**Suppl Table 4.** Transition ion ratio analysis of lipids identified in samples to reveal potential isomers

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Lipid** | **Formula** | **Precursor ion** | **Product ions (qualifiers)** | **Comments** | **Average ratio** | **SD** | **CV (%)** | **Isomer presence** |
| Aldosterone | C21H28O5 | 361.5 | 79.2 | Not identified in any samples | NA | NA | NA | NA |
| Estriol | C18H24O3 | 287 | 145 | Not identified in any samples | NA | NA | NA | NA |
| Dehydroepiandrosterone-sulphate | C19H28O5S | NA | NA | Only quantifier transition | NA | NA | NA | NA |
| Cortisone | C21H28O5 | 361 | 91 | Not identified in any samples | NA | NA | NA | NA |
| 361 | 163 | Not identified in any samples | NA | NA | NA |
| 11-deoxycortisol | C21H30O4 | 313 | 283 | Not present in all analyses | NA | NA | NA | NA |
| 313 | 285 | Not present in all analyses | NA | NA | NA |
| γ-linolenic acid | C18H30O2 | 279.2 | 149.2 | Not present in all analyses | NA | NA | NA | NA |
| 279.2 | 77.2 | Not present in all analyses | NA | NA | NA |
| 5α-androstane-3,17-dione | C19H28O2 | 327.2 | 41.2 | Not present in all analyses | NA | NA | NA | NA |
| 327.2 | 43.1 | Not present in all analyses | NA | NA | NA |
| 327.2 | 58.1 | Not present in all analyses | NA | NA | NA |
| 289.4 | 160.9 | Not present in all analyses | NA | NA | NA |
| Testosterone | C19H28O2 | 289 | 109 | Not present in all analyses | 74.23 | 30.52 | 4.10 | Potentially but not DHEA as these are chromatographically separated |
| Estradiol | C18H24O2 | 271 | 183 | Not identified in any samples | NA | NA | NA | NA |
| Estrone | C18H22O2 | 269 | 253 | Not identified in any samples | NA | NA | NA | NA |
| 17α-hydroxypregnenolone | C21H32O3 | 350.5 | 45.1 | Not present in all analyses | NA | NA | NA | NA |
| 350.5 | 73.1 | Not present in all analyses | NA | NA | NA |
| 350.5 | 104.9 | Not present in all analyses | NA | NA | NA |
| 350.5 | 186.9 | Not present in all analyses | NA | NA | NA |
| 17α-hydroxyprogesterone | C21H30O3 | 331 | 109 | Not identified in any samples | NA | NA | NA | Potentially, could be 11-deoxycorticosterone |
| Progesterone | C21H30O2 | 315.2 | 109 | TIR analysis | 48.54 | 6.66 | 13.71 | Potentially |
| Pregnenolone | C21H32O2 | 339.5 | 43.2 | Not present in all analyses | NA | NA | NA | NA |
| 5α-dihydrotestosterone | C19H30O2 | 313.4 | 59 | Not present in all analyses | NA | NA | NA | Potentially, could be androsterone |
| 313.4 | 105.1 | Not present in all analyses | NA | NA | NA |
| 313.4 | 269.1 | Not present in all analyses | NA | NA | NA |
| Dihydrocholesterol | C27H48O | NA | NA | Only quantifier transition | NA | NA | NA | NA |
| D-sphingosine | C18H37NO2 | 300.5 | 55.1 | Not present in all analyses | NA | NA | NA | NA |
| 300.5 | 56.1 | Not present in all analyses | NA | NA | NA |
| Dehydroepiandrosterone | C19H28O2 | NA | NA | Only quantifier transition | NA | NA | NA | NA |
| 25-hydroxycholesterol | C27H46O2 | 420.7 | 43.2 | TIR analysis | 4.92 | 0.22 | 4.44 | No |
| 420.7 | 57 | TIR analysis | 36.29 | 1.44 | 3.96 |
| 441.6 | 59 | Not present in all analyses | NA | NA | NA |
| Allopregnanolone | C21H34O2 | 341.5 | 57 | Not present in all analyses | NA | NA | NA | Potentially |
| 341.5 | 41.1 | TIR analysis | 57.16 | 17.37 | 30.4 |
| 4-cholesten-3-one | C27H44O | 385.7 | 79 | Not present in all analyses | NA | NA | NA | No |
| 385.7 | 81 | Not present in all analyses | NA | NA | NA |
| 385.7 | 109.1 | TIR analysis | 84.81 | 4.99 | 5.89 |
| Leukotriene C4 | C30H47N3O9S | 664.3 | 57.2 | Not identified in any samples | NA | NA | NA | No |

NA = not applicable.