Supplementary Materials

We are presenting an example output for three different searches in order to improve transparency of the applied software. The first search was performed for small phospholipid with low number of candidates. The second search did not produce any possitive targets. So chromatographic peak does not represent PL. The third search produced a large number of possible candidates.

```
Python 3.9.10 (tags/v3.9.10:f2f3f53, Jan 17 2022, 15:14:21) [MSC v.1929 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or "license()" for more information.
>>>
= RESTART: C:\Users\sijanecan\OneDrive - Univerza v Ljubljani\Namizje\FAKS\MAGISTRSKI ŠTUDIJ\MAGISTRSKA NALOGA\PL.py
Please enter the molar mass: 518.3239
(21:3) LPE, M: 518.32429, d: 0.00039
(18:3) LPC, M: 518.32426, d: 0.00036
>>>
= RESTART: C:\Users\sijanecan\OneDrive - Univerza v Ljubljani\Namizje\FAKS\MAGISTRSKI ŠTUDIJ\MAGISTRSKA NALOGA\PL.py
Please enter the molar mass: 333.2365
Peak does not correspond to PL.
>>>
= RESTART: C:\Users\sijanecan\OneDrive - Univerza v Ljubljani\Namizje\FAKS\MAGISTRSKI ŠTUDIJ\MAGISTRSKA NALOGA\PL.py
Please enter the molar mass: 760.5848
(14:0-23:1) PE, M: 760.58542, d: 0.00062
(14:1-23:0) PE, M: 760.58542, d: 0.00062
(15:0-22:1) PE, M: 760.58542, d: 0.00062
(15:1-22:0) PE, M: 760.58542, d: 0.00062
(16:0-21:1) PE, M: 760.58542, d: 0.00062
(16:1-21:0) PE, M: 760.58542, d: 0.00062
(17:0-20:1) PE, M: 760.58542, d: 0.00062
(17:1-20:0) PE, M: 760.58542, d: 0.00062
(18:0-19:1) PE, M: 760.58542, d: 0.00062
(18:1-19:0) PE, M: 760.58542, d: 0.00062
(19:0-18:1) PE, M: 760.58542, d: 0.00062
(19:1-18:0) PE, M: 760.58542, d: 0.00062
(20:0-17:1) PE, M: 760.58542, d: 0.00062
(20:1-17:0) PE, M: 760.58542, d: 0.00062
(21:0-16:1) PE, M: 760.58542, d: 0.00062
(21:1-16:0) PE, M: 760.58542, d: 0.00062
(22:0-15:1) PE, M: 760.58542, d: 0.00062
(22:1-15:0) PE, M: 760.58542, d: 0.00062
(23:0-14:1) PE, M: 760.58542, d: 0.00062
(23:1-14:0) PE, M: 760.58542, d: 0.00062
(14:0-20:1) PC, M: 760.58539, d: 0.00059
(14:1-20:0) PC, M: 760.58539, d: 0.00059
(15:0-19:1) PC, M: 760.58539, d: 0.00059
(15:1-19:0) PC, M: 760.58539, d: 0.00059
(16:0-18:1) PC, M: 760.58539, d: 0.00059
(16:1-18:0) PC, M: 760.58539, d: 0.00059
(17:0-17:1) PC, M: 760.58539, d: 0.00059
(17:1-17:0) PC, M: 760.58539, d: 0.00059
(18:0-16:1) PC, M: 760.58539, d: 0.00059
(18:1-16:0) PC, M: 760.58539, d: 0.00059
(19:0-15:1) PC, M: 760.58539, d: 0.00059
(19:1-15:0) PC, M: 760.58539, d: 0.00059
(20:0-14:1) PC, M: 760.58539, d: 0.00059
(20:1-14:0) PC, M: 760.58539, d: 0.00059
>>>
```

Figure S1. Example output for three different searches with Python code.