

Supplementary Table 6 Differential metabolites between the CaOx and struvite group

No.	Metabolite	Mode	Regulate	FC	<i>P</i> value	VIP value
1	(Z)-3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one	pos	up	1.0373	0.04786	1.0472
2	N-Acetyl-O-methyl-L-tyrosine	pos	up	1.1168	0.0468	1.6919
3	N-Acetylaspartylglutamic acid	pos	up	1.1238	0.0319	1.8527
4	(5R)-5-Hydroxyhexanoylcarnitine	pos	up	1.057	0.04821	1.2733
5	Vibunazole	pos	up	1.0544	0.02842	1.3739
6	Trimethylamine N-Oxide	pos	up	1.0558	0.04826	1.3285
7	Fructose lactate	pos	up	1.0411	0.02469	1.1893
8	Ethyl-4-hydroxymethyl-3(2H)-Furanone	pos	up	1.056	0.04285	1.314
9	3,7,8,15-Scirpenetetrol	pos	up	1.0661	0.04139	1.4746
10	4-Hydroxy-6-octenoylcarnitine	pos	up	1.0652	0.04184	1.3655
11	Valganciclovir, (S)-	pos	up	1.2584	0.01715	2.721
12	Cefepime	pos	up	1.2549	0.02341	2.4325
13	N-Methyl-14-O-demethylepiporphyroxine	pos	up	1.0912	0.03447	1.7027
14	7,4'-Dihydroxyflavone	pos	up	1.2023	0.03568	2.2269
15	A-Methyldopamine	pos	up	2.9271	0.008008	4.2054
16	N-(2,5-dimethylphenyl)-2-(5-pyrazin-2-yl-1,3,4-oxadiazol-2-yl)acetamide	pos	up	1.2304	0.02612	2.4108

17	Glycylprolylarginine	pos	up	1.1142	0.001476	2.2808
18	1-[4-(4-hydroxybenzoyl)piperazin-1-yl]ethanone	pos	up	1.3164	0.03159	2.4797
19	Buspirone	pos	up	1.0545	0.03794	1.3859
20	Sibrafiban	pos	up	1.1743	0.0429	2.11
21	Erythrogran	pos	down	0.831	0.001631	2.6221
22	LIPEGFILGRASTIM	pos	down	0.8442	0.0003025	2.5236
23	7-[(1R,2R,3R)-3-Hydroxy-2-[(3S)-3-hydroxyoctyl]-5-oxocyclopentyl]heptanoylcarnitine	pos	up	1.2345	0.03979	2.5557
24	(15Z)-tetracosenoate	pos	up	1.0706	0.005062	1.8014
25	Diphenhydramine N-glucuronide	pos	up	1.1536	0.000852	2.4945
26	Clarithromycin	pos	down	0.908	0.001657	1.9646
27	PS(20:3(5Z,8Z,11Z)/15:0)	pos	down	0.9466	0.02174	1.3711
28	2-[2-[2-[2-[2-[2-[(Z)-2-[2-[2-(2-Octadecoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	pos	down	0.609	1.10E-05	4.2833
29	[4-(3-Benzyl-4-hydroxybenzyl)-3,5-dimethylphenoxy]acetic acid	pos	down	0.8177	0.00852	2.6056
30	Ile-Glu-Thr-Asp-fluoromethyl ketone	pos	up	1.2037	0.004585	2.72
31	Menthyl pyrrolidone carboxylate	pos	up	1.0572	0.02687	1.3253
32	Butyl (S)-3-hydroxybutyrate glucoside	pos	up	1.3017	0.004482	2.9044

---

33	12-Oxo-2,3-dinor-10,15-phytodienoic acid	pos	up	1.082	0.03395	1.5434
34	Curdione	pos	up	1.1197	0.04972	1.7682
35	Tsangane L 3-glucoside	pos	up	1.7405	1.17E-05	4.5474
36	O-(13-Carboxytridecanoyl)carnitine	pos	up	1.0402	0.01538	1.3339
37	7-Hydroxytrideca-9,11-dienoylcarnitine	pos	up	1.0432	0.01917	1.4264
38	Neocnidilide	pos	up	1.0574	0.01862	1.3974
39	6-Keto-prostaglandin F1a	pos	up	1.0584	0.04752	1.4406
40	11-Hydroxyyohimbine	pos	up	1.0896	0.01302	1.7954
41	5(6)-Epoxy Prostaglandin E1	pos	up	1.0521	0.03417	1.4243
42	8-Hydroxydodecanoylcarnitine	pos	up	1.0452	0.02226	1.3423
43	4-phenylbutanic acid-O-sulphate	pos	down	0.8483	0.02347	2.0566
44	M-Aminobenzoic acid	pos	up	1.247	0.0206	2.359
45	Dalbergin	pos	up	1.2517	0.003627	2.7663
46	Latrunculin B	pos	up	1.113	0.02461	1.9927
47	N-(((2,7-Dimethyl-9H-fluoren-9-yl)methoxy)carbonyl)-L-leucine	pos	down	0.617	0.004978	3.7102
48	Methyl 4-mercaptobutyrimidate	pos	up	1.1751	0.03246	1.8925
49	Diacetoxyscirpenol	pos	up	1.1134	0.03529	1.8674
50	Laurenoniolide	pos	up	1.1409	0.003806	2.3926

---

---

51	Uridine, 2'-deoxy-2'-fluoro-2'-methyl-, (2'R)-	pos	up	1.297	0.04639	2.3831
52	10,11-dihydro-20-trihydroxy- leukotriene B4	pos	up	1.2046	0.01803	2.4266
53	17-Hydroxymethylethisterone	pos	up	1.3397	0.01543	2.7297
54	2-(Quinolin-8-yloxy)propanoic acid	pos	up	1.1444	0.01398	2.3002
55	3-Des(dimethylaminoethyl)-3-acetic acid zolmitriptan	pos	up	1.3528	0.01989	2.9267
56	5-methyl-N-(4-phenyl-1,3-thiazol-2- yl)furan-2-carboxamide	pos	up	1.223	0.01945	2.4466
57	Cysteinyl-Tyrosine	pos	up	1.3071	0.01841	2.741
58	2beta,9xi-Dihydroxy-8-oxo- 1(10),4,11(13)-germacatrien- 12,6alpha-olide	pos	up	1.5008	0.04371	2.7537
59	(5E)-3-Hydroxyhept-5-enoylcarnitine	pos	up	1.0476	0.04406	1.2346
60	H-D-Arg(NO2)-OH	pos	up	1.1186	0.03927	1.9239
61	L-beta-aspartyl-L-phenylalanine	pos	up	1.138	0.02933	1.8004
62	Captopril-cysteine disulfide	pos	up	1.3189	0.002905	3.1351
63	Adenosine	pos	up	1.0789	0.02401	1.542
64	Vicine	pos	up	1.1868	0.01161	2.1945
65	N-(2,6-dimethylphenyl)-N2-Ethenyl- N2-Ethylglycinamide	pos	down	0.8788	0.005338	2.1239
66	Perindoprilat glucuronide	pos	up	1.3884	0.02048	2.8057

---

67	Humulinic acid A	pos	up	1.0916	0.005924	1.9339
68	(9E)-7-Hydroxydodec-9-enoylcarnitine	pos	up	1.0338	0.04897	1.1197
69	Acetylcysteine	pos	up	1.0946	0.009943	1.9801
70	Erythromycin C	pos	down	0.7934	7.95E-07	3.2985
71	Zeranol	pos	up	1.0842	0.006582	1.7849
72	1-[4,5-BIS(Hydroxymethyl)-3-Methoxy-2-Methylphenoxy]-3-Methylbutane-2,3-Diol	neg	up	1.0733	0.007469	1.7487
73	N(epsilon)-(carboxyethyl)lysine	neg	up	1.3083	0.03667	2.4756
74	Levetiracetam	neg	down	0.9108	0.01648	1.6265
75	N-(3-Amino-3-oxopropyl)-L-valine	neg	down	0.9268	0.04236	1.0437
76	2-Methylthioadenosine	neg	up	1.2149	0.03906	2.1644
77	Norepinephrine sulfate	neg	down	0.8234	0.0271	2.6912
78	10-Methyl-9-(10-methyl-1H-acridin-9-yl)-1H-acridine	neg	down	0.9256	0.02362	1.8485
79	Abscisic alcohol 11-glucoside	neg	down	0.92	0.04219	1.6809
80	Gramineal	neg	up	1.0743	0.02679	1.833
81	Pyocyanin	neg	up	12.570 4	0.000249	4.9553
82	2-Hydroxydecanedioic acid	neg	up	1.1376	0.0198	2.4763
83	(Z)-2-Methyl-2-butene-1,4-diol 4-O-beta-D-Glucopyranoside	neg	up	1.1276	0.01953	2.4344

---

84	N,O-Didesmethyltramadol	neg	down	0.445	0.02303	3.9772
85	Hydroxychloroquine	neg	up	1.1159	0.0118	2.4399
86	4-Methylaminorex	neg	up	1.2177	0.03513	2.4829
87	LysoPA(22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	neg	up	1.1825	0.01106	2.7367
88	Traumatin	neg	down	0.9542	0.008344	1.3416
89	Gemfibrozil 1-O-beta-Glucuronide	neg	up	1.0686	0.04077	1.5824
90	16-alpha-Hydroxyandrosterone	neg	down	0.9343	0.009274	1.6612
91	4-ene-Valproic acid	neg	up	1.0507	0.01423	1.5988
92	9(S)-HpODE	neg	down	0.8179	0.01434	2.4374
93	Lobucavir	neg	up	1.2307	0.04197	2.5938
94	Blumenol C glucoside	neg	up	1.0777	0.01315	1.8754
95	3-Oxododecanoic acid	neg	down	0.9608	0.01683	1.2839
96	Isoforskolin	neg	up	1.2433	0.009365	2.3613
97	Arphamenine B	neg	up	1.0784	0.01115	1.8185
98	Beta-Funaltrexamine	neg	up	1.1273	0.02917	2.2767
99	5-Methoxytryptamine	neg	up	1.3331	0.01613	3.2155
100	Alongside	neg	up	1.3504	0.02087	1.8266
101	2-Methyl-5-hydroxytryptamine	neg	up	1.3487	0.009461	3.2253
102	Cifostodine	neg	up	1.503	0.004929	3.6645

---

103	Prostaglandin B2	neg	up	1.6976	0.03425	2.1262
104	Siguazodan	neg	up	1.203	0.03768	2.2068
105	Tryptophyl-Threonine	neg	up	1.7677	0.04364	3.3851
106	Cysteinyl-Leucine	neg	up	1.198	0.008556	2.3391
107	Exatecan	neg	up	1.206	0.01847	2.8358
108	1-Naphthalenesulfonic acid, 4-hydroxy-3-nitroso-	neg	up	1.1528	0.01373	2.3298
109	N-Biotinyl-4-aminobenzoic acid	neg	down	0.8888	0.01583	2.1189
110	3-(3-Indolyl)-2-oxopropanoic acid	neg	up	1.1615	0.03503	2.1949
111	N-hydroxy-L-tryptophan	neg	down	0.941	0.04556	1.5644
112	2-Isopropylmalic acid	neg	down	0.9511	0.005863	1.1193
113	Sesamol	neg	up	1.13	0.02754	2.0237
114	3,4-Dihydroxybenzaldehyde	neg	up	1.0936	0.03803	1.322
115	Maleic acid	neg	up	1.0479	0.03637	1.2519
116	Tyrosine-tyrosinate	neg	up	1.2221	0.03816	2.4165
117	5-Deoxymyricanone	neg	up	1.2302	0.01854	2.5628
118	(1R,2R,4S,6R)-2,6-Fenchanediol 2-O-b-D-glucoside	neg	up	1.1653	0.03185	1.9052