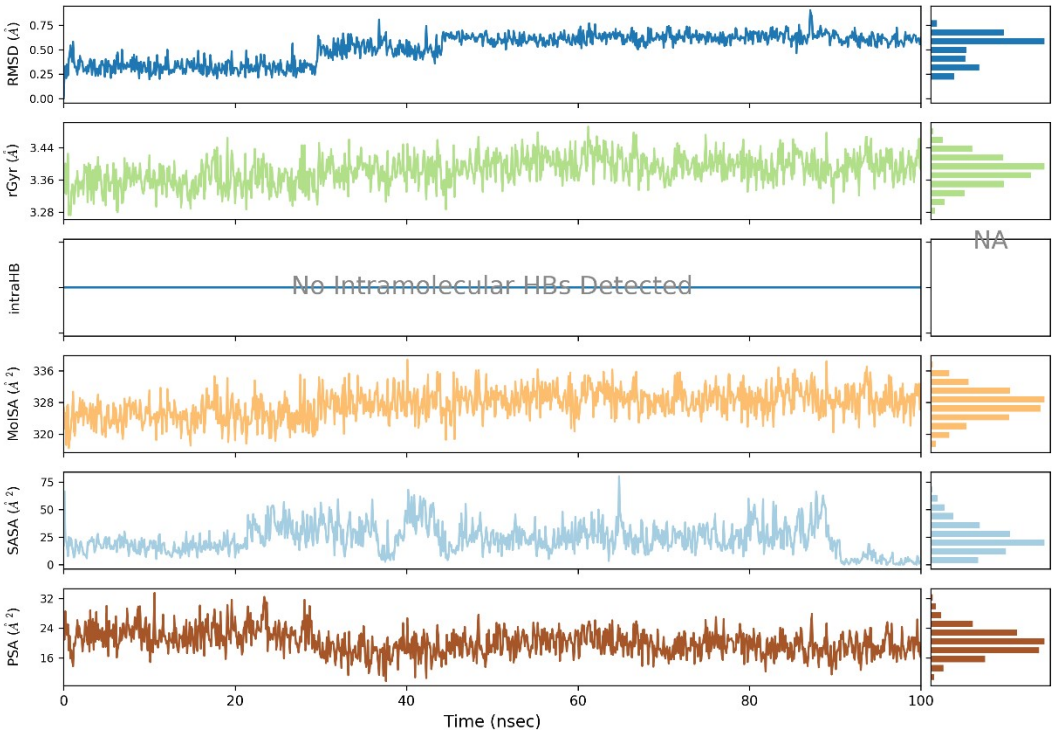
Supplementary figure S3; [13] C-NMR of incensole acetate



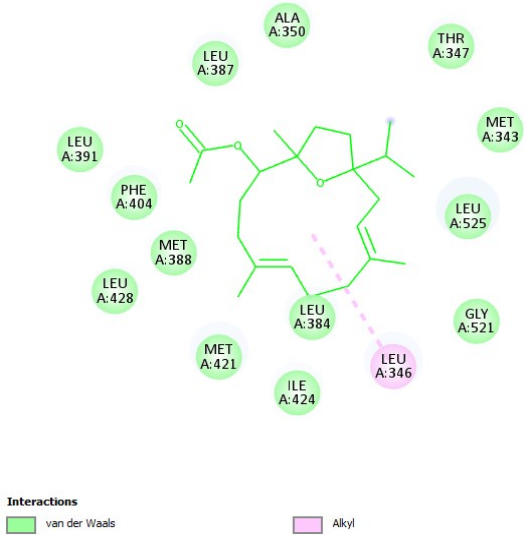
Supplementary figure S4; MD simulation supporting figure



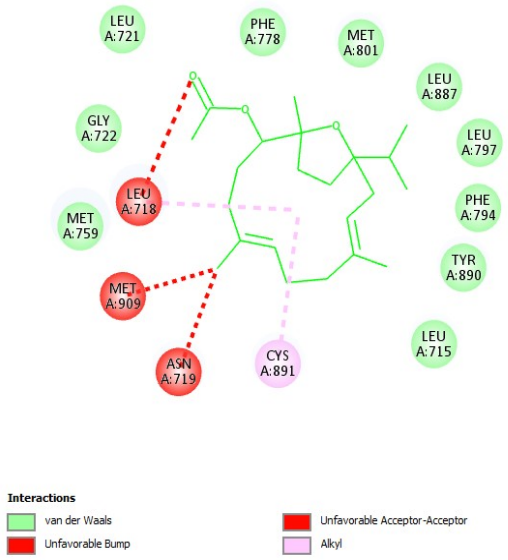
Supplementary figure S5; Protein secondary structure elements (SSE) such as alpha-helices marked by orange and the beta-strands were labeled by cyan.



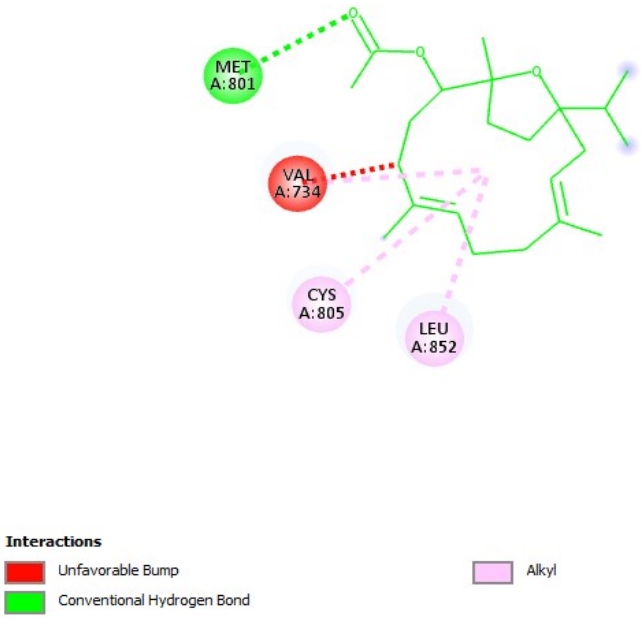
Supplementary figure S6; MD simulation Ligand properties



A

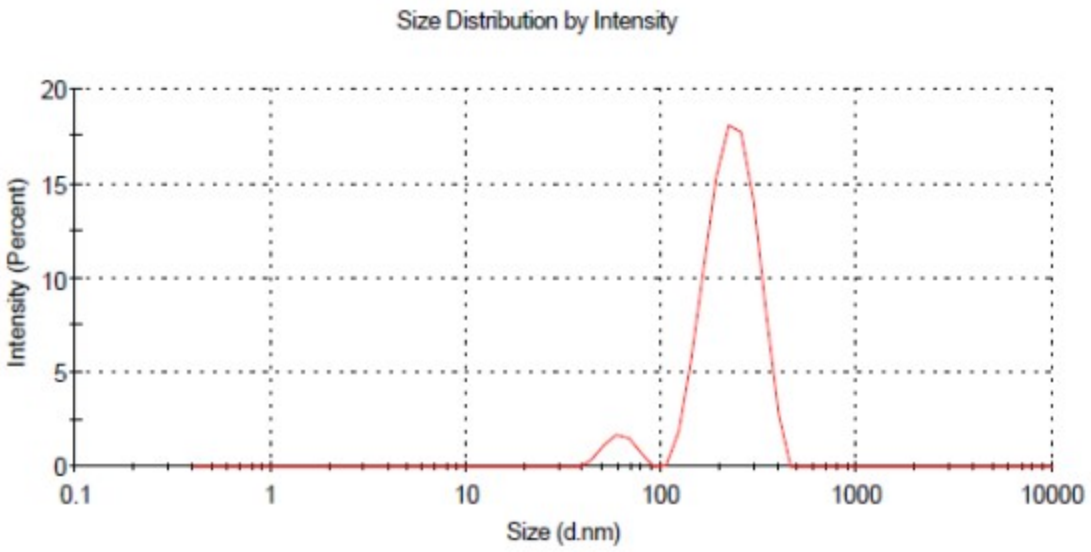


B

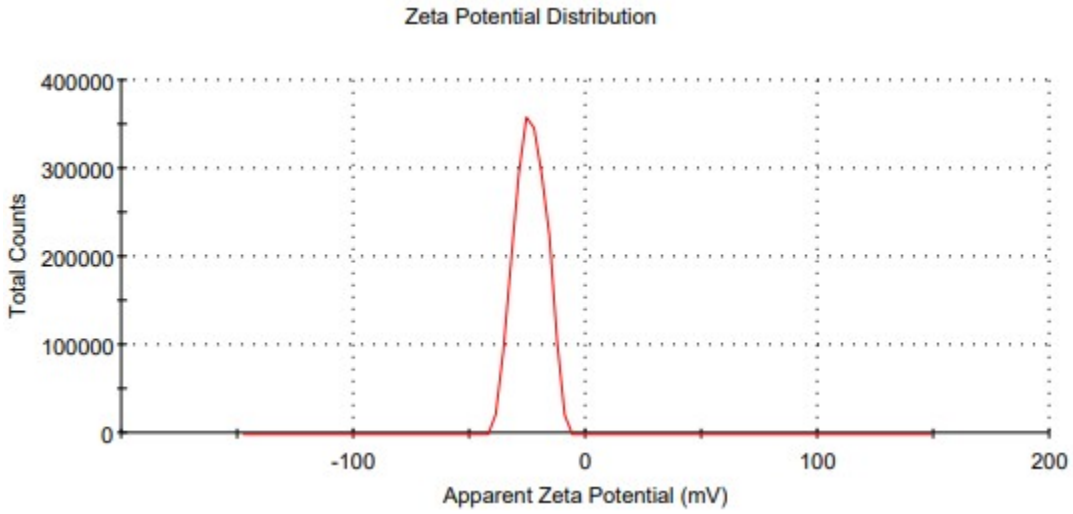


C

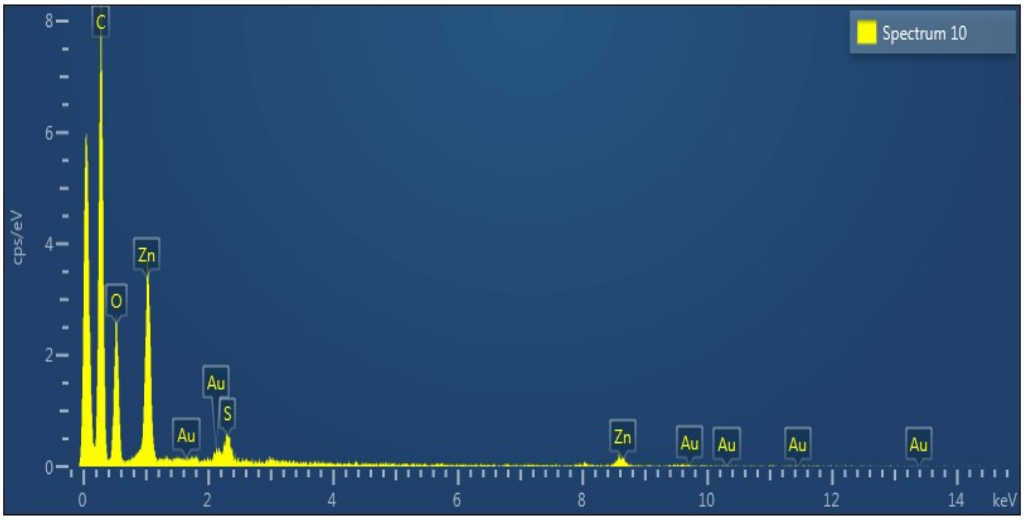
Supplementary figure S7; 2D diagram of incensole acetate interactions with (A) Estrogen receptor (B) Progesterone receptor (C) HER2 receptor.



Supplementary figure S8; Size-distribution analysis of NE



Supplementary figure S9; Zeta potential analysis of NE



Supplementary figure S10; EDX of Terpene I Nanoemulsion