Running title: Lipidomics of Lupinus luteus

Analysis of phospholipids, lysophospholipids and their linked fatty acyl chains

in yellow lupin seeds (Lupinus luteus L.) by liquid chromatography and tandem

mass spectrometry

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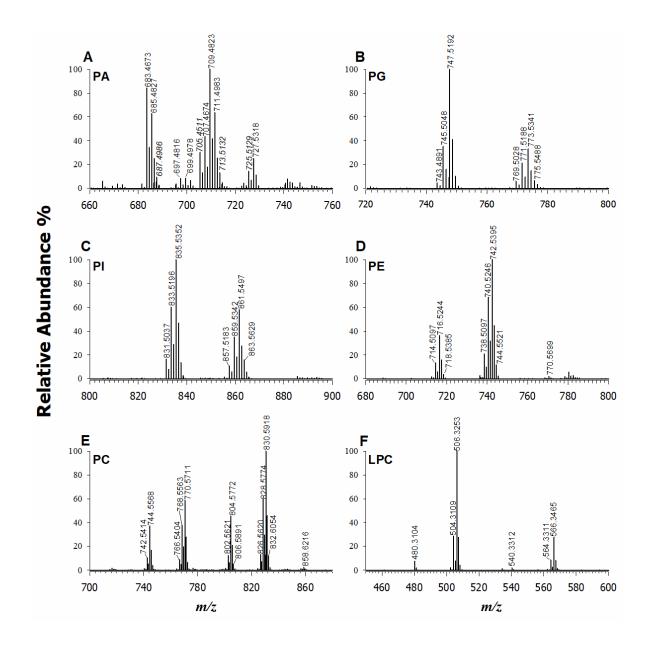


Figure S1.

Figure S1. ESI(-)-FTMS spectra of a purified lipid extract of *L. Luteus* seeds relevant to PA (A), PG (B), PI (C), PE (D), PC (E) and LPC (F) in negative ion mode averaged under the corresponding chromatographic band (see Figure 1).

Α 391.2 MS/MS @ m/z 671.5 391.2 MS/MS @ m/z 673.5 100 255.2 80 279.2 281.2 60 435.3 Relative Abundance % 40 20 0 200 300 400 500 600 700 250 350 450 550 650 C 415.2 281.2 MS/MS @ m/z 727.5 100 7 MS/MS @ m/z 695.5 463.3 80 60 x10 40 431.2 413.2 417.3 281.2 20 0 250 350 450 550 650 750 650 250 350 450 550 750

Phosphatidic acids (PA)

Figure S2. Tandem MS spectra obtained by ESI(-)-CID of representative PA identified in the lipid extract of *L. Luteus* seeds.

m/z

m/z

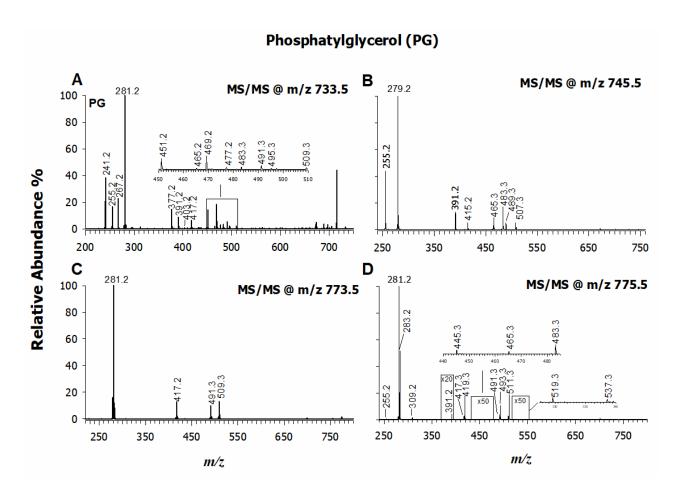


Figure S3. Tandem MS spectra obtained by ESI(-)-CID of representative PG identified in the lipid extract of *L. Luteus* seeds.

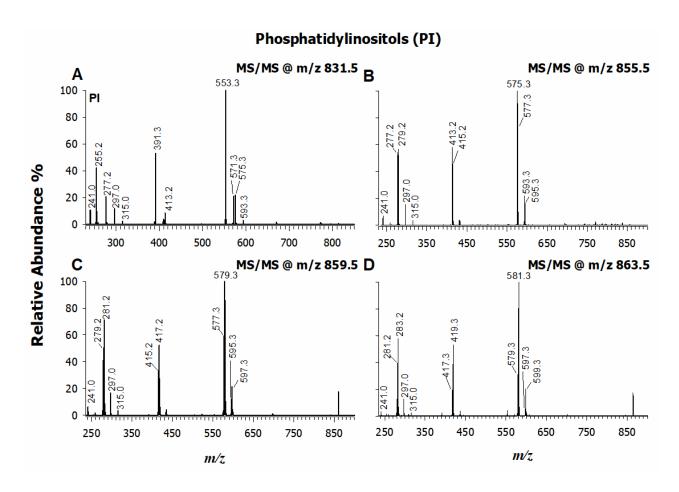


Figure S4. Tandem MS spectra obtained by ESI(-)-CID of representative PI identified in the lipid extract of *L. Luteus* seeds.

MS/MS @ m/z 714.5 B MS/MS @ m/z 738.5 Α 279.2 PΕ 456.3 458.3 460.3 Relative Abundance % C MS/MS @ m/z 744.5 D MS/MS @ m/z 770.5 281.2 281.2 506.3 309.3 283.2 m/z

Phosphatidylethanolamines (PE)

Figure S5. Tandem MS spectra obtained by ESI(-)-CID of representative PE identified in the lipid extract of *L. Luteus* seeds.

m/z

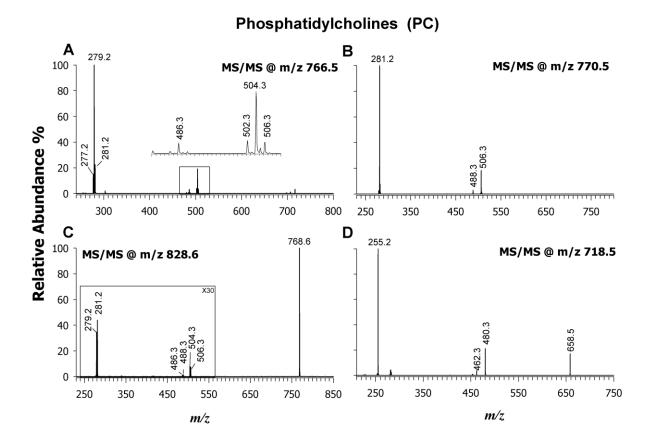


Figure S6. Tandem MS spectra obtained by ESI(-)-CID of representative PC identified in the lipid extract of *L. Luteus* seeds.

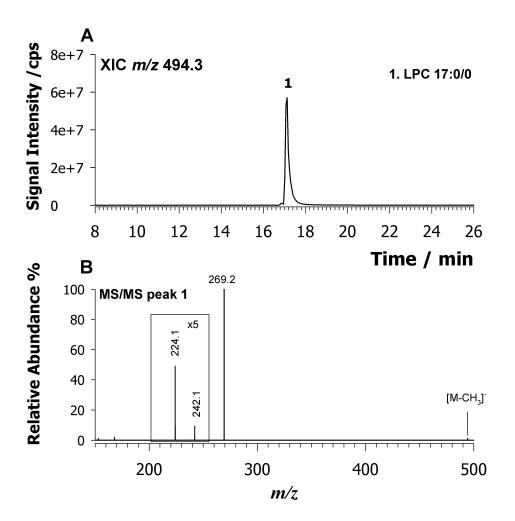


Figure S7.

Figure S7. XIC chromatogram of a standard LPC 17:0/0 observed as demethylated molecule at m/z 494.3 (A) and its relevant tandem MS spectrum (B).

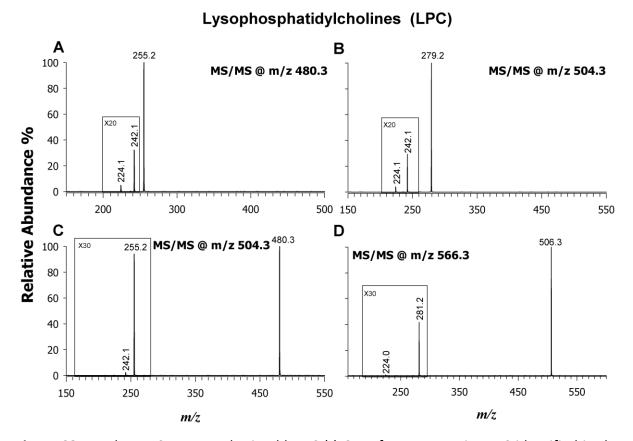


Figure S8. Tandem MS spectra obtained by ESI(-)-CID of representative LPC identified in the lipid extract of *L. Luteus* seeds.

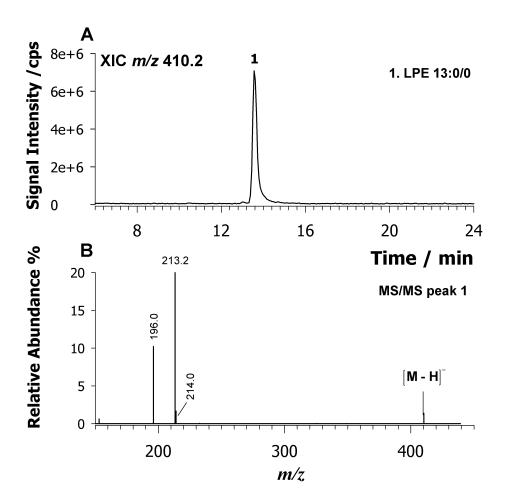


Figure S9. XIC chromatogram for LPE 13:0/0:0 observed as demethylated molecule at m/z 410.2 (A) and its relevant tandem MS spectrum (B).