

SUPPLEMENTARY DOCUMENT

Analysis of Polar Lipids in Hemp (*Cannabis sativa* L.) By-Products by Ultra-High Performance Liquid Chromatography and High-Resolution Mass Spectrometry

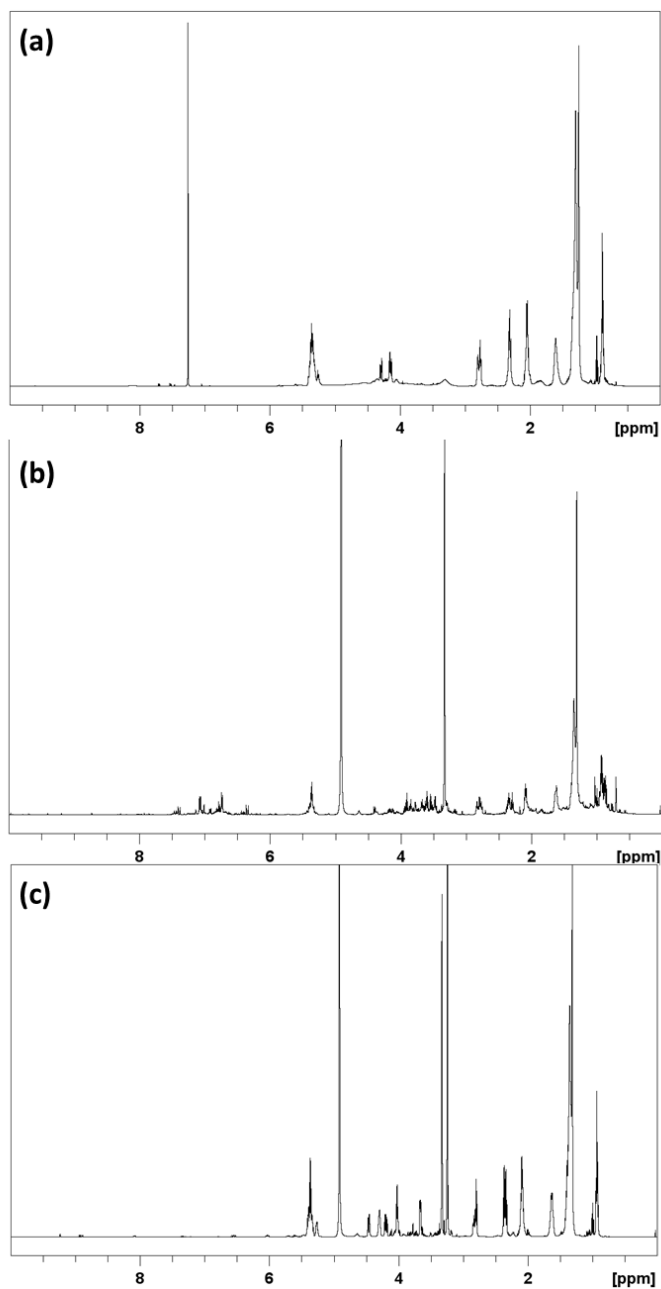


Figure S1. ^1H NMR spectrum of hemp cake SPE fractions chloroform (a) acetone (b) and MeOH (c).

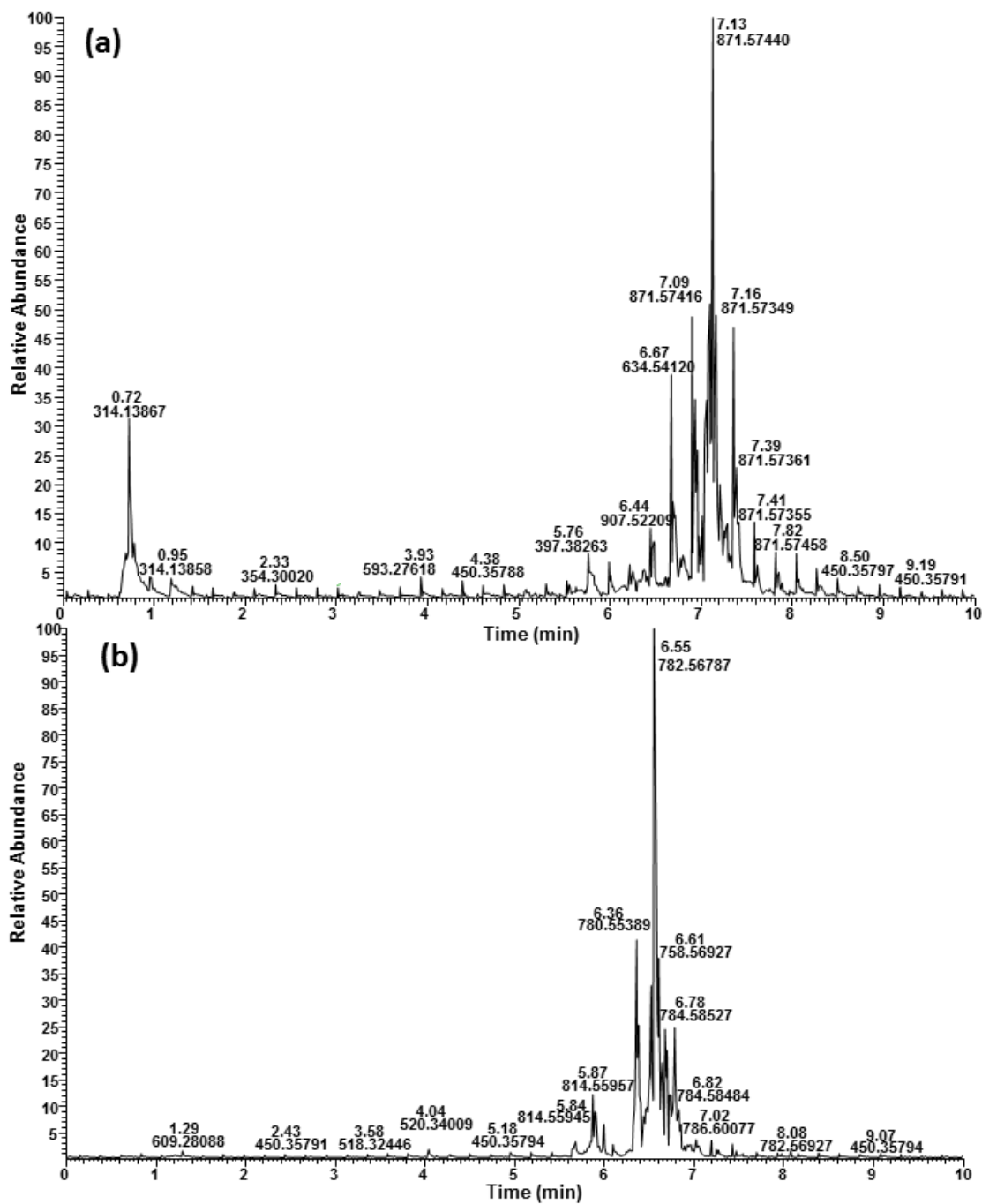


Figure S2. TICs of hemp cake SPE fractions acetone (a) and MeOH (b) in positive mode.

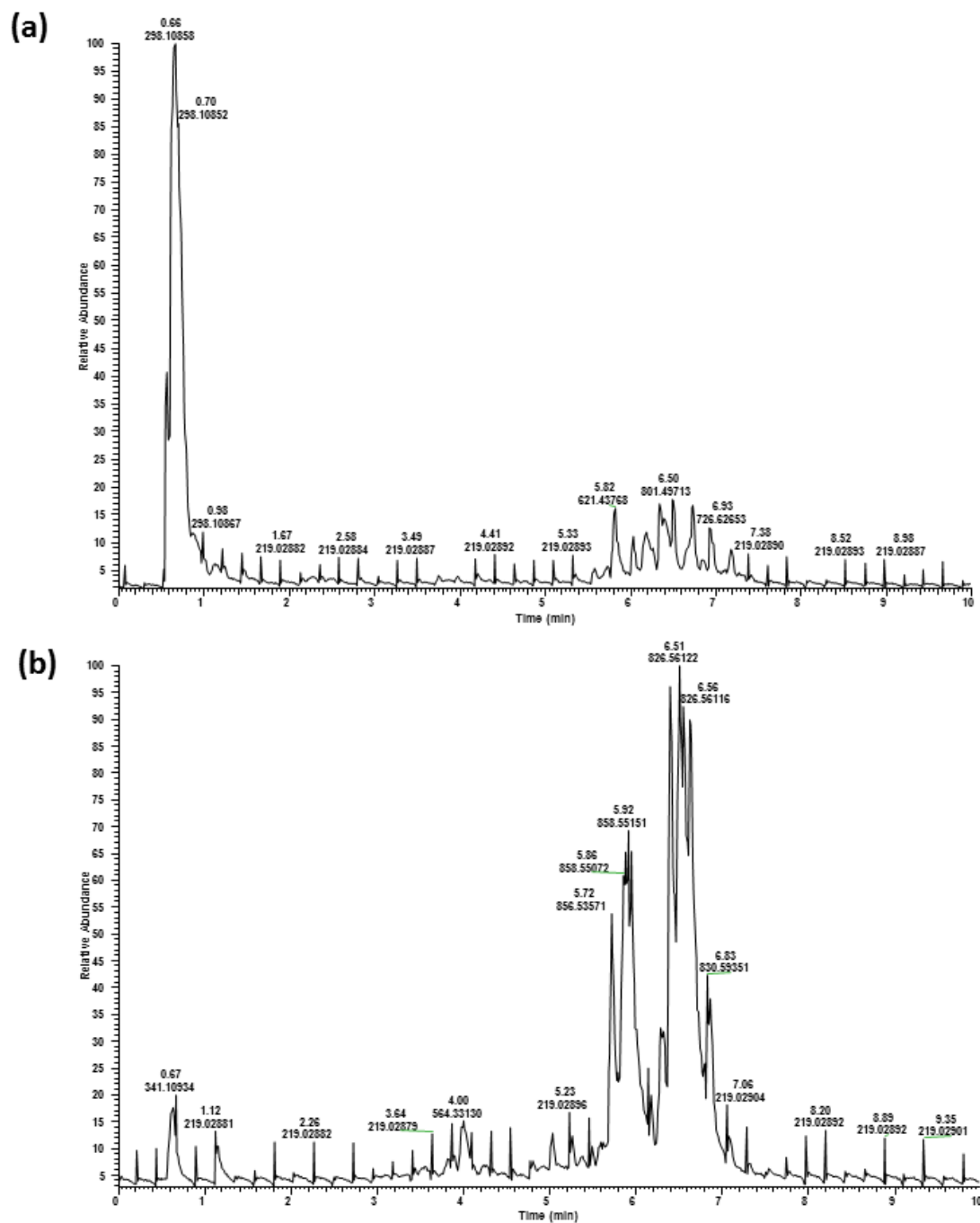


Figure S3. TICs of hemp cake SPE fractions acetone (a) and MeOH (b) in negative mode.

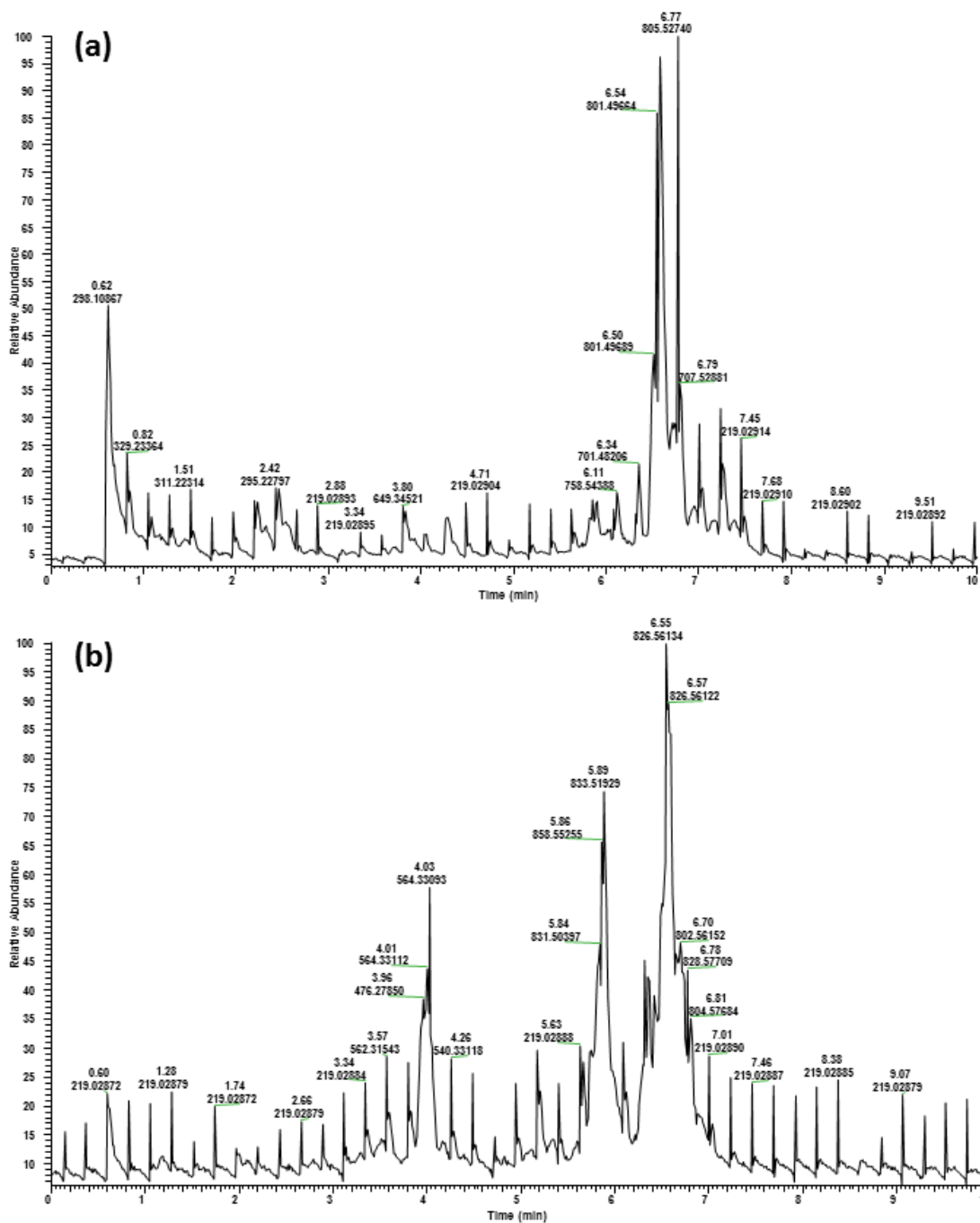


Figure S4. TICs of hemp seed hulls SPE fractions acetone (a) and MeOH (b) in negative mode.

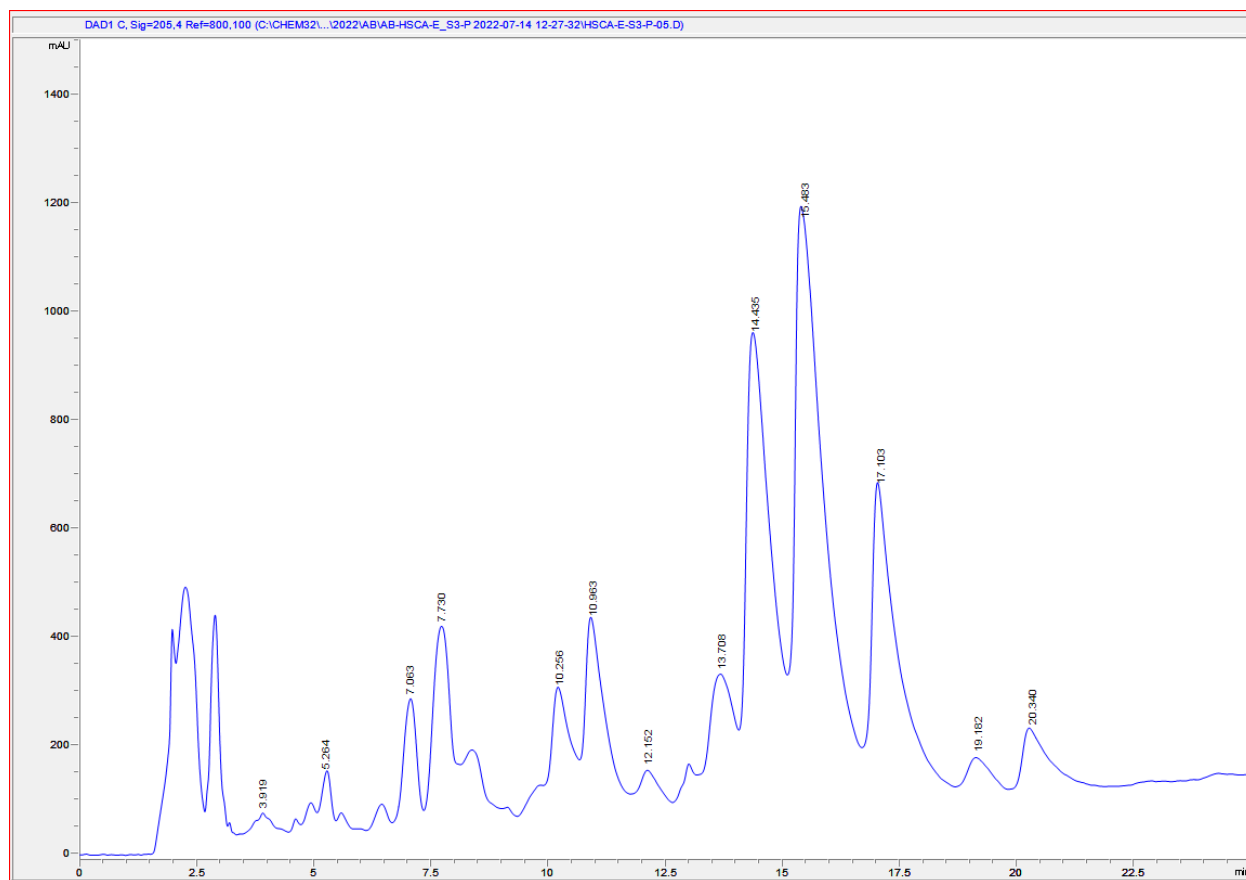


Figure S5. HPLC chromatogram of MeOH fraction of hemp cake.

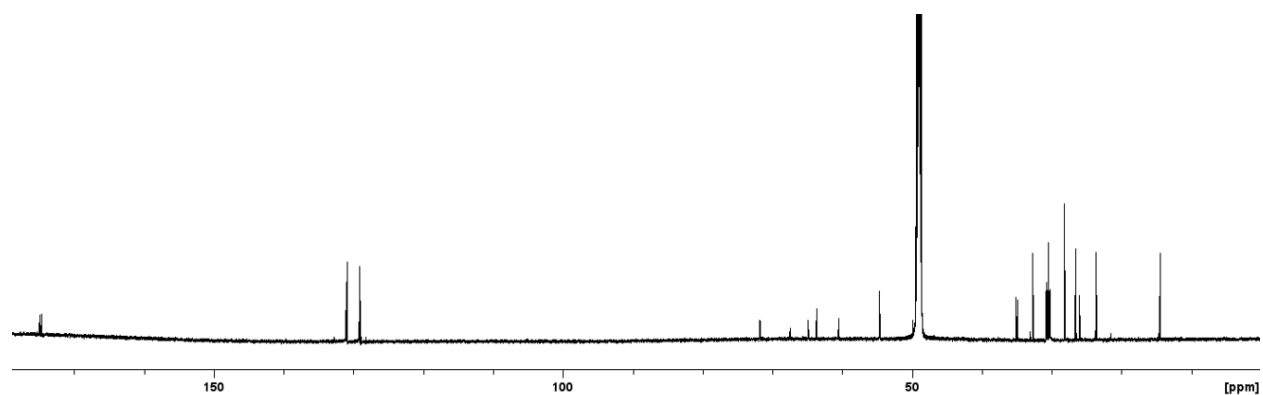
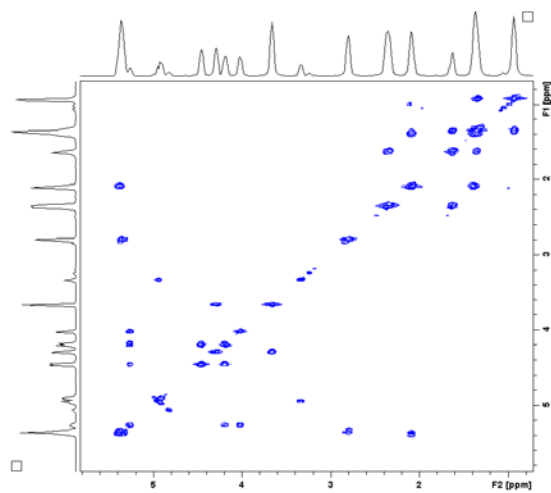
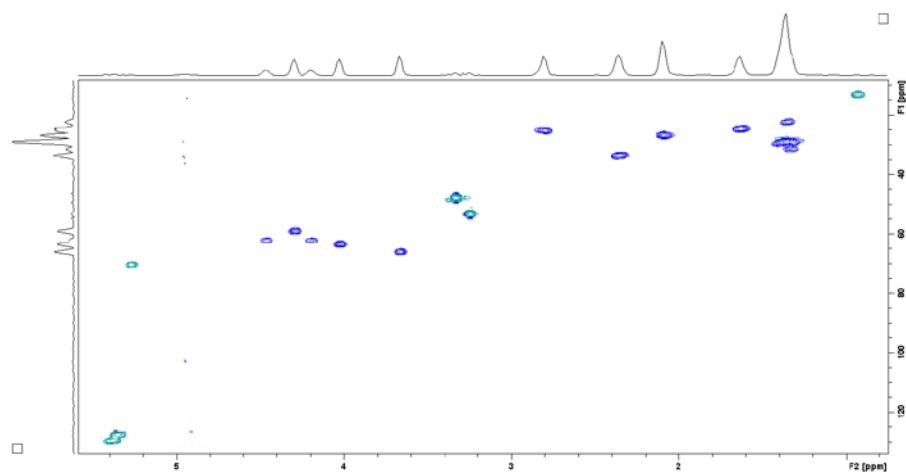


Figure S6. The ^{13}C NMR spectrum of 1,2-di-linoleoylphosphatidylcholine (PC 18:2/18:2) measured in CD_3OD .

(a)



(b)



(c)

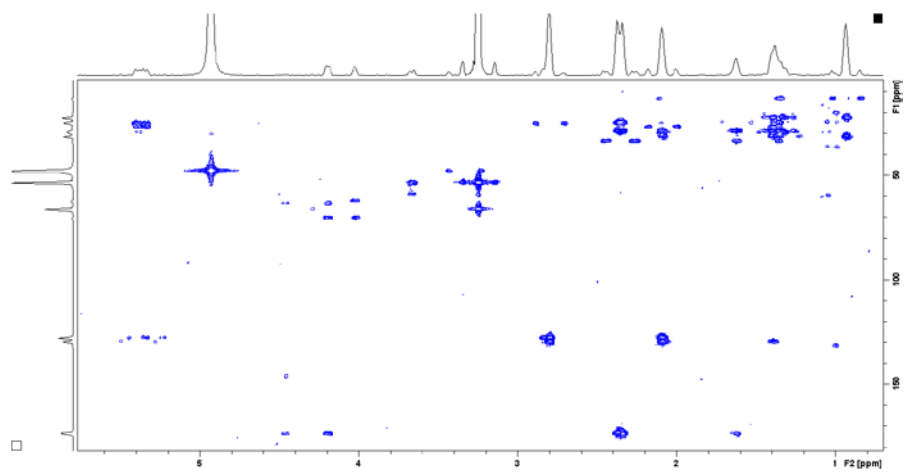
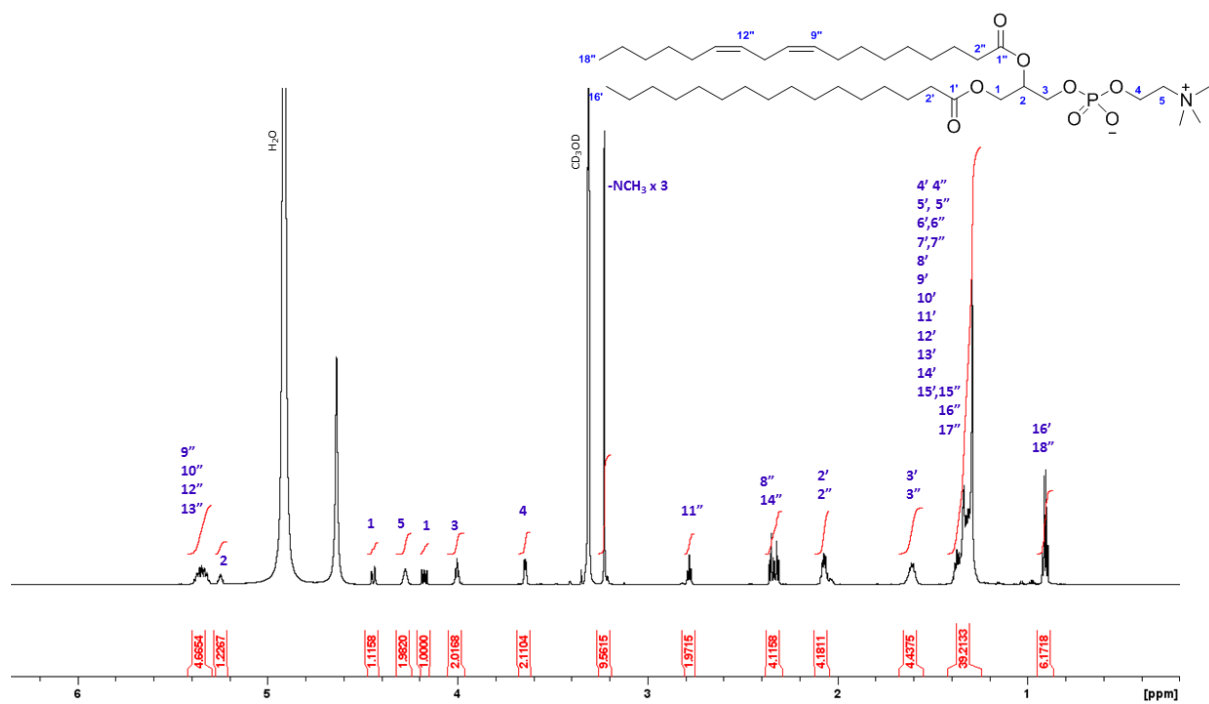


Figure S7. 2D-NMR spectra of 1,2-di-linoleoylphosphatidylcholine COSY (a) HSQC (b) and HMBC (c) measured in CD₃OD.

(a)



(b)

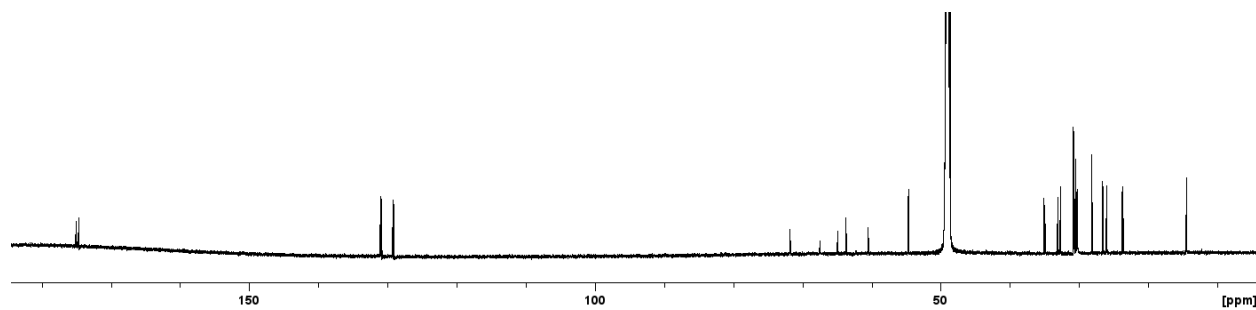
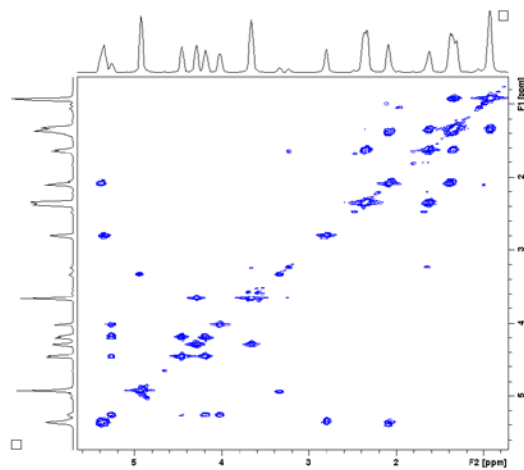
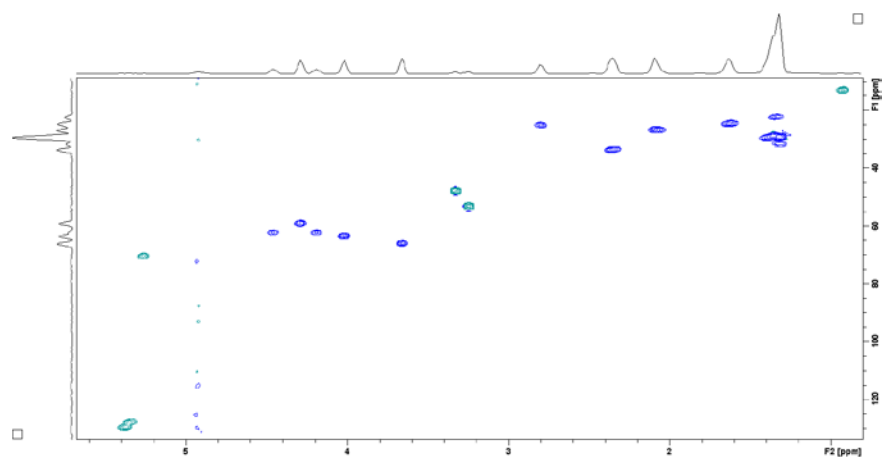


Figure S8. ^1H - (a) and ^{13}C -NMR spectrum of 1-palmitoyl-2-linoleoylphosphatidylcholine measured in CD_3OD . HRMS m/z 758.56768 [calcd for $\text{C}_{42}\text{H}_{81}\text{NO}_8\text{P}$ ($\text{M} + \text{H}$) $^+$ 758.56943].

(a)



(b)



(c)

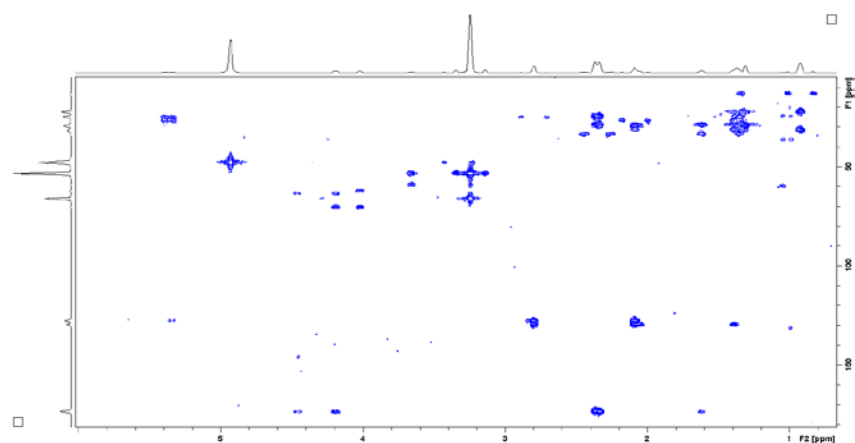


Figure S9. 2D-NMR spectra of 1- palmitoyl-2-linoleoylphosphatidylcholine COSY (a) HSQC (b) and HMBC (c) measured in CD₃OD.

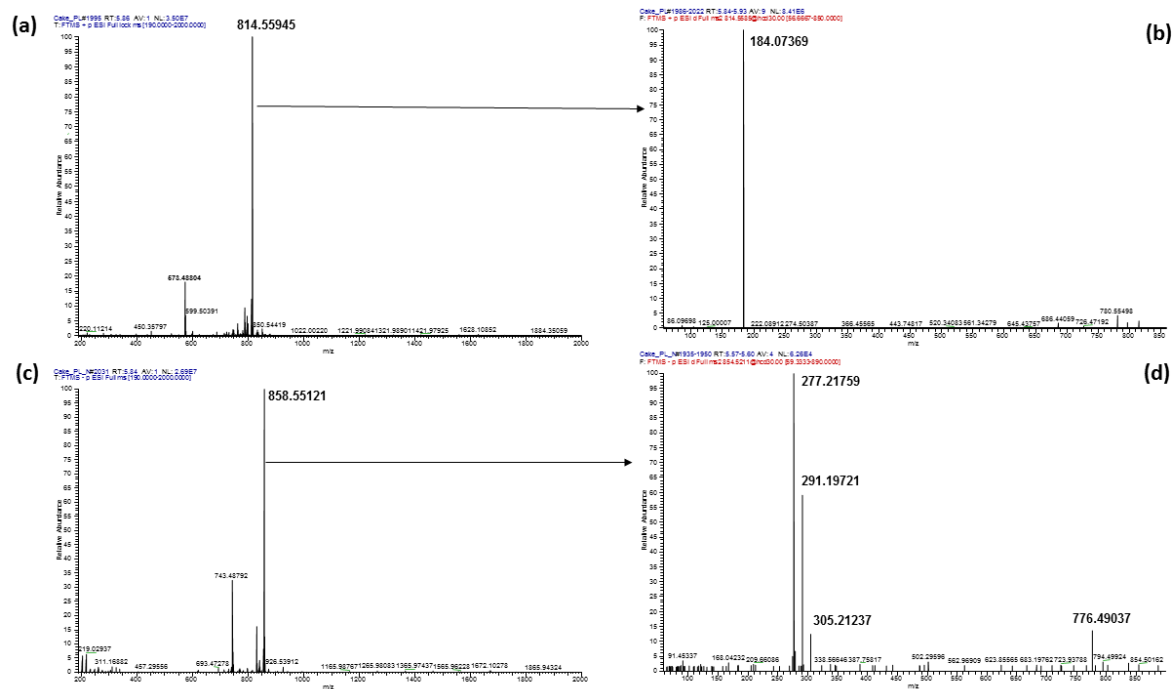


Figure S10. Mass spectrum of unknown phospholipid eluted around 6.00 min with molecular ion at m/z 814.55988 in positive mode (a) fragmentation ions of m/z 814.55988 in positive mode (b), mass spectrum of unknown phospholipid with molecular ion at m/z 858.55121 in negative mode (c) fragmentation ions of m/z 858.55121 (d).