

1 Supplementary Table 1 – Metabolites associated with the occurrence of acute kidney
2 injury up to 24h

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4 Glycerin

5 L-(-)-Serine

6 Fumaric acid

7 L-(-)-Malic acid

8 1-Methylnicotinamide

9 alpha-Ketoglutaric acid

10 2-Oxoadipic acid

11 N-Formyl-L-methionine

12 Citric acid

13 Corticosterone

14 Acrylic acid

15 2-Furoic acid

16 L-Lysine

17 Paracetamol

18 Tranexamic acid

19 7-Methylguanine

20 Pyridoxamine

21 N-Acetylaspartic acid

22 2-Hydroxyhippuric acid

23 4-Acetamidoantipyrine

24 Decanoylcarnitine

25 Glycerophospho-N-palmitoyl ethanolamine

- 1 5Î±-Dihydrotestosterone glucuronide
- 2 2-Oxobutyric acid
- 3 L-a-Amino-ε-caprolactam
- 4 Vigabatrin
- 5 Timonacic
- 6 2347
- 7 3-Thiomorpholinecarboxylic acid
- 8 (.+/-)-Tartaric acid
- 9 Dezaguanine
- 10 Vanillin
- 11 ST2975000
- 12 hydroxyacetone phosphate
- 13 ARECOLINE
- 14 8-Hydroxyoctanoic acid
- 15 S-Allyl-L-cysteine
- 16 TBHQ
- 17 BZ7175000
- 18 N-Nitrosoguvacoline
- 19 XT5075000
- 20 1774244
- 21 EDDA
- 22 UF7990000
- 23 D-Glucono-delta-lactone
- 24 Theophylline
- 25 Lanthionine ketimine

- 1 Kynurenic acid
- 2 N-Acetyl-L-glutamic acid
- 3 Prenisteine
- 4 carglumic acid
- 5 4-Methoxy-1H,1'H-2,2'-bipyrrole-5-carbaldehyde
- 6 Ser-Ser
- 7 (2E)-2-Cyano-N-(ethylcarbamoyl)-2-(methoxyimino)acetamide
- 8 Itaconate
- 9 (1S,6S)-6-Aminooctahydro-1-indolizinyll acetate
- 10 1640340
- 11 MFCD00025555
- 12 1,2,3,4-tetrahydro-beta-carboline-3-carboxylic acid
- 13 piroximone
- 14 Butopyronoxyl
- 15 Myristoleic acid
- 16 1872050
- 17 Leu-Val
- 18 Sulbactam
- 19 (E)-3,4,5-Trimethoxycinnamic acid
- 20 2-Isocapryloyl-3R-hydroxymethyl-gamma-butyrolactone
- 21 3-Oxotetradecanoic acid
- 22 Threonylglutamine
- 23 4-[(2-Isopropyl-5-methylcyclohexyl)oxy]-4-oxobutanoic acid
- 24 Imazapyr
- 25 Gln-Gln

- 1 lys-gln
- 2 (10S)-Juvenile hormone III diol
- 3 1083877
- 4 5955761
- 5 asn-arg
- 6 3-[(2,6-Dimethylheptanoyl)oxy]-4-(trimethylammonio)butanoate
- 7 3-hydroxyoctanoylcarnitine
- 8 Monocerin
- 9 METIPRANOLOL
- 10 N2-Dimethylguanosine
- 11 (4S)-4-[(2E,4Z)-2,4-Decadienoyloxy]-4-(trimethylammonio)butanoate
- 12 15,16-DiHODE
- 13 9-Decenoylcarnitine
- 14 3-[(3-Hydroxydecanoyl)oxy]-4-(trimethylammonio)butanoate
- 15 1886839
- 16 3-indole carboxylic acid glucuronide
- 17 glycidyl oleate
- 18 trans-2-Dodecenoylcarnitine
- 19 4147610
- 20 Tetrahydrocortisone
- 21 3, 5-Tetradecadiencarnitine
- 22 3-Hydroxy-cis-5-tetradecenoylcarnitine
- 23 1-Oleoyl-lysophosphatidic acid
- 24 2-Hydroxy-3-(phosphonoxy)propyl stearate
- 25 MFCD00083068

- 1 2-Hydroxy-3-(phosphonooxy)propyl (4Z,7Z,10Z,13Z,16Z)-4,7,10,13,16-
- 2 docosapentaenoate
- 3 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphocholine
- 4 MFCD00678983
- 5 2-[(2E,6E,10E,14E,18E,22E,26E,30E)-3,7,11,15,19,23,27,31,35-Nonamethyl-
- 6 2,6,10,14,18,22,26,30,34-hexatriacontanonaen-1-yl]-1,4-naphthoquinone