|  |  |
| --- | --- |
| Peak | m/z 191 compound |
| 1 | C19 Tricyclicterpane |
| 2 | C20 Tricyclicterpane |
| 3 | C21 Tricyclicterpane |
| 4 | C22 Tricyclicterpane |
| 5 | C23 Tricyclicterpane |
| 6 | C24 Tricyclicterpane |
| 7 | C25 (22S+22R) Tricyclicterpane |
| 8 | C24Tetracyclichopane (Seco) |
| 9 | C2622(S) Tricyclicterpane |
| 10 | C2622(R) Tricyclicterpane |
| 11 | C28 Tricyclicterpane |
| 12 | C29 Tricyclicterpane |
| 13 | C27 18α(H)-22,29,30-Trisnorneohopane (Ts) |
| 14 | C27 17α(H)-22,29,30-Trisnorhopane (Tm) |
| 15 | 17 α(H)-29,30-Bisnohopane |
| 16 | C30 Tricyclicterpane |
| 17 | 17 α(H)-28,30-Bisnohopane |
| 18 | C2917 α(H)-21β(H)-30-Norhopane |
| 19 | C29 Ts (18 α(H)-30-Noneorhopane |
| 20 | C30(17 α(H)-Diahopane) |
| 21 | C2917 β (H), 21α (H)-30 Normoratene |
| 22 | Oleanane |
| 23 | C3017 α(H), 21β(H)-Hopane |
| 24 | C3017 β (H), 21α (H)-Moretane |
| 25 | C3117 α (H), 21β (H)-30-Homohopane (22S) |
| 26 | C3117 α (H), 21β (H)-30-Homohopane (22R) |
| 27 | Gammacerane |
| 28 | Homomoretane |
| 29 | C3217 α (H), 21β (H)-30,31-Bishomohopane (22S) |
| 30 | C3217 α (H), 21β (H)-30,31-Bishomohopane (22R) |
| 31 | C3317 α (H), 21β (H)-30,31,32-Trishomohopane (22S) |
| 32 | C3317 α (H), 21β (H)-30,31,32-Trishomohopane (22R) |
| 33 | C3417 α (H), 21β (H)-30,31,32,33-Tetrakishomohopane (22S) |
| 34 | C3417 α (H), 21β (H)-30,31,32,33-Tetrakishomohopane (22R) |
| 35 | C3517 α (H), 21β (H)-30,31,32,33,34-Pentakishomohopane (22S) |
| 36 | C3517 α (H), 21β (H)-30,31,32,33,34-Pentakishomohopane (22R) |

**SI Table.**  m/z 191, m/z 217, m/z 178, 192, 178, 184, 231 and 253 ion fragmentogram identification

**SI Table** continued

|  |  |
| --- | --- |
| Peak m/z 217 compound | |
| 1 | C27 13β (H)- 17 α(H)-Diasterane (20S) |
| 2 | C27 13β (H)- 17 α(H)-Diasterane (20R) |
| 3 | C27 13α (H)- 17 β (H)-Diasterane (20S) |
| 4 | C27 13α (H)- 17 β (H)-Diasterane (20R) |
| 5 | C28 13β (H)- 17 α(H)-Diasterane (20S) |
| 6 | C28 13β (H)- 17 α(H)-Diasterane (20R) |
| 7 | C28 13α (H)- 17 β (H)-Diasterane (20S) |
| 8 | C27 5α (H), 14α (H), 17α (H) - Sterane(20S)+C2813α (H), 17 β (H)-Diasterane (20S) |
| 9 | C27 5α (H), 14β (H), 17β (H) - Sterane(20R)+C2913β (H), 17 α (H)-Diasterane (20S) |
| 10 | C27 5α (H), 14β (H), 17β (H) - Sterane(20S)+C2813α (H), 17 β (H)-Diasterane (20R) |
| 11 | C27 5α (H), 14α (H), 17α (H) - Sterane(20R) |
| 12 | C29 13β (H)- 17 α(H)-Diasterane (20R) |
| 13 | C29 13α (H)- 17 β (H)-Diasterane (20S) |
| 14 | C28 5α (H), 14α (H), 17α (H) - Sterane(20S) |
| 15 | C28 5α (H), 14β (H), 17β (H) - Sterane(20R)+C2913α (H), 17 β (H)-Diasterane (20R) |
| 16 | C28 5α (H), 14β (H), 17β (H) – Sterane (20S) |
| 17 | C28 5α (H), 14α (H), 17α (H) – Sterane (20R) |
| 18 | C29 5α (H), 14α (H), 17α (H) – Sterane (20S) |
| 19 | C29 5α (H), 14β (H), 17β (H) – Sterane (20R) |
| 20 | C29 5α (H), 14β (H), 17β (H) – Sterane (20S) |
| 21 | C29 5α (H), 14α (H), 17α (H) – Sterane (20R) |
| 22 | C305α (H), 14α (H), 17α (H) – Sterane (20S) |
| 23 | C30 5α (H), 14β (H), 17β (H) – Sterane (20R) |
| 24 | C30 5α (H), 14β (H), 17β (H) – Sterane (20S) |
| 25 | C305α (H), 14α (H), 17α (H) – Sterane (20R) |

**SI Table** continued

|  |  |
| --- | --- |
| m/z 178+192 Ion fragmentogram identification | |
| Compound no | Compound name |
| P | Phenanthrene |
| 3MP | 3-Methyl- Phenanthrene |
| 2MP | 2- Methyl - Phenanthrene |
| 9MP | 9- Methyl - Phenanthrene |
| 1MP | 1- Methyl - Phenanthrene |
| m/z 184+198 Ion fragmentogram identification | |
| Compound no | Compound name |
| DBT | Dibenzotiyofen |
| 1MDBT | 1- Methyl -Dibenzothiophene |
| 2MDBT | 2- Methyl -Dibenzothiophene |
| 4MDBT | 4- Methyl -Dibenzothiophene |
| m/z 231 Ion fragmentogram identification | |
| Compound no | Compound name |
| 1 | C20 Pregnan |
| 2 | C21 Methyl-pregnan |
| 3 | C22 Epimers |
| 4 | C26 20S |
| 5 | C26 20R + C27 20S |
| 6 | C28 20S |
| 7 | C27 20R |
| 8 | C28 20R |
| 9 | C29 20S Epimers |
| 10 | C29 20R |
| m/z 253 Ion fragmentogram identification | |
| Compound no | Compound name |
| 1 | C21 |
| 2 | C22 |
| 3 | C23 |
| 4 | C27 20S 5B |
| 5 | C27 20S 5B DIA-MA |
| 6 | C27 20S 5B + C27 20R 5B DIA-MA |
| 7 | C27 20S 5A |
| 8 | C28 20S 5B + C28 20S 5B DIA-MA |
| 9 | C28 20R 5A |
| 10 | C28 20S 5A |
| 11 | C28 20R 5B +C28 20R 5B DIA-MA |
| 12 | C29 20R 5B +C28 20R 5B DIA-MA |
| 13 | C29 20S 5A |
| 14 | C28 20R 5A |
| 15 | C29 20R 5B + C29 20R 5B DIA-MA |
| 16 | C29 20R 5A |