

Supplementary Table S3. Phospholipids identified in the “oxysterol window” of the plasma metabolome

Measured <i>m/z</i> (RA ^a)	Retention time/min	Elemental composition	Lipid Maps hit ^b	Metlin Library hit ^{c,d}	Measured MS ² fragments (RA)	Postulated structure
494.3240 (3.75)	9.52	C ₂₄ H ₄₉ O ₇ NP	GPCho 16:1(9Z)/0:0	GPCho 16:1(9E)/0:0 ^d	476 (100), 417 (0.86), 184 (33.4)	GPCho 16:1/0:0
496.3402 (100)	10.57	C ₂₄ H ₅₁ O ₇ NP	GPCho 16:0/0:0 GPEtn 19:0/0:0	GPCho 16:0/0:0 ^d	478 (100), 419 (0.30), 313 (0.13), 258 (0.52), 184 (29.27)	GPCho 16:0/0:0
520.3400 (58.26)	10.02	C ₂₆ H ₅₁ O ₇ NP	GPCho 18:2(9Z,12Z)/0:0	GPCho 18:2(9Z,12Z)/0:0 ^d	502 (100), 443 (0.26), 337 (0.11), 258 (0.61), 184 (29.60)	GPCho 18:2/0/0
522.3553 (32.38)	10.99	C ₂₆ H ₅₃ O ₇ NP	GPCho 18:1(9Z)/0:0	GPCho 18:1(9Z)/0:0 ^d	504 (100), 339 (0.47), 258 (0.83), 184 (28.21)	GPCho 18:1/0:0
524.3711	12.52	C ₂₆ H ₅₅ O ₇ NP	GPCho 18:0/0:0	GPCho 18:0/0:0 ^d	506 (100), 447	GPCho

(23.39)					(0.37), 341 (0.30), 258 (0.46), 184 (24.53)	18:0/0:0
544.3395 (9.34)	9.95	C ₂₈ H ₅₁ O ₇ NP	GPCho 20:4(5Z,8Z,11Z,14Z)/0:0	GPCho 20:4(5Z,8Z,11Z,14Z)/0:0 ^d	526 (100), 467 (0.25), 258 (0.32), 184 (27.49)	GPCho 20:4/0:0
568.3400 (1.26)	9.90	C ₃₀ H ₅₁ O ₇ NP	GPCho 22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0	GPCho 22:6(4E,7E,10E,13E,16E,19E)/0:0 ^c	550 (100), 385 (3.03), 184 (19.43)	GPCho 22:6/0:0
570.3556 (0.56)	10.34	C ₃₀ H ₅₃ O ₇ NP	NA	NA	NA	GPCho 22:5/0:0

^a Relative abundance as determined by peak area.

^b From a search of *m/z* value against the Lipid Maps^{S4} database <http://www.lipidmaps.org/tools/index.html>

PGCho x:y/x:y is an abbreviation for glycerophosphocholine where the number of carbons in the acyl chains are indicated by x and the number of double bonds by y.

^c From a search of *m/z* against the METLIN metabolite library¹⁷ <http://metlin.scripps.edu/index.php>.

^d From a search of M against the METLIN metabolite library¹⁷ <http://metlin.scripps.edu/index.php>