**Table S1.** Expected ions of QC mix and buffer

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **QC mix ions** | | |  | **QC mix ions** | | | | |
| **#** | **compound** | **m/z** | **type** |  | **#** | **compound** | **m/z** | **type** |
| 1 | *Caffeine* | 193.0725 | isotope |  | 25 | *Perfluorodecanoic acid* | 512.9594 | isotope |
| 2 | 194.0759 | isotope |  | 26 | 513.9628 | isotope |
| 3 | 195.0792 | isotope |  | 27 | 514.9662 | isotope |
| 4 | 179.0569 | fragment |  | 28 | 468.9696 | fragment |
| 5 | *Fluconazole* | 305.0962 | isotope |  | 29 | *Tricosa-fluorododecanoic acid* | 612.9531 | isotope |
| 6 | 306.0995 | isotope |  | 30 | 613.9564 | isotope |
| 7 | 307.1029 | isotope |  | 31 | 614.9598 | isotope |
| 8 | 191.0681 | fragment |  | 32 | 568.9632 | fragment |
| 9 | *Albendazole* | 264.0806 | isotope |  | 33 | *Perfluorotetra-decanoic acid* | 712.9467 | isotope |
| 10 | 265.0840 | isotope |  | 34 | 713.9500 | isotope |
| 11 | 266.0873 | isotope |  | 35 | 714.9534 | isotope |
| 12 | 188.9996 | fragment |  | 36 | 668.9568 | fragment |
| 13 | 232.0544 | fragment |  | 37 | 646.9549 | fragment |
| 14 | *Triamcinolone acetonide* | 433.2026 | isotope |  |  | | | | |
| 15 | 434.2059 | isotope |  | **Buffer ions** | | | | |
| 16 | 435.2093 | isotope |  | **#** | **compound** | **m/z** | **type** |
| 17 | 453.2088 | adduct |  | 1 | *HOT (Homotaurine)* | 138.0224 | isotope |
| 18 | 337.1439 | fragment |  | 2 | 139.0258 | isotope |
| 19 | *Pentadeca-fluoroheptyl* | 368.9760 | isotope |  | 3 | 140.0291 | isotope |
| 20 | 369.9794 | isotope |  | 4 | *HEX (Hexakis (1H, 1H, 3H-tetrafluoro-propoxy) phosphazine)* | 940.0009 | isotope |
| 21 | 370.9827 | isotope |  | 5 | 941.0042 | isotope |
| 22 | *3-Heptadeca-fluorooctylaniline* | 510.0150 | isotope |  | 6 | 942.0076 | isotope |
| 23 | 511.0184 | isotope |  |  |  |  |  |
| 24 | 512.0217 | isotope |  |  |  |  |  |