

Supplementary Table 5 Differential metabolites between the struvite and control group

No.	Metabolite	Mode	Regulate	FC	<i>P</i> value	VIP value
1	Resolvin E2	pos	down	0.9385	0.03163	1.2981
2	12-oxo-PDA	pos	down	0.8511	0.008378	2.1467
3	Ketopinic acid	pos	down	0.9472	0.008697	1.3276
4	Asparaginyllarginine	pos	down	0.9505	0.02117	1.1911
5	3-Phenylpropanal	pos	down	0.9431	0.02326	1.1995
6	3,4-Dimethyl-5-pentyl-2-furanpropanoic acid	pos	down	0.9361	0.02931	1.3459
7	Indoleacrylic acid	pos	down	0.8428	0.01482	2.0604
8	Hexyl glucoside	pos	down	0.8362	0.004009	2.1766
9	(-)-trans-Carveol glucoside	pos	down	0.9486	0.04878	1.1196
10	Pazufloxacin	pos	down	0.8763	0.01073	1.9427
11	3,5,5-Trimethyl-1,2-cyclohexanedione	pos	down	0.8293	0.03914	1.8741
12	4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[(2R)-2-amino-2-(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-, (2S,5R,6R)-	pos	up	1.3812	0.01268	2.6212
13	Lidocaine	pos	up	1.1183	0.01903	1.9547
14	Tocainide	pos	down	0.8393	0.0418	1.9442
15	N-Acetyl-O-methyl-L-tyrosine	pos	down	0.8773	0.04949	1.6853
16	N-Acetylaspartylglutamic acid	pos	down	0.8946	0.03159	1.624

17	Antramycin	pos	up	1.1766	0.01086	2.0376
18	Vibunazole	pos	down	0.9607	0.02451	1.0338
19	Deoxyhypusine	pos	down	0.8985	0.0162	1.7898
20	1-Methyladenosine	pos	down	0.9661	0.03171	1.0028
21	2',3'-Dideoxy-3'-fluorouridine	pos	down	0.8935	0.04826	1.6022
22	TETRAHYDROURIDINE	pos	down	0.9631	0.03742	1.0048
23	O-Glutarylcarnitine	pos	down	0.9563	0.02533	1.179
24	Turicine	pos	down	0.8968	0.007175	1.6827
25	Sec-o-Glucosylhamaudol	pos	down	0.9137	0.0325	1.4307
26	Portulacaxanthin II	pos	down	0.877	0.02816	1.8456
27	2,3,4,5-Tetrahydro-2-pyridinecarboxylic acid	pos	up	1.0746	0.04717	1.2559
28	Fructose lactate	pos	down	0.9399	0.0004964	1.6195
29	5-Aminovaleric Acid	pos	down	0.9412	0.009144	1.3833
30	D-Dopachrome	pos	up	1.1353	0.04696	1.6508
31	Naepaine	pos	up	1.2801	0.02883	2.4442
32	Alpha-Methyl-m-tyrosine	pos	down	0.9393	0.04061	1.243
33	2-Methoxyestriol	pos	up	1.4854	0.001656	2.8269
34	Cysteinyl-Proline	pos	down	0.5609	0.01989	3.0677
35	N-Acetyl-1-aspartylglutamic acid	pos	down	0.9045	0.008723	1.9584

36	(2S)-2-[(2-Carboxy-2-oxoethyl)amino]pentanedioic acid	pos	down	0.8837	0.005981	1.9584
37	2-Dicyclohexylphosphino-2',6'-dimethoxybiphenyl	pos	down	0.8449	0.005395	2.2327
38	A-Methyldopamine	pos	down	0.3929	0.04298	2.8382
39	Metaraminol	pos	down	0.8831	0.03334	1.736
40	Phenyl-Alanine	pos	down	0.8982	0.03506	1.4676
41	Hydroxydesmethyltetrahydropiperine sulfate	pos	down	0.9024	0.03037	1.517
42	3-Methylindole	pos	down	0.7741	0.007007	2.6326
43	5-Isopropyl-2-(2-methylpropyl)-2-cyclohexen-1-one	pos	down	0.8432	0.02432	1.8487
44	(+)-cis-abscisic aldehyde	pos	down	0.8806	0.02929	1.5767
45	2-Pentyl-3-phenyl-2-propenal	pos	down	0.8871	0.04412	1.5124
46	Polyoxyethylene 40 monostearate	pos	down	0.8009	0.004999	2.3758
47	3,4-Dihydroxy-2-methoxy-4-methyl-3-[2-methyl-3-(3-methyl-but-2-enyl)-oxiranyl]-cyclohexanone	pos	down	0.9392	0.02857	1.3245
48	20-Cooh ltb4	pos	down	0.9369	0.03653	1.2572
49	Clarithromycin	pos	up	1.1149	0.01084	1.6146
50	PA(14:1(9Z)/24:1(15Z))	pos	up	1.1536	0.01561	1.8156
51	2,3-Dipalmitoyl-S-glycerylcysteine	pos	up	1.1041	0.005577	1.6312
52	P-Menthane-3,8-diol	pos	down	0.8231	0.02668	1.6909

53	PE(15:0/20:0)	pos	up	1.1208	0.03002	1.4881
54	Cer(d18:2(4E,14Z)/6 keto-PGF1alpha)	pos	up	1.0543	0.04109	1.1002
55	Gibberellin A53	pos	down	0.8822	0.001394	1.9832
56	Cromakalim	pos	down	0.8469	0.00203	2.0921
57	2-[2-[2-[2-[2-[2-[(Z)-2-[2-[2-(2-Octadecoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	pos	up	1.2046	0.04297	1.9948
58	Ketorolac	pos	down	0.721	0.003784	2.7049
59	2,3-Dihydroxypropyl dodecanoate	pos	down	0.8682	0.01352	1.7159
60	Menthyl pyrrolidone carboxylate	pos	down	0.9173	0.01259	1.5296
61	7-Epi-12-hydroxyjasmonic acid	pos	down	0.9348	0.009248	1.442
62	Butyl (S)-3-hydroxybutyrate glucoside	pos	down	0.7433	0.004116	2.7204
63	12-Oxo-2,3-dinor-10,15-phytodienoic acid	pos	down	0.9077	0.01651	1.6412
64	Curdione	pos	down	0.8778	0.04167	1.6105
65	Oxyglutinosone	pos	down	0.9233	0.02431	1.3299
66	7-Hydroxytrideca-9,11-dienoylcarnitine	pos	down	0.9627	0.03519	1.1079
67	Abscisic acid	pos	down	0.9195	0.02594	1.4853
68	6-Hydroxydodeca-8,10-dienoylcarnitine	pos	down	0.9426	0.01176	1.4495

69	3,3-Bis(carboxymethyl)hexadecanedioic acid	pos	down	0.8464	0.006214	2.0066
70	(R)-Methysticin	pos	down	0.8551	0.01954	1.8702
71	Gln Leu Gln	pos	down	0.8473	0.01607	2.0192
72	Guanadrel	pos	down	0.7687	0.01985	2.2409
73	(1S,2S,4R)-p-Menth-8-ene-1,2,10-triol 2-glucoside	pos	down	0.8411	0.0497	1.7901
74	8-Deoxy-11-hydroxy-13-chlorogrosheimin	pos	down	0.8734	0.04918	1.6722
75	N-(((2,7-Dimethyl-9H-fluoren-9-yl)methoxy)carbonyl)-L-leucine	pos	up	1.3844	0.02049	2.6108
76	3,4-Epoxy cyclohexylmethyl 3,4-Epoxy cyclohexanecarboxylate	pos	down	0.8832	0.02083	1.7541
77	Glucosaminic acid	pos	down	0.9223	0.008373	1.6021
78	Asparaginyl-Proline	pos	down	0.9436	0.03884	1.1665
79	Methyl 4-mercaptobutyrimidate	pos	down	0.8791	0.04915	1.3823
80	Gein	pos	down	0.6865	0.009851	2.6895
81	4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one	pos	down	0.7813	0.007645	2.6245
82	D-Cathine	pos	down	0.8539	0.008578	1.858
83	(10betaH,11xi)-11-Hydroxy-13-nor-6-eremophilin-8-one	pos	down	0.6999	0.04959	2.3506
84	Baicalin	pos	down	0.6172	0.02746	2.7962

85	10-hydroxy-(2E,8E)-decadien-4-ynoic Acid	pos	down	0.8925	0.03828	1.4512
86	Polygonal	pos	down	0.7797	0.02063	2.2191
87	Methyldopate	pos	down	0.9391	0.03679	1.0916
88	2-(Quinolin-8-yloxy)propanoic acid	pos	down	0.897	0.01986	1.7404
89	Paclobutrazol	pos	down	0.9417	0.0209	1.3169
90	2-hydroxy-3-methylbutanedioylcarnitine	pos	down	0.8893	0.0165	1.6879
91	2-Amino-6-[(1R,2S)-1,2,3-trihydroxypropyl]-7,8-dihydro-3H-pteridin-4-one	pos	down	0.8317	0.01717	2.148
92	Xi-2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	pos	down	0.8684	0.007194	1.9954
93	Sarmentosin	pos	down	0.7449	0.03949	2.066
94	Octa-2,6-dienedioylcarnitine	pos	down	0.8229	0.0459	1.9005
95	3-Des(dimethylaminoethyl)-3-acetic acid zolmitriptan	pos	down	0.744	0.005877	2.821
96	4-Quinolinecarboxylic acid	pos	down	0.9486	0.0004014	1.3814
97	7-Hydroxyetodolac	pos	down	0.7356	0.02863	2.3163
98	Octa-3,6-dienedioylcarnitine	pos	down	0.4687	0.01754	3.3922
99	2-succinylbenzoate	pos	down	0.6925	0.00625	2.7453
100	Genipic acid	pos	down	0.8331	0.0198	1.9491

101	5-methyl-N-(4-phenyl-1,3-thiazol-2-yl)furan-2-carboxamide	pos	down	0.8328	0.01183	2.1035
102	Cysteinyl-Tyrosine	pos	down	0.7823	0.01779	2.3421
103	4-(3-Tert-Butylamino-2-hydroxypropoxy)benzimidazol-2-one	pos	down	0.8356	0.0221	2.0303
104	Harmalol	pos	down	0.7955	0.002635	2.3788
105	H-D-Arg(NO ₂)-OH	pos	down	0.9099	0.03257	1.5632
106	2-Quinolinecarboxylic acid	pos	down	0.8528	0.001098	2.2533
107	Pyridoxal	pos	down	0.8874	0.02966	1.6137
108	Adenosine	pos	down	0.9078	0.01231	1.5241
109	N-Acetyltyrosine	pos	down	0.9005	0.0253	1.6442
110	3',5'-Cyclic AMP	pos	down	0.9428	0.004063	1.3437
111	Vicine	pos	down	0.8436	0.02963	1.7312
112	Delta-Valerolactone	pos	up	1.0696	0.02834	1.422
113	N-iminoethyl-l-ornithine	pos	down	0.9179	0.009655	1.8279
114	Lys Pro Leu	pos	down	0.8743	0.02579	1.7805
115	Trigonelline	pos	down	0.775	0.02302	2.208
116	2-(Methylamino)ethanol	pos	down	0.8874	0.01283	1.9432
117	Glycerylphosphorylcholine	pos	up	1.2556	0.01093	2.3692
118	Pyridin-3-yl sulfate	pos	down	0.8685	0.03886	1.7602

119	Glycyl-D-proline	pos	down	0.8718	0.04901	1.4558
120	N-(2,6-dimethylphenyl)-N2-Ethenyl-N2-Ethylglycinamide	pos	up	1.1356	0.02091	1.6713
121	Butorphanol	pos	up	1.1716	0.0168	2.1587
122	Loliolide	pos	down	0.9418	0.04827	1.1725
123	INDOPHENOL	pos	down	0.928	0.03307	1.3805
124	Indole-3-acetyl-glutamate	pos	down	0.8294	0.01994	2.1218
125	(S)-3-Octanol glucoside	pos	down	0.9469	0.04739	1.2116
126	Chlorhexidine	pos	up	1.3693	0.00132	2.9275
127	Blennin D	pos	down	0.9044	0.01092	1.6281
128	(+)-Nicotine	pos	down	0.6891	0.001782	2.7827
129	Artecanin	pos	down	0.7138	0.01509	2.1716
130	Erythromycin C	pos	up	1.2204	4.75E-05	2.573
131	Phenol	pos	down	0.9411	0.03459	1.1408
132	Zeranol	pos	down	0.9105	0.006972	1.7973
133	1-[4,5-BIS(HYDROXYMETHYL)-3-Methoxy-2-METHYLPHENOXY]-3-Methylbutane-2,3-Diol	neg	down	0.9397	0.00828	1.2969
134	Ala-Trp-OH	neg	up	1.1628	0.004665	2.1363
135	N(epsilon)-(carboxyethyl)lysine	neg	down	0.7437	0.02301	2.4433
136	1-Deoxy-D-xylulose-5-phosphate	neg	up	1.1211	0.03418	1.5681

137	Guanidoacetic acid	neg	down	0.8861	0.03045	1.5995
138	CAMP	neg	down	0.943	0.007598	1.3987
139	1-Oxononan-4-yl (2R)-2-acetamido-3-sulfanylpropanoate	neg	up	1.4311	0.01786	2.8122
140	2-Methylthioadenosine	neg	down	0.8402	0.02267	1.9294
141	L-Furosine	neg	down	0.872	0.04873	1.822
142	4-Hydroxyphenytoin glucuronide	neg	up	1.1696	0.02893	1.873
143	7-Amino-4-hydroxy-2-naphthalenesulfonic acid	neg	down	0.8842	0.03457	1.9352
144	Citrazinic acid	neg	down	0.8095	0.0239	1.8773
145	Quinolin-2-yl hydrogen sulfate	neg	down	0.8728	0.01539	1.9364
146	Methylgallic acid-O-sulphate	neg	down	0.8046	0.0254	2.2556
147	3-(5-(4-(1H-Imidazol-1-yl)phenyl)-1-(4-carbamoyl-2-methylphenyl)-1H-pyrrol-2-yl)propanoic acid	neg	down	0.8849	0.02483	1.8147
148	(S)-2-Amino-4-methylsulfanyl-butane-1-thiol	neg	down	0.8134	0.006654	2.3248
149	4-Hydroxy-5-(dihydroxyphenyl)-valeric acid-O-sulphate	neg	down	0.8767	0.02017	1.7776
150	Nivalenol	neg	down	0.8998	0.04329	1.5228
151	Pyocyanin	neg	down	0.1416	0.0357	2.6067
152	3,6-Dihydroxycyclohepta-2,4,6-trien-1-one	neg	down	0.8132	0.03104	2.13

153	(+/-)-2-(2-Furanyl)pyrrolidine	neg	down	0.9049	0.002604	1.539
154	2-Polyprenyl-6-methoxy-1,4-benzoquinone	neg	down	0.8433	0.008665	2.1585
155	L-Kynurenine	neg	down	0.8357	0.002882	2.3595
156	2-Phenylethanol glucuronide	neg	down	0.8673	0.01012	1.9304
157	2-Hydroxyphenethylamine	neg	down	0.9212	0.00499	1.4353
158	Indoximod	neg	down	0.7036	0.009499	2.4277
159	2-Hydroxyethyl methacrylate	neg	down	0.8848	0.003499	1.8265
160	2-Hydroxycampholonic acid	neg	down	0.9	0.04095	1.4351
161	Aspartyl-Tryptophan	neg	down	0.7995	0.02655	2.3159
162	Antipyrine	neg	down	0.7861	0.009648	2.7941
163	Isovaleric acid	neg	down	0.9154	0.02921	1.2397
164	N-(2,5-dioxocyclopentyl)acetamide	neg	up	1.1607	0.01229	2.1215
165	Lomefloxacin	neg	down	0.9656	0.03012	1.0109
166	Carmofur	neg	down	0.8006	0.02854	2.1576
167	2-n-Propyl-4-oxopentanoic acid	neg	down	0.9124	0.01374	1.4131
168	2-tert-Butyl-4-methoxyphenol	neg	down	0.948	0.01106	1.1952
169	Gemfibrozil 1-O-beta-Glucuronide	neg	down	0.9282	0.02409	1.3856
170	Nonate	neg	down	0.9118	0.004665	1.5806
171	4-ene-Valproic acid	neg	down	0.9517	0.01373	1.2431

172	12S-HHT	neg	down	0.9339	0.02299	1.2273
173	Buccoxime	neg	down	0.8949	0.0358	1.482
174	4-Tert-Amylphenol	neg	down	0.8974	0.01568	1.6287
175	9(S)-HpODE	neg	up	1.3592	0.0004861	2.897
176	Furanogermenone	neg	down	0.9204	0.001586	1.6827
177	4-Hydroxy-3-methoxy-2,10-bisaboladien-9-one	neg	down	0.9215	0.03493	1.2162
178	3,5,5-Trimethyl-2-cyclohexen-1-one	neg	down	0.9332	0.01811	1.2698
179	Sugeonol	neg	down	0.9391	0.01036	1.3206
180	Isopiperitenone	neg	down	0.938	0.03693	1.2808
181	Desacetyl-laurenobiolide	neg	down	0.9522	0.01085	1.171
182	6,15-Diketo,13,14-dihydro-PGF1a	neg	down	0.9387	0.0204	1.2243
183	(2E,4E)-2,4-Octadien-1-ol	neg	down	0.9341	0.01853	1.2325
184	6-(4-sulfophenyl)decanoic Acid	neg	down	0.9224	0.00705	1.5348
185	Tetranorprostanedioic acid	neg	down	0.9359	0.03473	1.1923
186	Blumealactone B	neg	down	0.9236	0.03621	1.3897
187	2-hydroxydesipramine	neg	down	0.9351	0.0486	1.3592
188	Phosphocreatine	neg	down	0.7319	0.009746	2.5155
189	Caprylic acid	neg	down	0.9138	0.0134	1.4021
190	Azelaic acid	neg	down	0.9467	0.01826	1.2305

191	1,2,3,4,5,6-Hexahydro-5-(1-hydroxyethylidene)-7H-cyclopenta[b]pyridin-7-one	neg	down	0.8685	0.04545	1.7694
192	11-Dehydro-2,3-dinor-txb2	neg	down	0.8781	0.01451	1.8803
193	5-Methoxytryptamine	neg	down	0.7727	0.02168	2.367
194	2-Methyl-5-hydroxytryptamine	neg	down	0.7753	0.02453	2.2411
195	3-(3,5-dihydroxyphenyl)-1-propanoic acid sulphate	neg	down	0.9464	0.005564	1.6186
196	1,2-Dihydroxy-3,4-epoxy-1,2,3,4-tetrahydronaphthalene	neg	down	0.8482	0.03256	1.7526
197	Cifostodine	neg	down	0.7072	0.04331	2.2448
198	9-Azabicyclo[3.3.1]nonan-3-one	neg	down	0.9403	0.01497	1.2702
199	Hydroxyethyl methacrylic acid	neg	down	0.8873	0.003916	1.833
200	(ent-6 α ,7 α)-6,7-Dihydroxy-16-kauren-19-oic acid	neg	down	0.7738	0.03026	2.0651
201	Siguazodan	neg	down	0.7923	0.008592	2.3362
202	Geniposide	neg	down	0.8919	0.03883	1.4333
203	D-Linalool 3-(6"-malonylglucoside)	neg	down	0.8904	0.01364	1.9447
204	1,2-Cyclohexanedicarboxylic acid, 4-methyl-	neg	down	0.8412	0.03763	1.8184
205	Eugenyl glucoside	neg	down	0.8568	0.01763	2.0074
206	Propofol glucuronide	neg	down	0.8324	0.01051	2.2893
207	Dihydrocaffeic acid 3-O-glucuronide	neg	down	0.7264	0.00857	2.6025

208	Aminomethanesulfonic acid	neg	down	0.8245	0.01001	2.5449
209	1-Naphthalenesulfonic acid, 4-hydroxy-3-nitroso-	neg	down	0.8888	0.02666	1.8245
210	Mecoprop	neg	down	0.881	0.01107	1.9525
211	Isoferuloyl C1-glucuronide	neg	down	0.7497	0.00818	2.5813
212	Ethyl 2-furanacrylate	neg	down	0.9051	0.005843	1.7733
213	Sumiki's acid	neg	down	0.5727	0.0185	3.2468
214	2-Pyrocatechuic acid	neg	down	0.9121	0.04122	1.5292
215	Indole-3-carboxylic acid-O-sulphate	neg	down	0.9043	0.04404	1.4882
216	Aspartyl-Gamma-glutamate	neg	up	1.2718	0.01658	2.4349
217	Xi-2,3-Dihydro-2-oxo-1H-indole-3-acetic acid	neg	up	1.565	0.01018	2.809
218	Protocatechuic acid 3-O-sulfate	neg	down	0.9309	0.02994	1.4555
219	6-Thiourate	neg	down	0.9221	0.02691	1.4965
220	Vinclozolin M2	neg	down	0.8199	0.03007	2.0868
221	Ferene triazine	neg	down	0.9488	0.01911	1.2413
222	Xanthosine	neg	down	0.9645	0.00246	1.1393
223	2,6-diamino-4-hydroxy-5-formamidopyrimidine	neg	down	0.7663	0.02093	2.6226
224	5-Megastigmen-7-yne-3,9-diol	neg	down	0.9521	0.02757	1.1014
225	Gamma-delta-Dioxovaleric acid	neg	down	0.8517	0.01499	2.2088

226	Tetrahydrodipicolinate	neg	up	1.1433	0.01153	1.7946
227	Raffinose	neg	down	0.8271	0.04792	2.0154
228	Oleoside	neg	down	0.9301	0.03685	1.2667
229	Tyrosine-tyrosinate	neg	down	0.7979	0.03733	2.1502
230	5-Deoxymyricanone	neg	down	0.7786	0.01038	2.4488
231	Cucumopine	neg	down	0.8962	0.02224	1.5004
232	Jasmolone glucoside	neg	down	0.9036	0.03128	1.4249
233	(6E,8S,10Z)-8-hydroxy-3-oxohexadecadienoic acid	neg	down	0.9434	0.01924	1.1908
234	Hydroxycortisol	neg	down	0.9142	0.03935	1.4557
235	(1R,2R,4S,6R)-2,6-Fenchenediol 2-O- β -D-glucoside	neg	down	0.8404	0.01052	1.9509
236	3-Hydroxyoctanoic acid	neg	down	0.8891	0.01528	1.6946
237	5-Methoxytryptophan	neg	down	0.8591	0.02681	2.0884
238	Valeric acid	neg	down	0.9313	0.03025	1.1987
239	4-Methyl-5-oxo-2-pentyl-2,5-dihydro-3-furancarboxylic acid	neg	down	0.9515	0.00215	1.2581
240	Tetranor-PGFM	neg	down	0.9341	0.03148	1.2106
241	Xi-7-Hydroxyhexadecanedioic acid	neg	down	0.9368	0.02867	1.225
242	Polyethylene, oxidized	neg	down	0.9549	0.03234	1.1596
243	Pyrocatechol	neg	down	0.9058	0.009777	1.6788
