

## **Urinary NMR profiling in pediatric acute kidney injury - a pilot study**

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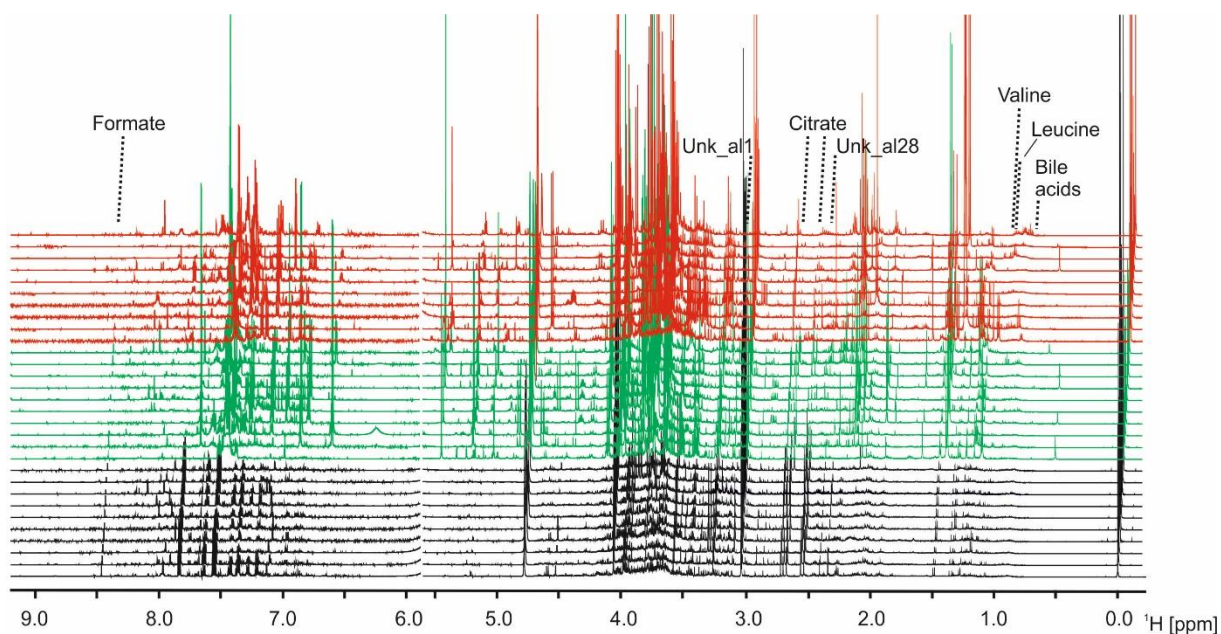
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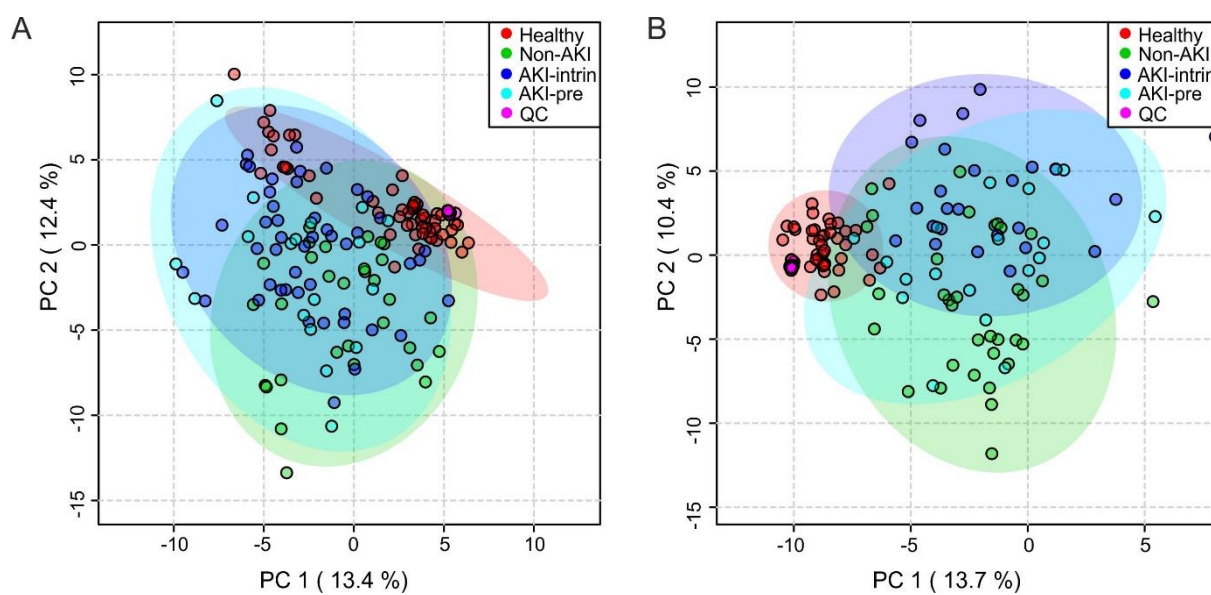
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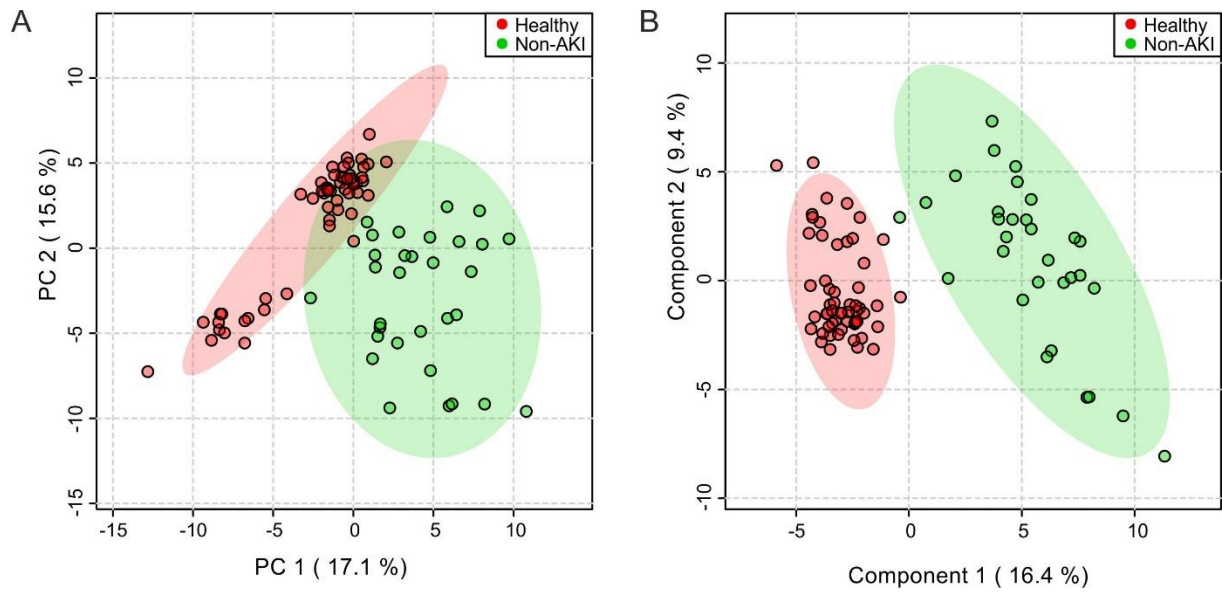
## **Supplemental Information**



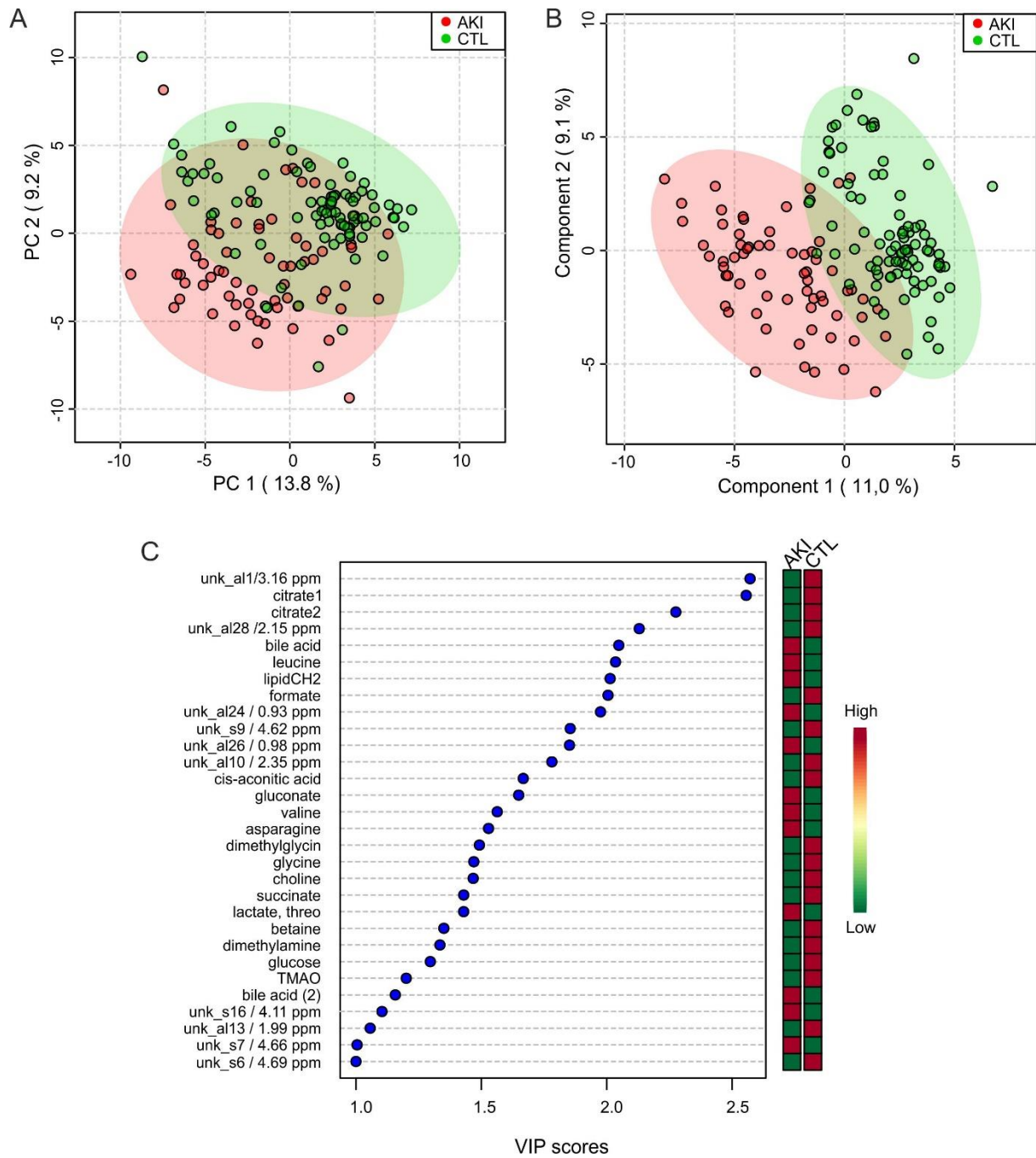
**Figure S1.** Ten representative spectra of each group: healthy control group – black, hospitalized patients without AKI – green, AKI – red.



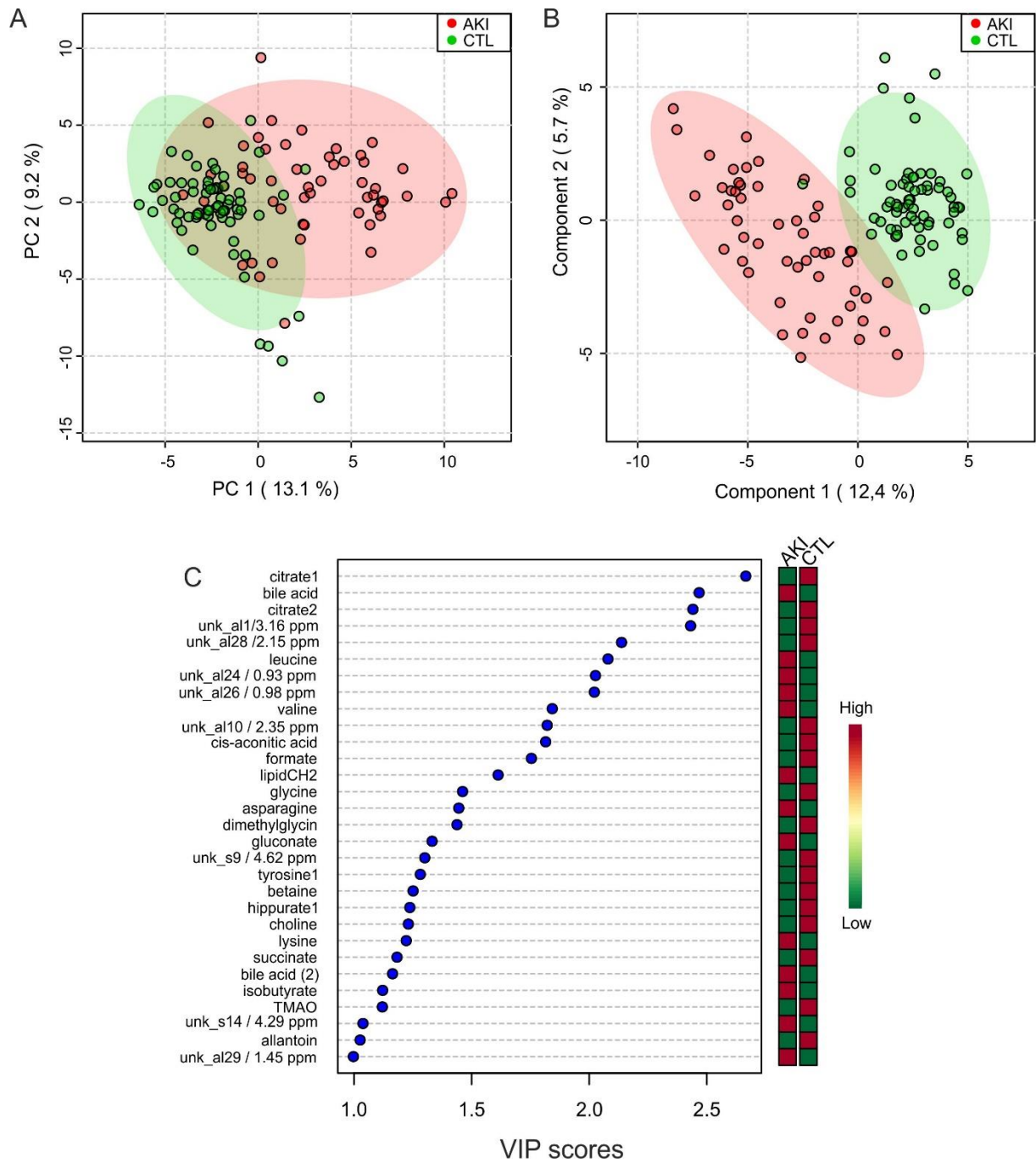
**Figure S2:** Principal component analysis. AKI classified into prerenal (AKI-pre) and intrinsic (AKI-intrin). A) Neonates included into study cohort, B) neonates excluded. Healthy – healthy control group. Non-AKI – hospitalized patients without AKI, QC – quality control.



**Figure S3:** Statistical analysis of healthy control group vs. hospitalized patients without AKI (Non-AKI): A) Principal component analysis. B) Partial least squares discriminant analysis.  $R^2$  0.97,  $Q^2$  0.87, 5 components, p value in permutation < 0.001.



**Figure S4.** AKI vs CTL after taking out buckets separating healthy control group from hospitalized patients without AKI. Non-AKI and healthy control groups were joined in one group CTL. A) Principal component analysis. B) Partial least squares discriminant analysis. C) Variable importance in projection plot.



**Figure S5.** Same as Figure S4, with neonatal spectra excluded. A) Principal component analysis. B) Partial least squares discriminant analysis. C) Variable importance in projection plot.

**Table S1.** Partial least squares discriminant analysis of healthy control group vs. hospitalized patients without AKI (Non-AKI): Variable importance in projection (VIP) values.

<b>Bucket</b>	<b>VIP</b>
Lactose/unk_s3 / 5.25 ppm	2.3
Mannitol-1	2.1
<i>Mannitol-2*</i>	1.7
<i>Mannitol-3*</i>	1.8
<i>mannitol-4*</i>	1.8
<i>Mannitol-5*/</i> guanidoacetic acid	1.6
Mandelic acid /phenyl-acetylglycine/phenylalanine	2.0
Glucose/taurine	1.9
HPPHA/phenol	1.9
glutamine	1.9
unk_a9 / 7.47 ppm	1.8
3-aminoisobutyrate	1.7
Hippurate-4*	1.7
creatinine	1.6
unk_s2 / 5.35 ppm	1.6
Indoxylsulfate-3*	1.5
Indoxylsulfate-4*	1.6
glycolic acid	1.6

\*Mannitol, hippurate and indoxylsulfate have more than one resonance. Due to overlap with resonances of other compounds the corresponding buckets do not behave in exactly the same way in multivariate analysis. All buckets of the respective compounds were omitted from further analysis.