

Supplementary materials

Table S1 More information about chemical elucidation of differential metabolites in LC-MS analysis

| Metabolite | Detected ion | Measured m/z | Formula | ppm ^a | MS/MS fragment ^b | Database ID ^c | | | |
|------------------------|--|--------------|--|------------------|--|--------------------------|---------|--------|------------|
| | | | | | | HMDB | KEGG | METLIN | ChemSpider |
| Creatine | [M+H] ⁺ | 132.0770 | C ₄ H ₁₀ N ₃ O ₂ ⁺ | 1.51 | 132[M+H] ⁺ /115/90/72/44 | 64 | C00300 | 7 | 566 |
| Trimethylglycine | [M+H] ⁺ | 118.0864 | C ₅ H ₁₂ NO ₂ ⁺ | 0.85 | 118[M+H] ⁺ /58/59 | 43 | C00719 | 287 | 242 |
| N-methylnicotinic acid | [M+H] ⁺ | 138.0541 | C ₇ H ₈ NO ₂ ⁺ | -6.52 | 138[M+H] ⁺ /94/92/78/65/53 | 875 | C01004 | 273 | - |
| Uric acid | [M+H] ⁺ | 169.0357 | C ₅ H ₅ N ₄ O ₃ ⁺ | 0.59 | 169[M+H] ⁺ /152/141/126/96/70/ 55/43 | 289 | C00366 | 88 | 1142 |
| 3-HIVC | [M+H] ⁺ | 262.1640 | C ₁₂ H ₂₄ NO ₅ ⁺ | -3.43 | 262[M+H] ⁺ /144/85/60/59 | - | - | 6505 | - |
| 2PY/4PY | [M-NH ₃ +H] ⁺ | 136.0398 | C ₇ H ₆ NO ₂ ⁺ | 3.68 | 153[M+H] ⁺ /136/108/92/80/53 | 04193/ | C05842/ | - | 62899/ |
| | [M-NH ₃ -CO+H] ⁺ | 108.0448 | C ₆ H ₆ NO ⁺ | 3.70 | | 04194 | C05843 | | 389671 |
| Kynurenic acid | [M-H ₂ O-CO+H] ⁺ | 144.0447 | C ₉ H ₆ NO ⁺ | 2.15 | 190[M+H] ⁺ /144/116/89/63 | 715 | C01717 | 5683 | 3712 |
| t(6)A | [M-ribosyl+H] ⁺ | 281.0989 | C ₁₀ H ₁₃ N ₆ O ₄ ⁺ | -1.35 | 413[M+H] ⁺ /281/162/136/120/ 119 | - | - | - | 141829 |
| Dihydroxyquinoline | [M+H] ⁺ | 162.0548 | C ₉ H ₈ NO ₂ ⁺ | -1.23 | 162[M+H] ⁺ /144/116/89 | 4077 | C05639 | - | 389609 |

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^a ppm=(measured m/z-theoretical m/z)/theoretical m/z × 10⁶; ^b The collision energy for MS/MS analysis was set at 20 eV; ^c Databases available on www.hmdb.ca/ for HMDB, www.kegg.com/ for KEGG, <http://metlin.scripps.edu/> for METLIN and www.chemspider.com/ for ChemSpider.

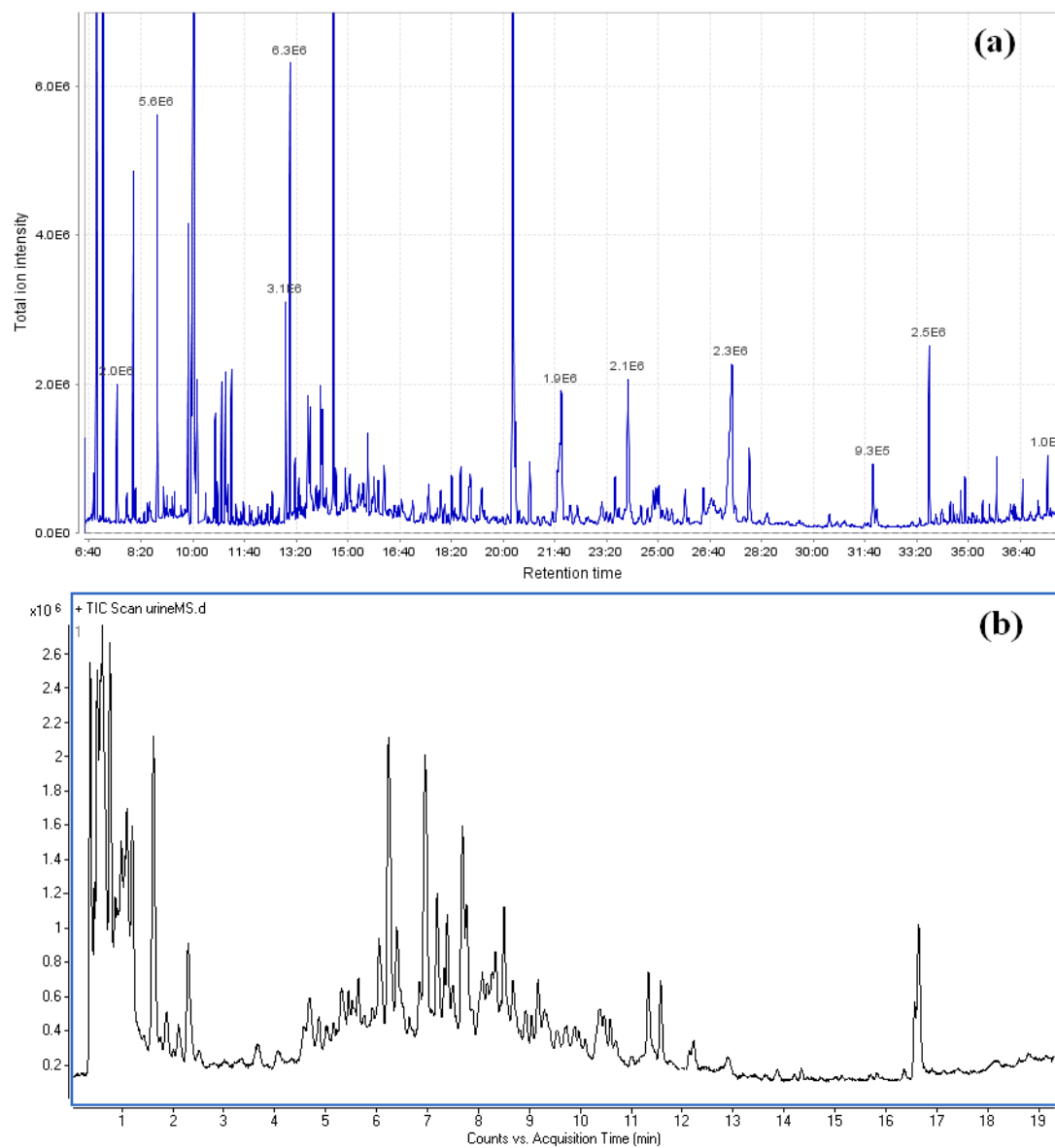


Fig. S1 Typical metabolic profiles of a rat urine (QC sample) acquired by GC-MS (a) and LC-MS (b).