

Electronic Supplementary Material

**[¹⁸F]Fluorocholine PET/CT Imaging of Liver Cancer: Radiopathologic Correlation
with Tissue Phospholipid Profiling**

Journal: Molecular Imaging and Biology

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Author Contributions: Conceived and designed experiments: SAK, MMS, YK, AF, LC, LLW.
Performed the experiments: SAK, AF, LC, KM. Analyzed the data: SAK, MMS, YK, AF, LC,
KM, LLW. Contributed materials/analysis tools: SAK, MMS, YK, AF, LC, LLW. Writing and
final manuscript approval: SAK, MMS, YK, AF, LC, KM, LLW.

Supplementary Table 1. Mass-to-charge (m/z) ratios that include phosphatidylcholine species with poly-unsaturated fatty acyls

| | | m/z ratio | | | | |
|-----------------------------------|-----------------------------------|---------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|-------------------------------------|
| 786.5677 | | 780.5573 | 782.5692 | 784.5815 | 786.6014 | 788.6106 |
| 14:1 [92] / 20:1 [112] | 18:2 [92,122] / 18:3 [92,122,152] | 22:4 [72,102,132,162] / 14:0 | 22:2 [132,162] / 14:1 [92] | 22:2 [132,162] / 14:1 [92] | 14:1 [92] / 22:1 [132] | 14:1 [92] / 22:1 [132] |
| 16:1 [92] / 18:1 [112] | 16:1 [92] / 20:4 [82,112,142,172] | 18:0 / 18:4 [62,92,122,152] | 18:0 / 18:4 [62,92,122,152] | 18:3 [92,122,152] / 18:0 | 18:1 [92] / 18:1 [112] | 18:1 [92] / 18:1 [112] |
| 18:1 [112] / 16:1 [92] | 18:3 [92,122,152] / 18:2 [92,122] | 20:3 [52,82,112] / 16:1 [92] | 20:3 [52,82,112] / 16:1 [92] | 18:1 [92] / 18:2 [92,122] | 14:0 / 22:2 [132,162] | 14:0 / 22:2 [132,162] |
| 18:2 [92,122] / 16:0 | 18:4 [62,92,122,152] / 18:1 [112] | 20:4 [52,82,112,142] / 16:0 | 20:4 [52,82,112,142] / 16:0 | 20:3 [82,112,142] / 16:0 | 18:0 / 18:2 [92,122] | 18:0 / 18:2 [92,122] |
| 20:1 [112] / 14:1 [92] | 20:4 [52,82,112,142] / 16:1 [92] | 18:3 [92,122,152] / 18:1 [92] | 18:3 [92,122,152] / 18:1 [92] | 20:2 [112,142] / 16:1 [92] | 20:1 [112] / 16:1 [92] | 20:1 [112] / 16:1 [92] |
| 16:0 / 18:2 [92,122] | 22:5 [42,72,102,132,162] / 14:0 | 22:5 [42,72,102,132,162] / 14:0 | 16:0 / 20:4 [52,82,112,142] | 16:0 / 20:4 [52,82,112,142] | 18:1 [112] / 18:2 [92,122] | 22:2 [132,162] / 14:0 |
| | 14:1 [92] / 22:4 [72,102,132,162] | 18:1 [112] / 18:3 [92,122,152] | 18:1 [112] / 18:3 [92,122,152] | 18:1 [112] / 18:3 [92,122,152] | 18:1 [112] / 18:1 [92] | 18:1 [112] / 18:1 [92] |
| | 20:5 [52,82,112,142,172] / 16:0 | 18:3 [62,92,122] / 18:1 [92] | 18:3 [62,92,122] / 18:1 [92] | 18:0 / 18:3 [92,122,152] | 18:4 [62,92,122,152] / 18:1 [92] | 18:4 [62,92,122,152] / 18:1 [92] |
| | 22:4 [72,102,132,162] / 14:1 [92] | 16:0 / 20:4 [82,112,142,172] | 16:0 / 20:4 [82,112,142,172] | 16:1 [92] / 20:2 [112,142] | 16:0 / 22:6 [42,72,102,132,162,192] | 16:0 / 22:6 [42,72,102,132,162,192] |
| | 18:4 [62,92,122,152] / 18:1 [92] | 18:2 [92,122] / 18:2 [92,122] | 18:2 [92,122] / 18:2 [92,122] | 18:2 [92,122] / 18:1 [112] | 20:4 [52,82,112,142] / 18:2 [92,122] | 20:2 [112,142] / 18:3 [62,92,122] |
| | 18:1 [92] / 18:4 [62,92,122,152] | 18:1 [92] / 18:3 [62,92,122] | 20:3 [52,82,112] / 16:0 | 20:3 [52,82,112] / 16:0 | 18:3 [62,92,122] / 20:3 [82,112,142] | 18:2 [92,122] / 20:3 [52,82,112] |
| | 14:0 / 22:5 [72,102,132,162,192] | 14:0 / 22:4 [72,102,132,162] | 16:0 / 20:3 [82,112,142] | 16:0 / 20:3 [82,112,142] | 18:1 [92] / 20:5 [52,82,112,142,172] | 18:1 [92] / 20:4 [82,112,142,172] |
| | 22:5 [72,102,132,162,192] / 14:0 | 18:3 [62,92,122] / 18:1 [112] | 18:3 [62,92,122] / 18:0 | 18:2 [92,122] / 20:4 [82,112,142,172] | 16:1 [92] / 22:5 [72,102,132,162,192] | 20:3 [52,82,112] / 18:2 [92,122] |
| | 18:1 [112] / 18:4 [62,92,122,152] | 20:3 [82,112,142] / 16:1 [92] | 18:0 / 18:3 [62,92,122] | 18:2 [92,122] / 20:4 [82,112,142,172] | 20:1 [112] / 18:4 [62,92,122,152] | 20:1 [112] / 18:4 [62,92,122,152] |
| | 14:0 / 22:5 [42,72,102,132,162] | 18:3 [92,122,152] / 18:1 [112] | 16:0 / 20:3 [52,82,112] | 20:3 [52,82,112] / 18:3 [92,122,152] | 20:3 [52,82,112] / 18:3 [92,122,152] | 20:4 [52,82,112,142] / 18:1 [112] |
| | 20:4 [82,112,142,172] / 16:1 [92] | 18:4 [62,92,122,152] / 18:0 | 14:1 [92] / 22:2 [132,162] | 18:1 [112] / 20:5 [52,82,112,142,172] | 18:1 [112] / 20:5 [52,82,112,142,172] | 18:4 [62,92,122,152] / 20:1 [112] |
| | 16:0 / 20:5 [52,82,112,142,172] | 20:4 [82,112,142,172] / 16:0 | 20:4 [82,112,142,172] / 16:0 | 16:1 [92] / 22:5 [42,72,102,132,162] | 20:4 [82,112,142,172] / 18:1 [112] | 20:4 [82,112,142,172] / 18:1 [112] |
| | 16:1 [92] / 20:4 [52,82,112,142] | 16:1 [92] / 20:3 [82,112,142] | 16:1 [92] / 20:3 [82,112,142] | 20:4 [82,112,142] / 18:3 [92,122,152] | 22:5 [42,72,102,132,162] / 16:0 | 22:5 [42,72,102,132,162] / 16:0 |
| | 18:3 [62,92,122] / 18:2 [92,122] | 18:1 [112] / 18:3 [62,92,122] | 18:1 [112] / 18:3 [62,92,122] | 22:6 [42,72,102,132,162,192] / 16:0 | 20:3 [82,112,142] / 18:2 [92,122] | 20:3 [82,112,142] / 18:2 [92,122] |
| | 16:1 [92] / 18:3 [92,122,152] | 16:1 [92] / 20:3 [52,82,112] | 16:1 [92] / 20:3 [52,82,112] | 18:3 [92,122,152] / 20:3 [82,112,142] | 18:1 [112] / 20:4 [52,82,112,142] | 18:1 [112] / 20:4 [52,82,112,142] |
| | | | | | 18:3 [92,122,152] / 20:2 [112,142] | |
| 780.5573 | | 782.5692 | 784.5815 | 806.5683 | 808.5808 | |
| 18:2 [92,122] / 18:3 [92,122,152] | 22:4 [72,102,132,162] / 14:0 | 22:2 [132,162] / 14:1 [92] | 20:5 [52,82,112,142,172] / 18:1 [112] | 20:5 [52,82,112,142,172] / 18:1 [112] | 16:0 / 22:5 [42,72,102,132,162] | |
| 16:1 [92] / 20:4 [82,112,142,172] | 18:0 / 18:4 [62,92,122,152] | 18:3 [92,122,152] / 18:0 | 20:3 [82,112,142] / 18:3 [62,92,122] | 20:3 [82,112,142] / 18:3 [62,92,122] | 18:3 [62,92,122] / 20:2 [112,142] | |
| 18:3 [92,122,152] / 18:2 [92,122] | 20:3 [52,82,112] / 16:1 [92] | 18:1 [92] / 18:2 [92,122] | 18:3 [92,122,152] / 20:3 [52,82,112] | 18:3 [92,122,152] / 20:3 [52,82,112] | 16:1 [92] / 22:4 [72,102,132,162] | |
| 18:4 [62,92,122,152] / 18:1 [112] | 20:4 [52,82,112,142] / 16:0 | 20:3 [82,112,142] / 16:0 | 20:2 [112,142] / 16:1 [92] | 20:2 [112,142] / 16:1 [92] | 18:2 [92,122] / 20:3 [82,112,142] | |
| 20:4 [52,82,112,142] / 16:1 [92] | 18:3 [92,122,152] / 18:1 [92] | 20:2 [112,142] / 16:1 [92] | 22:5 [72,102,132,162,192] / 16:1 [92] | 22:5 [72,102,132,162,192] / 16:1 [92] | 20:4 [52,82,112,142] / 18:1 [92] | |
| 22:5 [42,72,102,132,162] / 14:0 | 16:0 / 20:4 [52,82,112,142] | 18:1 [112] / 18:2 [92,122] | 20:3 [52,82,112] / 18:3 [62,92,122] | 20:3 [52,82,112] / 18:3 [62,92,122] | 20:5 [52,82,112,142,172] / 18:0 | |
| 14:1 [92] / 22:4 [72,102,132,162] | 18:3 [62,92,122] / 18:1 [92] | 18:2 [92,122] / 18:1 [92] | 20:5 [52,82,112,142,172] / 18:1 [92] | 20:5 [52,82,112,142,172] / 18:1 [92] | 18:1 [112] / 20:4 [82,112,142,172] | |
| 20:5 [52,82,112,142,172] / 16:0 | 18:3 [62,92,122] / 18:1 [92] | 18:0 / 18:3 [92,122,152] | 18:4 [62,92,122,152] / 20:2 [112,142] | 18:4 [62,92,122,152] / 20:2 [112,142] | 18:1 [92] / 20:4 [52,82,112,142] | |
| 22:4 [72,102,132,162] / 14:1 [92] | 16:0 / 20:4 [82,112,142,172] | 16:1 [92] / 20:2 [112,142] | 16:0 / 22:6 [42,72,102,132,162,192] | 16:0 / 22:6 [42,72,102,132,162,192] | 16:0 / 22:5 [72,102,132,162,192] | |
| 18:4 [62,92,122,152] / 18:1 [92] | 18:2 [92,122] / 18:2 [92,122] | 18:2 [92,122] / 18:1 [112] | 20:4 [52,82,112,142] / 18:2 [92,122] | 20:4 [52,82,112,142] / 18:2 [92,122] | 20:2 [112,142] / 18:3 [62,92,122] | |
| 18:1 [92] / 18:4 [62,92,122,152] | 18:1 [92] / 18:3 [62,92,122] | 20:3 [52,82,112] / 16:0 | 18:3 [62,92,122] / 20:3 [82,112,142] | 18:3 [62,92,122] / 20:3 [82,112,142] | 18:2 [92,122] / 20:3 [52,82,112] | |
| 14:0 / 22:5 [72,102,132,162,192] | 14:0 / 22:4 [72,102,132,162] | 16:0 / 20:3 [82,112,142] | 16:0 / 22:6 [42,72,102,132,162,192] | 16:0 / 22:6 [42,72,102,132,162,192] | 18:1 [92] / 20:4 [82,112,142,172] | |
| 22:5 [72,102,132,162,192] / 14:0 | 18:3 [62,92,122] / 18:1 [112] | 18:0 / 18:3 [62,92,122] | 18:2 [92,122] / 20:4 [82,112,142,172] | 18:2 [92,122] / 20:4 [82,112,142,172] | 20:3 [52,82,112] / 18:2 [92,122] | |
| 18:1 [112] / 18:4 [62,92,122,152] | 20:3 [82,112,142] / 16:1 [92] | 18:0 / 18:3 [62,92,122] | 20:3 [52,82,112] / 18:3 [92,122,152] | 20:3 [52,82,112] / 18:3 [92,122,152] | 20:1 [112] / 18:4 [62,92,122,152] | |
| 14:0 / 22:5 [42,72,102,132,162] | 18:3 [92,122,152] / 18:1 [112] | 16:0 / 20:3 [52,82,112] | 18:1 [112] / 20:5 [52,82,112,142,172] | 18:1 [112] / 20:5 [52,82,112,142,172] | 20:4 [52,82,112,142] / 18:1 [112] | |
| 20:4 [82,112,142,172] / 16:1 [92] | 18:4 [62,92,122,152] / 18:0 | 14:1 [92] / 22:2 [132,162] | 18:1 [112] / 20:5 [52,82,112,142,172] | 18:1 [112] / 20:5 [52,82,112,142,172] | 18:4 [62,92,122,152] / 20:1 [112] | |
| 16:0 / 20:5 [52,82,112,142,172] | 20:4 [82,112,142,172] / 16:0 | 20:4 [82,112,142,172] / 16:0 | 16:1 [92] / 22:5 [42,72,102,132,162] | 16:1 [92] / 22:5 [42,72,102,132,162] | 20:4 [82,112,142,172] / 18:1 [112] | |
| 16:1 [92] / 20:4 [52,82,112,142] | 16:1 [92] / 20:3 [82,112,142] | 16:1 [92] / 20:3 [82,112,142] | 20:4 [82,112,142] / 18:3 [92,122,152] | 20:4 [82,112,142] / 18:3 [92,122,152] | 22:5 [42,72,102,132,162] / 16:0 | |
| 18:3 [62,92,122] / 18:2 [92,122] | 18:1 [112] / 18:3 [62,92,122] | 18:1 [112] / 18:3 [62,92,122] | 22:6 [42,72,102,132,162,192] / 16:0 | 22:6 [42,72,102,132,162,192] / 16:0 | 20:3 [82,112,142] / 18:2 [92,122] | |
| 16:1 [92] / 18:3 [92,122,152] | 16:1 [92] / 20:3 [52,82,112] | 16:1 [92] / 20:3 [52,82,112] | 18:3 [92,122,152] / 20:3 [82,112,142] | 18:3 [92,122,152] / 20:3 [82,112,142] | 18:1 [112] / 20:4 [52,82,112,142] | |
| | | | | | 18:1 [112] / 20:4 [52,82,112,142] | |

Supplementary Table 1 (Cont'd). Mass-to-charge (m/z) ratios that include phosphatidylcholine species with poly-unsaturated fatty acyls

| | m/z ratio | |
|--|---|--|
| 810.5967 | 812.6067 | 832.5772 |
| 20:1 [11Z] / 18:3 [6Z,9Z,12Z] 16:0 / 22:4 [7Z,10Z,13Z,16Z] 18:0 / 20:4 [8Z,11Z,14Z,17Z] 20:4 [8Z,11Z,14Z,17Z] / 18:0 18:4 [6Z,9Z,12Z,15Z] / 20:0 20:4 [5Z,8Z,11Z,14Z] / 18:0 18:1 [11Z] / 20:3 [5Z,8Z,11Z] 18:2 [9Z,12Z] / 20:2 [11Z,14Z] 22:4 [7Z,10Z,13Z,16Z] / 16:0 18:1 [11Z] / 20:3 [8Z,11Z,14Z] 20:0 / 18:4 [6Z,9Z,12Z,15Z] 18:1 [9Z] / 20:3 [8Z,11Z,14Z] 20:1 [11Z] / 18:3 [9Z,12Z,15Z] 18:1 [9Z] / 20:3 [5Z,8Z,11Z] 20:3 [8Z,11Z,14Z] / 18:1 [11Z] 18:3 [6Z,9Z,12Z] / 20:1 [11Z] 20:3 [5Z,8Z,11Z] / 18:1 [11Z] 20:3 [8Z,11Z,14Z] / 18:1 [9Z] 20:3 [5Z,8Z,11Z] / 18:1 [9Z] 18:3 [9Z,12Z,15Z] / 20:1 [11Z] 18:0 / 20:4 [5Z,8Z,11Z,14Z] | 20:3 [8Z,11Z,14Z] / 18:0 18:0 / 20:3 [8Z,11Z,14Z] 18:1 [11Z] / 20:2 [11Z,14Z] 18:1 [9Z] / 20:2 [11Z,14Z] 18:3 [9Z,12Z,15Z] / 20:0 20:1 [11Z] / 18:2 [9Z,12Z] 22:2 [13Z,16Z] / 16:1 [9Z] 18:0 / 20:3 [5Z,8Z,11Z] 20:2 [11Z,14Z] / 18:1 [9Z] 20:0 / 18:3 [9Z,12Z,15Z] 20:2 [11Z,14Z] / 18:1 [11Z] 18:2 [9Z,12Z] / 20:1 [11Z] 20:2 [11Z,14Z] / 18:1 [9Z] 20:5 [5Z,8Z,11Z,14Z,17Z] / 16:0 18:2 [9Z,12Z] / 22:5 [4Z,7Z,10Z,13Z,16Z] 20:4 [8Z,11Z,14Z,17Z] / 20:3 [8Z,11Z,14Z] 20:5 [5Z,8Z,11Z,14Z,17Z] / 20:2 [11Z,14Z] 18:2 [9Z,12Z] / 22:5 [4Z,7Z,10Z,13Z,16Z] 20:4 [8Z,11Z,14Z,17Z] / 20:3 [5Z,8Z,11Z] 20:3 [5Z,8Z,11Z] / 20:4 [5Z,8Z,11Z,14Z] 18:3 [9Z,12Z,15Z] / 22:4 [7Z,10Z,13Z,16Z] 20:3 [8Z,11Z,14Z] / 20:4 [8Z,11Z,14Z,17Z] 18:1 [11Z] / 22:6 [4Z,7Z,10Z,13Z,16Z,19Z] 22:5 [4Z,7Z,10Z,13Z,16Z] / 18:2 [9Z,12Z] 20:3 [5Z,8Z,11Z] / 20:4 [8Z,11Z,14Z,17Z] 18:2 [9Z,12Z] / 22:5 [7Z,10Z,13Z,16Z,19Z] 18:3 [6Z,9Z,12Z] / 22:4 [7Z,10Z,13Z,16Z] 20:3 [8Z,11Z,14Z] / 20:4 [5Z,8Z,11Z,14Z] 20:4 [5Z,8Z,11Z,14Z] / 20:3 [5Z,8Z,11Z] 22:5 [7Z,10Z,13Z,16Z,19Z] / 18:2 [9Z,12Z] | 18:1 [9Z] / 22:6 [4Z,7Z,10Z,13Z,16Z,19Z] 20:2 [11Z,14Z] / 20:5 [5Z,8Z,11Z,14Z,17Z] 22:6 [4Z,7Z,10Z,13Z,16Z,19Z] / 18:1 [11Z] 22:4 [7Z,10Z,13Z,16Z] / 18:3 [9Z,12Z,15Z] 20:4 [5Z,8Z,11Z,14Z] / 20:3 [8Z,11Z,14Z] 22:6 [4Z,7Z,10Z,13Z,16Z,19Z] / 18:1 [9Z] 22:4 [7Z,10Z,13Z,16Z] / 18:3 [6Z,9Z,12Z] 20:4 [8Z,11Z,14Z,17Z] / 20:3 [8Z,11Z,14Z] 20:5 [5Z,8Z,11Z,14Z,17Z] / 20:2 [11Z,14Z] 18:2 [9Z,12Z] / 22:5 [4Z,7Z,10Z,13Z,16Z] 20:4 [8Z,11Z,14Z,17Z] / 20:3 [5Z,8Z,11Z] 20:3 [5Z,8Z,11Z] / 20:4 [5Z,8Z,11Z,14Z] 18:3 [9Z,12Z,15Z] / 22:4 [7Z,10Z,13Z,16Z] 20:3 [8Z,11Z,14Z] / 20:4 [8Z,11Z,14Z,17Z] 18:1 [11Z] / 22:6 [4Z,7Z,10Z,13Z,16Z,19Z] 22:5 [4Z,7Z,10Z,13Z,16Z] / 18:2 [9Z,12Z] 20:3 [5Z,8Z,11Z] / 20:4 [8Z,11Z,14Z,17Z] 18:2 [9Z,12Z] / 22:5 [7Z,10Z,13Z,16Z,19Z] 18:3 [6Z,9Z,12Z] / 22:4 [7Z,10Z,13Z,16Z] 20:3 [8Z,11Z,14Z] / 20:4 [5Z,8Z,11Z,14Z] 20:4 [5Z,8Z,11Z,14Z] / 20:3 [5Z,8Z,11Z] 22:5 [7Z,10Z,13Z,16Z,19Z] / 18:2 [9Z,12Z] |
| | 834.5969 | 836.6099 |
| | 18:1 [11Z] / 22:5 [7Z,10Z,13Z,16Z,19Z] 22:5 [4Z,7Z,10Z,13Z,16Z] / 18:1 [9Z] 20:3 [5Z,8Z,11Z] / 20:3 [8Z,11Z,14Z] 22:2 [13Z,16Z] / 18:4 [6Z,9Z,12Z,15Z] 18:1 [11Z] / 22:5 [4Z,7Z,10Z,13Z,16Z] 20:3 [8Z,11Z,14Z] / 20:3 [5Z,8Z,11Z] 22:5 [4Z,7Z,10Z,13Z,16Z] / 18:1 [11Z] 20:3 [8Z,11Z,14Z] / 20:3 [8Z,11Z,14Z] 18:2 [9Z,12Z] / 22:4 [7Z,10Z,13Z,16Z] 20:2 [11Z,14Z] / 20:4 [8Z,11Z,14Z,17Z] 20:5 [5Z,8Z,11Z,14Z,17Z] / 20:1 [11Z] 18:1 [9Z] / 22:5 [4Z,7Z,10Z,13Z,16Z] 18:4 [6Z,9Z,12Z,15Z] / 22:2 [13Z,16Z] 22:6 [4Z,7Z,10Z,13Z,16Z,19Z] / 18:0 20:1 [11Z] / 20:5 [5Z,8Z,11Z,14Z,17Z] 22:4 [7Z,10Z,13Z,16Z] / 18:2 [9Z,12Z] 22:5 [7Z,10Z,13Z,16Z,19Z] / 18:1 [9Z] 20:2 [11Z,14Z] / 20:4 [5Z,8Z,11Z,14Z] 18:0 / 22:6 [4Z,7Z,10Z,13Z,16Z,19Z] 22:2 [13Z,16Z] / 18:3 [6Z,9Z,12Z] 18:1 [11Z] / 22:4 [7Z,10Z,13Z,16Z] 20:2 [11Z,14Z] / 20:3 [8Z,11Z,14Z] 20:5 [5Z,8Z,11Z,14Z,17Z] / 20:0 20:3 [8Z,11Z,14Z] / 20:2 [11Z,14Z] | 18:3 [9Z,12Z,15Z] / 22:2 [13Z,16Z] 22:5 [7Z,10Z,13Z,16Z,19Z] / 18:0 20:1 [11Z] / 20:4 [5Z,8Z,11Z,14Z] 18:3 [6Z,9Z,12Z] / 22:2 [13Z,16Z] 20:4 [7Z,10Z,13Z,16Z] / 18:1 [11Z] 18:1 [9Z] / 22:4 [7Z,10Z,13Z,16Z] 20:2 [11Z,14Z] / 20:3 [5Z,8Z,11Z] 20:4 [5Z,8Z,11Z,14Z] / 20:1 [11Z] 22:1 [13Z] / 18:4 [6Z,9Z,12Z,15Z] 18:1 [9Z] / 22:4 [7Z,10Z,13Z,16Z] 20:2 [11Z,14Z] / 20:3 [5Z,8Z,11Z] 20:4 [5Z,8Z,11Z,14Z] / 20:1 [11Z] 22:4 [7Z,10Z,13Z,16Z] / 18:1 [9Z] 22:2 [13Z,16Z] / 18:3 [9Z,12Z,15Z] 20:4 [8Z,11Z,14Z,17Z] / 20:1 [11Z] 20:0 / 20:5 [5Z,8Z,11Z,14Z,17Z] 20:3 [5Z,8Z,11Z] / 20:2 [11Z,14Z] 22:5 [4Z,7Z,10Z,13Z,16Z] / 18:0 18:4 [6Z,9Z,12Z,15Z] / 22:1 [13Z] 18:0 / 22:5 [4Z,7Z,10Z,13Z,16Z] 22:2 [13Z,16Z] / 18:3 [6Z,9Z,12Z] 18:1 [11Z] / 22:4 [7Z,10Z,13Z,16Z] 20:2 [11Z,14Z] / 20:3 [8Z,11Z,14Z] 20:5 [5Z,8Z,11Z,14Z,17Z] / 20:0 20:3 [8Z,11Z,14Z] / 20:2 [11Z,14Z] |

Supplementary Table 2. Mass-to-charge (m/z) ratios that include only phosphatidylcholine species with saturated and mono-unsaturated fatty acyl groups.

| | m/z ratio | |
|--|---|--|
| 732.5537 | 734.5667 | 760.5814 |
| 18:1 [9Z] / 14:0 18:1 [11Z] / 14:0 18:0 / 14:1 [9Z] 14:1 [9Z] / 18:0 14:0 / 18:1 [9Z] 16:1 [9Z] / 16:0 14:0 / 18:1 [11Z] 16:0 / 16:1 [9Z] | 16:0 / 16:0 18:0 / 14:0 14:0 / 18:0 20:0 / 14:1 [9Z] 16:0 / 18:1 [9Z] 14:1 [9Z] / 20:0 18:0 / 16:1 [9Z] 16:1 [9Z] / 18:0 18:1 [11Z] / 16:0 14:0 / 20:1 [11Z] | 18:1 [9Z] / 16:0 20:1 [11Z] / 14:0 16:0 / 18:1 [11Z] 20:0 / 14:1 [9Z] 16:0 / 18:1 [9Z] 14:1 [9Z] / 20:0 18:0 / 16:1 [9Z] 16:1 [9Z] / 18:0 18:1 [11Z] / 16:0 14:0 / 20:1 [11Z] |