Supplementary data 3

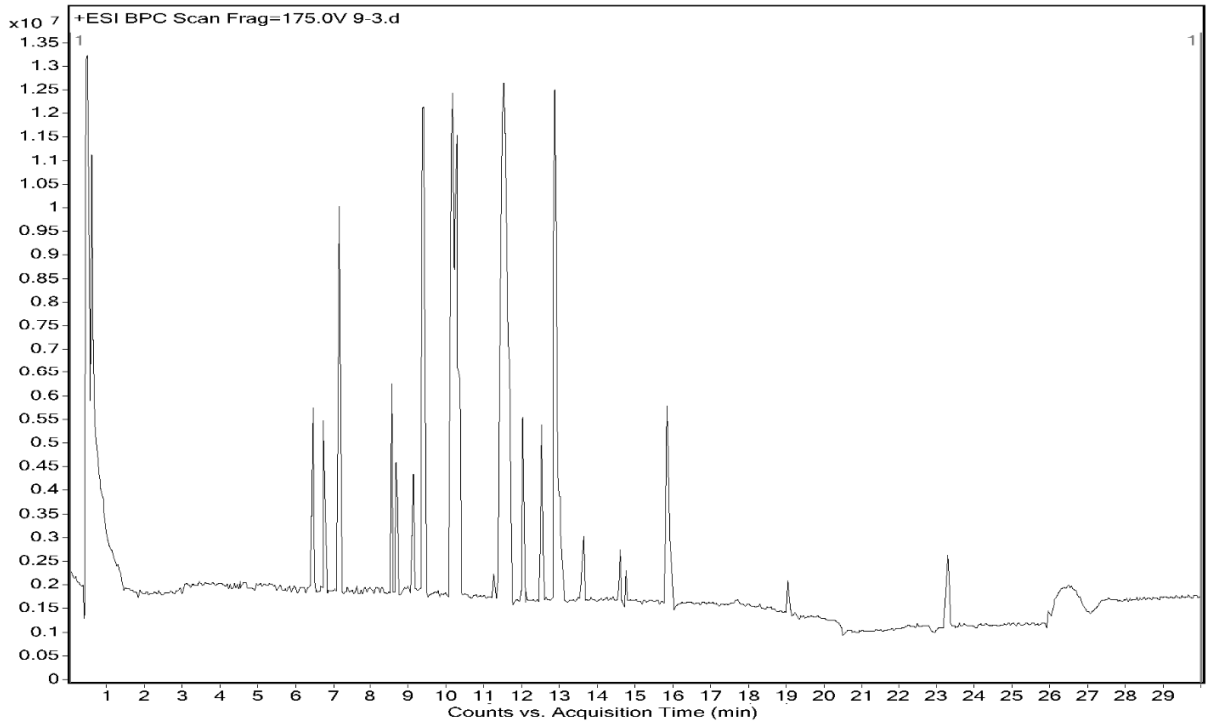


Figure S3 Chromatograms of chemical constituents presented in CA-M

Table S3 Phytochemical constituents in CA-M identified by UPLC-HRMS

Cpd #	RT	Mass	Name	Formula	Classification
Cpd 1	0.472	360.1225	Elephantopin	$C_{19}H_{20}O_7$	Terpenoids
Cpd 2	0.489	238.2148	N/A	-	-
Cpd 3	0.539	118.0851	Betaine	$C_5H_{12}NO_2$	Amino acid related compounds
Cpd 4	1.867	131.0931	Leucine	$C_6H_{13}NO_2$	Amino acid related compounds
Cpd 5	2.920	188.0663	Ethyl oxalacetate	$C_8H_{12}O_5$	Fatty acids related compounds
Cpd 6	4.909	357.2589	Ile Leu Leu	$C_{18}H_{35}N_3O_4$	Amino acid related compounds
Cpd 7	5.829	559.3736	(6R)-Vitamin D3 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct / (6R)-cholecalciferol 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) adduct	$C_{35}H_{49}N_3O_3$	Terpenoids
Cpd 8	6.034	607.3711	N/A	-	-
Cpd 9	6.346	355.1503	Ala Glu His	$C_{14}H_{21}N_5O_6$	Amino acid related compounds
Cpd 10	6.469	217.2016	N/A		
Cpd 11	6.777	261.2276	N/A		

Cpd 12	6.808	170.131	Citronellic acid	$C_{10}H_{18}O_2$	Terpenoids
Cpd 13	6.814	228.1722	3-oxo-Tridecanoic acid	$C_{13}H_{24}O_3$	Fatty acids related compounds
Cpd 14	6.836	226.1568	Dihydrojasmonic acid, methyl ester	$C_{13}H_{22}O_3$	Fatty acids related compounds
Cpd 15	6.870	250.1541	Gemfibrozil	$C_{15}H_{22}O_3$	Fatty acids related compounds
Cpd 16	7.025	305.2531	N/A	-	-
Cpd 17	7.052	298.1387	Benzenehexanoic acid, 2,5-dihydroxy-3,4-dimethoxy-6-methyl-	$C_{15}H_{22}O_6$	Others
Cpd 18	7.167	226.1567	Dihydrojasmonic acid, methyl ester	$C_{13}H_{22}O_3$	Fatty acids related compounds
Cpd 19	7.297	228.1722	3-oxo-Tridecanoic acid	$C_{13}H_{24}O_3$	Fatty acids related compounds
Cpd 20	7.453	222.1254	Hydroxyibuprofen	$C_{13}H_{18}O_3$	Others
Cpd 21	7.547	226.1567	Dihydrojasmonic acid, methyl ester	$C_{13}H_{22}O_3$	Fatty acids related compounds
Cpd 22	7.560	230.1879	13-Hydroxy-tridecanoic acid	$C_{13}H_{26}O_3$	Fatty acids related compounds
Cpd 23	7.755	250.1541	Gemfibrozil	$C_{15}H_{22}O_3$	Fatty acids related compounds
Cpd 24	7.793	224.1409	Methyl jasmonate	$C_{13}H_{20}O_3$	Terpenoids
Cpd 25	8.069	266.149	Gemfibrozil M1	$C_{15}H_{22}O_4$	Others
Cpd 26	8.087	228.1722	3-oxo-Tridecanoic acid	$C_{13}H_{24}O_3$	Fatty acids related compounds
Cpd 27	8.553	245.2328	N/A	-	-
Cpd 28	8.831	230.1881	13-Hydroxy-tridecanoic acid	$C_{13}H_{26}O_3$	Fatty acids related compounds
Cpd 29	8.843	333.284	N/A		
Cpd 30	9.122	280.1282	Gemfibrozil M3	$C_{15}H_{20}O_5$	Fatty acids related compounds
Cpd 31	9.394	184.1831	9-Dodecen-1-ol	$C_{12}H_{24}O$	Fatty acid related compound (fatty alcohol)
Cpd 32	9.395	212.1775	3-n-Decyl acrylic acid	$C_{13}H_{24}O_2$	Fatty acid related compound
Cpd 33	9.396	252.17	Punctaporin B	$C_{15}H_{24}O_3$	Others
Cpd 34	9.525	563.3116	Dihydroergocornine	$C_{31}H_{41}N_5O_5$	Others
Cpd 35	9.526	568.2669	Swietenine	$C_{32}H_{40}O_9$	Terpenoids
Cpd 36	9.781	230.188	13-Hydroxy-tridecanoic acid	$C_{13}H_{26}O_3$	Fatty acids related compounds
Cpd 37	9.840	450.2204	Methyldopexamine sulfate	$C_{23}H_{34}N_2O_5S$	Others
Cpd 38	9.852	248.1386	Amiloxate	$C_{15}H_{20}O_3$	Fatty acids related compounds
Cpd 39	10.045	157.1446	N/A	-	-
Cpd 40	10.163	273.2639	Hexadecasphinganine	$C_{16}H_{35}NO_2$	Fatty acid related compound
Cpd 41	10.212	210.1623	3-Tridecynoic acid	$C_{13}H_{22}O_2$	Fatty acids related compounds
Cpd 42	10.221	229.2382	N/A	-	-
Cpd 43	10.271	317.2896	Phytosphingosine	$C_{18}H_{39}NO_3$	Fatty acid related compound
Cpd 44	10.359	357.3438	N-(2-fluro-ethyl)-eicosanoyl amine	$C_{22}H_{44}FNO$	Fatty acid related compound

Cpd 45	10.361	333.2843	N/A	-	-
Cpd 46	10.361	289.2586	N/A	-	-
Cpd 47	10.650	342.2845	Prostaglandin F1a alcohol	$C_{20}H_{38}O_4$	Fatty acids related compounds
Cpd 48	10.658	228.1724	3-oxo-Tridecanoic acid	$C_{13}H_{24}O_3$	Fatty acids related compounds
Cpd 49	10.885	250.1546	Gemfibrozil	$C_{15}H_{22}O_3$	Fatty acids related compounds
Cpd 50	11.084	196.1467	3-Dodecynoic acid	$C_{12}H_{20}O_2$	Fatty acids related compounds
Cpd 51	11.108	144.0428	(E)-2-Methylglutaconic acid	$C_6H_8O_4$	Fatty acids related compounds
Cpd 52	11.271	270.1316	2-[3-Carboxy-3-(methylammonio)propyl]-L-histidine	$C_{11}H_{18}N_4O_4$	Amino acid related compound
Cpd 53	11.496	184.183	9-Dodecen-1-ol	$C_{12}H_{24}O$	Fatty acid related compound (fatty alcohol)
Cpd 54	11.502	252.1701	Punctaporin B	$C_{15}H_{24}O_3$	Others
Cpd 55	11.509	128.1209	Octanal	$C_8H_{16}O$	Fatty acid related compound (fatty aldehyde)
Cpd 56	11.511	170.1311	Citronellic acid	$C_{10}H_{18}O_2$	Terpenoids
Cpd 57	11.516	156.1157	6E-Nonenoic acid	$C_9H_{16}O_2$	Fatty acids related compounds
Cpd 58	11.518	100.0898	4-Methylpentanal	$C_6H_{12}O$	Others (Carbohydrate)
Cpd 59	11.520	230.1881	13-Hydroxy-tridecanoic acid	$C_{13}H_{26}O_3$	Fatty acids related compounds
Cpd 60	11.522	212.1777	3-n-Decyl acrylic acid	$C_{13}H_{24}O_2$	Fatty acids related compounds
Cpd 61	11.613	301.2949	Dihydrosphingosine	$C_{18}H_{39}NO_2$	Fatty acid related compound
Cpd 62	11.689	345.3204	N/A	-	-
Cpd 63	11.759	389.3462	N/A	-	-
Cpd 64	11.807	320.1955	QH2	$C_{19}H_{28}O_4$	Others
Cpd 65	12.040	210.162	3-Tridecynoic acid	$C_{13}H_{22}O_2$	Fatty acids related compounds
Cpd 66	12.045	246.1229	Val Glu	$C_{10}H_{18}N_2O_5$	Amino acid related compounds
Cpd 67	12.046	134.0587	Deoxyribose	$C_5H_{10}O_4$	Others (Carbohydrate)
Cpd 68	12.046	224.1413	Methyl jasmonate	$C_{13}H_{20}O_3$	Terpenoids
Cpd 69	12.115	212.1778	3-n-Decyl acrylic acid	$C_{13}H_{24}O_2$	Fatty acids related compounds
Cpd 70	12.539	432.2102	6β,11β,16α,17α,21-Pentahydroxypregna-1,4-diene-3,20-dione-16,17-acetonide	$C_{24}H_{32}O_7$	Terpenoids
Cpd 71	12.542	392.218	Phe Ala Arg	$C_{18}H_{28}N_6O_4$	Amino acid related compounds
Cpd 72	12.542	449.2368	Phe Gln Arg	$C_{20}H_{31}N_7O_5$	Amino acid related compounds
Cpd 73	12.542	114.1053	4-Heptanone	$C_7H_{14}O$	Fatty acid related compound (ketone)
Cpd 74	12.542	470.1657	7-Hydroxymethotrexate	$C_{20}H_{22}N_8O_6$	Others
Cpd 75	12.894	216.1491	Val Val	$C_{10}H_{20}N_2O_3$	Amino acid related compounds

Cpd 76	13.008	329.3258	N/A	-	-
Cpd 77	13.068	373.3518	N/A	-	-
Cpd 78	13.138	417.3773	N/A	-	-
Cpd 79	13.221	212.1778	3-n-Decyl acrylic acid	$C_{13}H_{24}O_2$	Fatty acids related compounds
Cpd 80	13.372	355.341	N-(2-Hydroxyethyl) icosanamide	$C_{22}H_{45}NO_2$	Fatty acids related compounds
Cpd 81	13.419	399.3667	N/A	-	-
Cpd 82	13.639	226.157	Dihydrojasmonic acid, methyl ester	$C_{13}H_{22}O_3$	Fatty acids related compounds
Cpd 83	13.639	144.0794	Hydroxycyclohexanecarboxylic acid	$C_7H_{12}O_3$	Others
Cpd 84	13.757	252.17	Punctaporin B	$C_{15}H_{24}O_3$	Others
Cpd 85	13.940	226.1571	Dihydrojasmonic acid, methyl ester	$C_{13}H_{22}O_3$	Fatty acids related compounds
Cpd 86	14.518	354.2371	Prostaglandin H1	$C_{20}H_{34}O_5$	Fatty acids related compounds
Cpd 87	14.652	212.1778	3-n-Decyl acrylic acid	$C_{13}H_{24}O_2$	Fatty acids related compounds
Cpd 88	15.448	384.247	Ibutilide	$C_{20}H_{36}N_2O_3S$	Others
Cpd 89	15.876	296.1591	Lactone of PGF-MUM	$C_{16}H_{24}O_5$	Terpenoids
Cpd 90	15.877	144.0427	(E)-2-Methylglutaconic acid	$C_6H_8O_4$	Fatty acids related compounds
Cpd 91	16.902	296.2343	12-Hydroxy-10-octadecynoic acid	$C_{18}H_{32}O_3$	Fatty acids related compounds
Cpd 92	18.112	424.3141	N/A	-	-
Cpd 93	18.422	397.2211	GPEtn(12:0/0:0)	$C_{17}H_{36}NO_7P$	Fatty acid related compound
Cpd 94	18.966	482.3551	N/A	-	-
Cpd 95	19.027	438.3294	27-nor-5β-Cholestane-3α,7α,12α,24,25-pentol	$C_{26}H_{46}O_5$	Terpenoid (Sterol Lipids)
Cpd 96	19.094	434.2963	1α-Hydroxy-24-(dimethylphosphoryl)-25,26,27-trinorvitamin D3	$C_{26}H_{43}O_3P$	Terpenoids
Cpd 97	23.284	430.2653	Gln Lys Arg	$C_{17}H_{34}N_8O_5$	Amino acid related compounds
Cpd 98	23.287	408.2832	3β,6α,7α -Trihydroxy-5β-cholan-24-oic acid	$C_{24}H_{40}O_5$	Terpenoids (steroid)
Cpd 99	26.000	141.9924	N/A	-	-
Cpd 100	26.017	125.0135	Taurine	$C_2H_7NO_3S$	Amino acid related compounds

N/A indicates not applicable of non-identified compound