Table 1S: The distribution of AO metabolites in different sample and different method

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak | tR | Theoretical Mass *m/z* | Formula [M-H]- | Identification/Reactions | T0.5 | T1 | T2 | T4 | Heart | liver | spleen | lung | kidney | brain | 1 | 2 | 3 |
| 1 | 11.67 | 329.06557 | C17H13O7 | AO | + | + | + | + | + | + | + | + | + | + | + | + | + |
| 2 | 11.49 | 329.06557 | C17H13O7 | Isomer of AO | + | + | + | + | - | - | - | - | - | - | + | + | + |
| 3 | 11.86 | 329.06557 | C17H13O7 | Isomer of AO | - | + | + | + | - | - | - | - | - | - | + | + | - |
| 4 | 10.96 | 299.05611 | C16H11O6 | Demethoxylation of AO | - | + | + | + | - | - | - | - | - | - | + | + | + |
| 5 | 11.57 | 299.05611 | C16H11O6 | Demethoxylation of AO | + | + | + | + | + | + | + | + | + | + | + | + | - |
| 6 | 7.47 | 345.06159 | C17 H13 O8 | Hydroxylation of AO | + | + | + | + | - | - | - | - | - | - | + | + | + |
| 7 | 7.57 | 345.06159 | C17H13O8 | Hydroxylation of AO | - | + | + | + | - | - | - | - | - | - | + | + | + |
| 8 | 7.75 | 345.06159 | C17H13O8 | Hydroxylation of AO | - | - | - | + | - | - | - | - | - | - | + | + | + |
| 9 | 5.34 | 409.02326 | C17H13O10S | Sulfation of AO | - | - | - | + | - | - | - | - | - | - | + | + | + |
| 10 | 7.37 | 409.02326 | C17H13O10S | Sulfation of AO | + | + | + | + | - | - | - | - | - | - | + | + | + |
| 11 | 8.16 | 409.02326 | C17H13O10S | Sulfation of AO | - | + | + | + | + | + | + | + | + | + | + | + | + |
| 12 | 6.86 | 475.08820 | C22H19O12 | Glucuronidation and Demethoxylation of AO | + | + | + | + | + | + | + | + | + | + | + | + | + |
| 13 | 7.21 | 475.08820 | C22H19O12 | Glucuronidation and Demethoxylation of AO | + | + | + | + | - | - | - | - | - | - | + | + | - |
| 14 | 8.99 | 475.08820 | C22H19O12 | Glucuronidation and Demethoxylation of AO | + | + | + | + | + | - | - | - | - | - | + | + | - |
| 15 | 6.09 | 491.08311 | C22H19O13 | Glucuronidation and Demethylation of AO | - | + | + | + | - | - | - | - | - | - | + | + | - |
| 16 | 6.72 | 491.08311 | C22 H19 O13 | Glucuronidation and Demethylation of AO | + | + | + | + | + | + | - | + | + | - | + | + | + |
| 17 | 6.94 | 491.08311 | C22 H19 O13 | Glucuronidation and Demethylation of AO | + | + | + | + | + | + | + | + | + | + | + | + | + |
| 18 | 7.04 | 491.08311 | C22 H19 O13 | Glucuronidation and Demethylation of AO | - | + | + | + | + | - | - | + | + | - | + | + | - |
| 19 | 6.46 | 505.09876 | C23H21O13 | Glucuronidation of AO | + | + | + | + | + | + | + | + | + | - | + | + | + |
| 20 | 6.77 | 505.09876 | C23H21O13 | Glucuronidation of AO | + | + | + | + | + | + | + | + | + | + | + | + | + |
| 21 | 6.90 | 505.09876 | C23H21O13 | Glucuronidation of AO | + | + | + | + | + | + | + | + | + | + | + | + | + |
| 22 | 7.30 | 505.09876 | C23H21O13 | Glucuronidation of AO | + | + | + | + | + | + | - | + | + | - | + | + | + |
| 23 | 5.44 | 521.09258 | C23H21O14 | Glucuronidation and Hydroxylation AO | + | + | + | + | + | + | - | + | + | - | + | + | - |
| 24 | 7.57 | 521.09258 | C23H21O14 | Glucuronidation and Hydroxylation of AO | + | + | + | + | - | - | - | - | - | - | + | + | - |
| 25 | 7.85 | 521.09258 | C23H21O14 | Glucuronidation and Hydroxylation of AO | - | - | - | + | - | - | - | - | - | - | + | + | - |
| 26 | 5.36 | 585.05418 | C23H21O16S | Glucuronidation and Sulfation of AO | + | + | + | + | - | - | - | - | - | - | + | + | + |
| 27 | 5.60 | 585.05418 | C23H21O16S | Glucuronidation and Sulfation of AO | + | + | + | + | - | - | - | - | - | - | + | + | + |
| 28 | 5.17 | 681.13109 | C29H29O19 | Diglucuronidation of AO | + | + | + | + | + | + | + | + | + | + | + | + | + |
| 29 | 5.15 | 651.12029 | C28H27O18 | Diglucuronidation and Demethoxylation of AO | + | + | + | + | - | + | - | - | + | - | + | + | - |
| 30 | 5.39 | 651.12029 | C28H27O18 | Diglucuronidation and Demethoxylation of AO | + | + | + | + | + | + | - | + | + | - | + | + | - |
| 31 | 5.45 | 651.12029 | C28H27O18 | Diglucuronidation and Demethoxylation of AO | - | + | + | + | - | - | - | - | - | - | + | + | - |
| 32 | 5.10 | 667.11520 | C28H27O19 | Diglucuronidation and demethylation of AO | + | + | + | + | - | - | - | - | - | - | + | + | + |
| 33 | 5.22 | 667.11520 | C28H27O19 | Diglucuronidation and demethylation of AO | + | + | + | + | - | - | - | - | - | - | + | + | - |
| 34 | 5.33 | 697.12577 | C29H29O20 | Diglucuronidation and Hydroxylation of AO | - | - | - | + | - | - | - | - | - | - | + | + | - |
| 35 | 4.96 | 697.12577 | C29H29O20 | Diglucuronidation and Hydroxylation of AO | - | - | - | + | - | - | - | - | - | - | + | + | - |
| 36 | 12.08 | 315.05102 | C16H11O7 | Demethylation of AO | - | - | - | + | + | + | + | + | + | + | + | + | + |

T0.5: 0.5h after drug administration; T1: 1h after drug administration; T2: 2h after drug administration; T4: 4h after drug administration;

1: method 1; 2: method 2; 3: method 3.