

**S5 Table.** Number of used MS/MS spectra for training in negative ion mode.

| <b>Liebisch</b> | <b>LMID</b>  | <b>Number MS/MS spectra</b> |
|-----------------|--------------|-----------------------------|
| Cer(16:0_d18:0) | LMSP02020001 | 15                          |
| Cer(16:0_d18:1) | LMSP02010004 | 21                          |
| Cer(d18:0_18:0) | LMSP02020008 | 17                          |
| Cer(d18:0_18:1) | LMSP02020015 | 30                          |
| Cer(d18:0_22:0) | LMSP02020010 | 9                           |
| Cer(d18:0_24:0) | LMSP02020012 | 10                          |
| Cer(d18:0_24:1) | LMSP02020011 | 14                          |
| Cer(d18:1_22:0) | LMSP02010008 | 26                          |
| Cer(d18:1_24:0) | LMSP02010012 | 19                          |
| Cer(d18:1_24:1) | LMSP02010009 | 28                          |
| PC(16:0_16:1)   | LMGP01010566 | 11                          |
| PC(16:0_18:1)   | LMGP01010581 | 10                          |
| PC(16:0_20:4)   | LMGP01012136 | 13                          |
| PC(16:0_22:5)   | LMGP01010647 | 11                          |
| PC(16:0_22:6)   | LMGP01012137 | 8                           |
| PC(18:0_18:1)   | LMGP01010761 | 10                          |
| PC(18:0_20:4)   | LMGP01012144 | 11                          |
| PC(18:1_18:1)   | LMGP01010855 | 4                           |
| PC(18:1_18:2)   | LMGP01012149 | 4                           |
| PE(16:0_16:1)   | LMGP02011228 | 7                           |
| PE(16:0_17:1)   | LMGP02011226 | 11                          |
| PE(16:0_18:1)   | LMGP02010311 | 13                          |
| PE(17:1_17:1)   | LMGP02011209 | 2                           |
| PE(18:1_18:1)   | LMGP02010109 | 7                           |
| PE(18:1_19:1)   | LMGP02010646 | 6                           |
| PG(16:0_16:1)   | LMGP04010910 | 10                          |
| PG(16:0_17:1)   | LMGP04010908 | 10                          |
| PG(16:0_18:1)   | LMGP04010987 | 10                          |
| PG(16:0_19:1)   | LMGP04010196 | 1                           |
| PG(17:1_18:1)   | LMGP04010328 | 6                           |
| PG(18:1_18:1)   | LMGP04010985 | 4                           |
| PI(16:0_18:1)   | LMGP06010001 | 11                          |
| PI(16:0_18:2)   | LMGP06010959 | 13                          |
| PI(16:0_18:3)   | LMGP06010944 | 11                          |
| PI(18:0_18:2)   | LMGP06010956 | 14                          |
| PI(18:0_18:3)   | LMGP06010284 | 19                          |
| PI(18:2_18:2)   | LMGP06010927 | 10                          |
| PS(18:0_18:1)   | LMGP03010025 | 7                           |
| PS(18:0_20:4)   | LMGP03010039 | 8                           |
| PS(18:0_22:4)   | LMGP03010883 | 12                          |
| PS(18:1_18:1)   | LMGP03010030 | 9                           |