|  |  |  |  |
| --- | --- | --- | --- |
|  |  | **Tandem MS Analysis** | |
| **Analyte** | ***m/z* of precursor ion** | **Scan Type** | **MRM product ion *m/z*** |
| Phe | 166.1 | Neutral loss 46 | NA |
| Leu | 132.1 | Neutral loss 46 | NA |
| Met | 150.1 | Neutral loss 46 | NA |
| Tyr | 182.1 | Neutral loss 46 | NA |
| Val | 118.1 | Neutral loss 46 | NA |
| Cit | 176.1 | NA | 113.1 |
| Arg | 175.1 | NA | 70.1 |
| Ala | 90.1 | Neutral loss 46 | NA |
| SUAC | 155.1 | NA | 137.1 |
| C0 | 162.1 | NA | 103.0 |
| C2 | 204.1 | NA | 85.0 |
| C3 | 218.1 | NA | 85.0 |
| C4 | 232.2 | Precursor 85 | NA |
| C3DC+C4OH | 248.2 | Precursor 85 | NA |
| C5 | 246.2 | Precursor 85 | NA |
| C5OH | 262.2 | Precursor 85 | NA |
| C5DC | 276.2 | Precursor 85 | NA |
| C6 | 260.2 | Precursor 85 | NA |
| C8 | 288.3 | Precursor 85 | NA |
| C10 | 316.3 | Precursor 85 | NA |
| C12 | 344.3 | Precursor 85 | NA |
| C14 | 372.3 | Precursor 85 | NA |
| C16 | 400.4 | Precursor 85 | NA |
| C16OH | 416.4 | Precursor 85 | NA |
| C18 | 428.4 | Precursor 85 | NA |
| C18OH | 444.4 | Precursor 85 | NA |
| C26:0-LPC | 636.5 | NA | 104.1 |

Supplementary Table I. Tandem mass spectrometric analyses of amino acids, acylcarnitines, succinylacetone, and hexacosanoyl lysophosphatidylcholine.