**S2 Table. Number of SRM substances and samples for 3-class, 9-class, and 16-class categorizations.**

|  |  |  |  |
| --- | --- | --- | --- |
| Prediction class type | Class | Number of SRM substances | Number of classified samples |
| 3-class | 1 | 12 | 36 |
| 2 | 3 | 9 |
| 3 | 5 | 15 |
| 9-class | 1 | 2 | 6 |
| 2 | 2 | 6 |
| 3 | 3 | 9 |
| 4 | 1 | 3 |
| 5 | 3 | 9 |
| 6 | 3 | 9 |
| 7 | 1 | 3 |
| 8 | 2 | 6 |
| 9 | 3 | 9 |
| 16-class | 1 | 1 | 3 |
| 2 | 1 | 3 |
| 3 | 1 | 3 |
| 4 | 1 | 3 |
| 5 | 1 | 3 |
| 6 | 3 | 9 |
| 7 | 1 | 3 |
| 8 | 1 | 3 |
| 9 | 1 | 3 |
| 10 | 1 | 3 |
| 11 | 1 | 3 |
| 12 | 1 | 3 |
| 13 | 1 | 3 |
| 14 | 1 | 3 |
| 15 | 3 | 9 |
| 16 | 1 | 3 |