Electronic Supplementary Material (ESI) for RSC Advances.


Table S1.Theinformationoflipidmarkersrelated with KYDS rats model identified in positive and negative mode.

| NO. | Rt/min | m/z | Metabolite name | Scan | Proposed composition | LIPID code | Change trend |
|---|---|---|---|---|---|---|---|
| 1 | 2.34 | 480.3071 | LysoPE(0:0/18:1(11Z)) | ESI+ | $C_{23}H_{46}NO_7P$ | LMGP02050039 | ↑ |
| 2 | 3.6 | 414.2992 | N-Docosahexaenoyl GABA | ESI+ | $C_{26}H_{39}NO_3$ | LMFA08020105 | ↓ |
| 3 | 4.57** | 395.2774 | 15-HETE-G | ESI+ | $C_{23}H_{38}O_5$ | LMGP06050010 | ↓ |
| 4 | 5.32* | 468.344 | PE(O-18:0/0:0) | ESI+ | $C_{23}H_{50}NO_6P$ | LMGP02060003 | ↓ |
| 5 | 7.25 | 317.2473 | 5beta-pregnane-3,20-dione | ESI+ | $C_{21}H_{32}O_2$ | LMST02030146 | ↓ |
| 6 | 7.42* | 701.5579 | SM(d16:1/18:1) | ESI+ | $C_{39}H_{77}N_2O_6P$ | LMSP03010040 | ↓ |
| 7 | 7.95 | 510.3894 | PC(O-18:0/0:0) | ESI+ | $C_{26}H_{56}NO_6P$ | LMGP01060014 | ↓ |
| 8 | 8.98 | 355.2131 | 5-hydroperoxy-7-[3,5-epidioxy-2-(2-octenyl)-cyclopentyl]-6-heptenoic acid | ESI+ | $C_{19}H_{30}O_6$ | LMFA01040028 | ↓ |
| 9 | 9.22 | 427.3198 | (25S)-3-oxo-cholest-1,4-dien-26-oic acid | ESI+ | $C_{28}H_{42}O_3$ | LMST04030213 | ↓ |
| 10 | 9.3* | 758.5694 | PC(16:0/18:2(9Z,12Z)) | ESI+ | $C_{42}H_{80}NO_8P$ | LMGP01010594 | ↓ |
| 11 | 9.97* | 235.169 | Sugeonol | ESI+ | $C_{15}H_{22}O_2$ | LMPR0103450003 | ↑ |
| 12 | 10.59** | 149.0269 | 2-Oxo-4-methylthiobutanoic acid | ESI+ | $C_5H_8O_3S$ | LMFA01060170 | ↑ |
| 13 | 10.59** | 391.2847 | 12α-Hydroxy-3-oxo-5β-cholan-24-oic Acid | ESI+ | $C_{24}H_{38}O_4$ | LMST04010168 | ↑ |
| 14 | 10.59 | 803.583 | PG(18:1(9Z)/20:1(11Z)) | ESI+ | $C_{44}H_{83}O_{10}P$ | LMGP04010958 | ↑ |
| 15 | 10.62** | 393.2997 | Allodeoxycholic acid | ESI+ | $C_{24}H_{40}O_4$ | LMST04010044 | ↓ |
| 16 | 10.88 | 536.1779 | Davallioside A | ESI+ | $C_{25}H_{29}NO_{12}$ | LMPK12020044 | ↓ |
| 17 | 11.11* | 768.5892 | PC(P-16:0/20:3(5Z,8Z,11Z)) | ESI+ | $C_{44}H_{82}NO_7P$ | LMGP01030129 | ↓ |
| 18 | 11.24 | 707.1791 | Kaempferol3-[2‴,3‴,5‴-triacetyl-alpha-L-arabinofuranosyl-(1->6)-glucoside | ESI+ | $C_{32}H_{34}O_{18}$ | LMPK12111800 | ↓ |
| 19 | 2.72* | 343.0978 | Sanaganone | ESI- | $C_{22}H_{16}O_4$ | LMPK12110058 | ↓ |
| 20 | 6.95 | 315.2325 | Pregnenolone | ESI- | $C_{21}H_{32}O_2$ | LMST02030088 | ↑ |
| 21 | 8.93 | 506.3235 | PE(0:0/20:1(11Z)) | ESI- | $C_{25}H_{50}NO_7P$ | LMGP02050046 | ↑ |
| 22 | 10.84 | 283.2588 | Linoleic acid(d4) | ESI- | $C_{18}H_{28}D_4O_2$ | LMFA01030809 | ↑ |

Compared with model group,* stands for significant difference ($p<0.05$) ,**stands for very significant difference($p<0.01$).

↑ ↓ stands for the relative content of ions which is increased or decreased.