

**Supplementary Table 1. Differentially expressed metabolites in all 3 AKI stages versus healthy control groups**

No.	Metabolite	m/z (mass/charge)	Retention time (sec)	P value <sup>a)</sup>	Log fold change	Mode
1	Unannotated	416.21	1.85	0.03	1.01	HILIC POS
2	Unannotated	416.88	1.55	0.03	-0.62	HILIC NEG
3	Unannotated	484.88	1.53	0.04	-0.58	HILIC NEG
4	Unannotated	804.59	1.25	0.04	0.62	HILIC NEG
5	Unannotated	298.29	18.57	0.01	-0.8	C-18 POS
6	Unannotated	450.31	10.98	0.04	-1.3	C-18 POS
7	Unannotated	762.59	21.2	0.02	1.2	C-18 POS
8	Unannotated	267.12	11.95	0.01	-1.3	C-18 NEG
9	11a-hydroxyprogesterone	329.25	18.53	0.01	-0.67	C-18 NEG
10	Unannotated	365.27	16.41	0.03	-0.7	C-18 NEG
11	Unannotated	401.29	19.14	0.05	0.87	C-18 NEG
12	1-hexadecanoyl-2-sn-glycero-3-phosphate	409.24	14.98	0.05	-0.75	C-18 NEG
13	Unannotated	448.31	10.96	0.05	-1.05	C-18 NEG
14	1-palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	452.28	15	0.03	0.62	C-18 NEG
15	1-oleoyl-sn-glycero-3-phosphoethanolamine	478.29	15.43	0.03	0.67	C-18 NEG
16	Unannotated	524.28	13.97	0.02	0.75	C-18 NEG
17	Unannotated	559.47	18.65	0.05	-0.81	C-18 NEG
18	Unannotated	804.57	23.23	0.02	1.94	C-18 NEG

AKI, acute kidney injury; HILIC, hydrophilic interaction liquid chromatography; POS, positive; NEG, negative.

<sup>a)</sup>Unpaired *t* test.