|  |  |  |
| --- | --- | --- |
| **Amino acids and Biogenic amines** | **Acylcarnitines** | **Lipids** |
| Asp | C3-OH | lysoPC a C14:0 |
| Ac-Orn | C3:1 | lysoPC a C24:0 |
| c4-OH-Pro | C4:1 | PC aa C24:0 |
| Carnosine | C5-M-DC | PC aa C26:0 |
| DOPA | C5-OH (C3-DC-M) | PC aa C30:2 |
| Dopamine | C5:1 | PC aa C40:1 |
| Histamine | C5:1-DC | PC ae C30:2 |
| Met-SO | C6:1 | PC ae C42:0 |
| Nitro-Tyr | C8 | SM C22:3 |
| PEA | C9 |   |
| Serotonin | C10:1 |   |
| Spermidine | C10:2 |   |
| Spermine | C12 |   |
|   | C12-DC |   |
|   | C12:1 |   |
|   | C14:1-OH |   |
|   | C14:2-OH |   |
|   | C16-OH |   |
|   | C16:1-OH |   |
|   | C16:2 |   |
|   | C16:2-OH |   |
|   | C18:1-OH |   |

**Tab. S1**:44 metabolites that were excluded from further analysis because of missing concentrations or levels below the lower limit of detection.