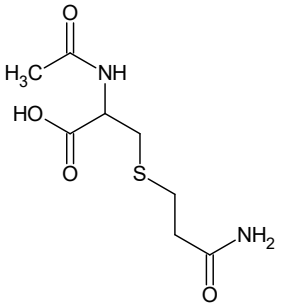
ELECTRONIC SUPPLEMENTARY MATERIAL

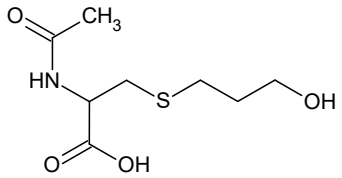
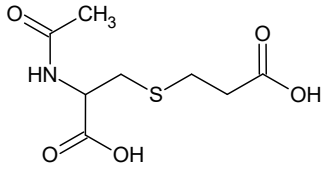
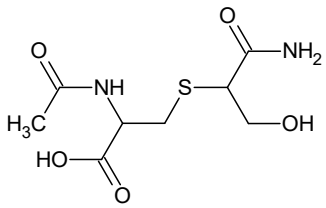
Biomarkers of fried food intake: a systematic review of *in vivo* studies

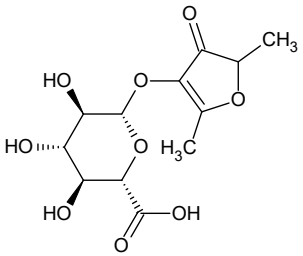
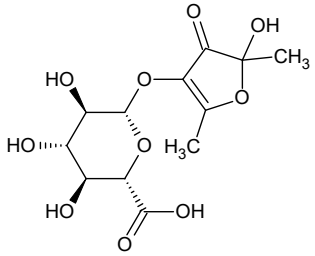
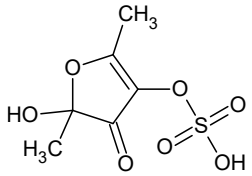
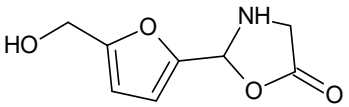
Aline G. A. Carvalho[a,b], Luana O. Oliveira[c], Hygor M. R. de Souza[b], Gabriela R. A. Soliz[b], Maria Fernanda C. Guimarães[b], Fabio A. Oroski[d], Vanessa N. Castelo-Branco[c], Tatiana El-Bacha[b,e], and Alexandre G. Torres[a,b,]

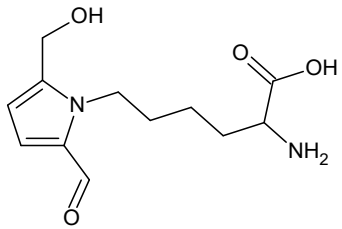
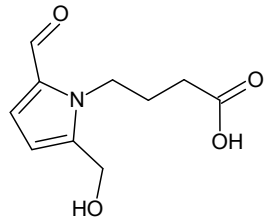
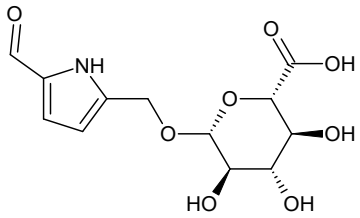
[a.] *Laboratório de Bioquímica Nutricional e de Alimentos, Instituto de Química, Universidade Federal do Rio de Janeiro.*
[b.] *Lipid Biochemistry and Lipidomics Laboratory (LipBio), Instituto de Química, Universidade Federal do Rio de Janeiro.*
[c.] *Laboratório de Biotecnologia de Alimentos, Faculdade de Farmácia, Universidade Federal Fluminense.*
[d.] *Grupo de Estudos em Bioeconomia da Escola de Química. Escola de Química, Universidade Federal do Rio de Janeiro.*
[e.] *LeBioME-Bioactives, Mitochondria and Placental Metabolism Core, Institute of Nutrition Josué de Castro, Universidade Federal do Rio de Janeiro.*

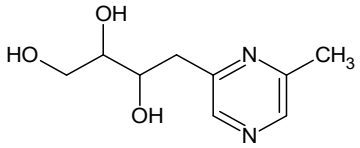
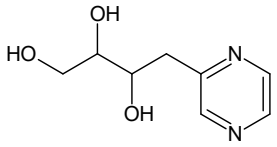
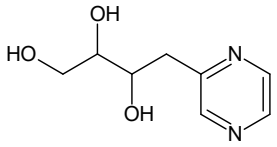
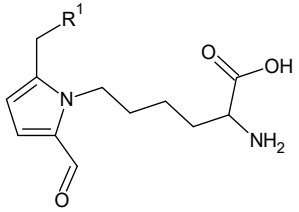
Table S1. Biomarkers of fried food intake, their molecular formula, and chemical structures.

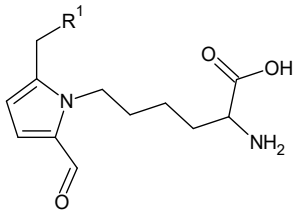
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Mercapturic acids of acrolein and acrylamide				
N-acetyl-S-(2-carbamoylethyl) cysteine (AAMA)	$C_8H_{14}N_2O_4S$		↑	$C_{predose}$: 0.08 ± 0.05 µmol/g creatinine (Study 1)[23] C_{max}: 1.16 ± 0.47 µmol/g creatinine (Study 1) [23] $C_{predose}$: 0.05 ± 0.02 µmol/g creatinine (Study 2) [23] C_{max}: 0.16 ± 0.03 µmol/g creatinine (Study 2) [23]

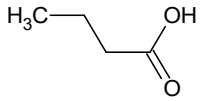
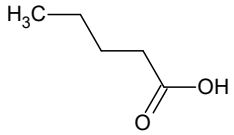
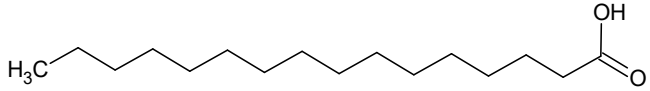
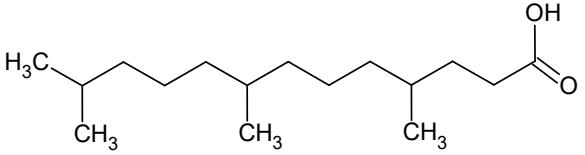
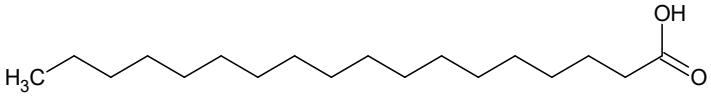
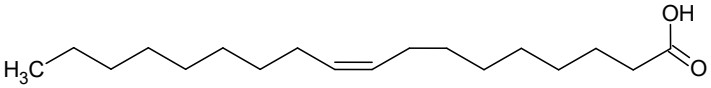
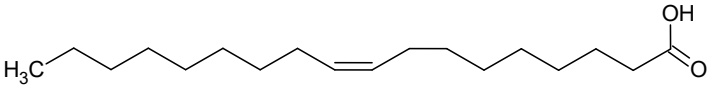
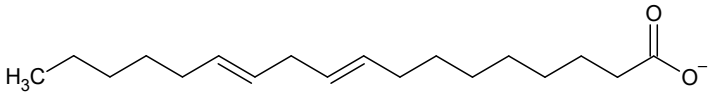
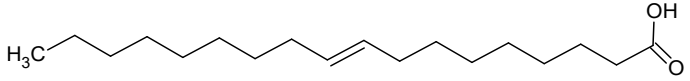
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
N-acetyl-S-(3-hydroxypropyl) cysteine (3-HPMA)	$C_8H_{15}NO_4S$		↑	$C_{predose}$: 114.4 - 185.7 ng/mL [20] C_{max}: 194.7 – 277.3 ng/mL [20] $C_{predose}$: 11.6 ± 28.8 µmol/g creatinine (Study 1) [23] C_{max}: 66.6 ± 44.1 µmol/g creatinine (Study 1) [23] $C_{predose}$: 0.18 ± 0.02 µmol/g creatinine (Study 2) [23] C_{max}: 0.47 ± 0.15 µmol/g creatinine (Study 2) [23]
N-acetyl-S-(carboxyethyl) cysteine (CEMA)	$C_8H_{13}NO_5S$		↑	$C_{predose}$: 0.06 ± 0.01 µmol/g creatinine (Study 2) [23] C_{max}: 0.35 ± 0.11 µmol/g creatinine (Study 2) [23]
N-acetyl-S-(1/2-carbamoyl-2-hydroxyethyl) cysteine (GAMA)	$C_8H_{14}N_2O_5S$		↑	$C_{predose}$: 0.02 ± 0.01 µmol/g creatinine (Study 1) C_{max}: 0.08 ± 0.05 µmol/g creatinine (Study 1) [23] $C_{predose}$: 0.02 ± 0.01 µmol/g creatinine (Study 2) C_{max}: 0.03 ± 0.02 µmol/g creatinine (Study 2) [23]

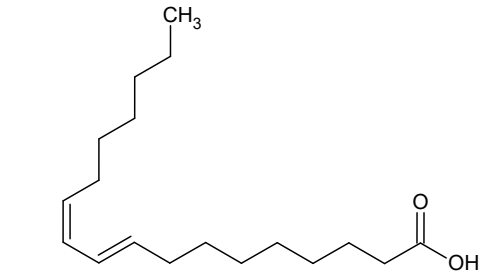
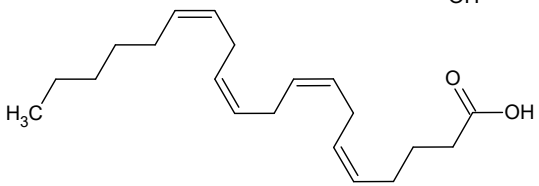
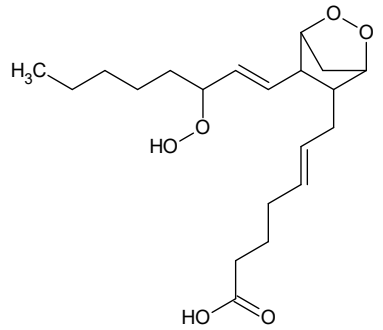
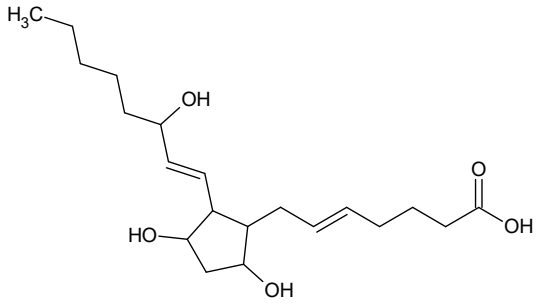
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Furan, pyrrole, and pyrazine metabolites				
Furaneol glucuronide	$C_{12}H_{16}O_9$		↑	In potato chips: $C_{predose}$: 0.002 area unit (AU) [22] C_{max}: 0.011 AU [22] In French fries: $C_{predose}$: 0.002 AU [22] C_{max}: 0.007 AU [22]
2,4-Dihydroxy-2,5-dimethyl-3(2H)-furanone glucuronide	$C_6H_8O_4$		↑	In potato chips: $C_{predose}$: 0.000 - 0.001 AU [22] C_{max}: 0.01 – 0.08 AU [22] In French fries: $C_{predose}$: 0.000 - 0.001AU [22] C_{max}: 0.005 – 0.06 AU [22]
2,4-Dihydroxy-2,5-dimethyl-3(2H)-furanone sulfate	$C_6H_8SO_7$		↑	In potato chips: $C_{predose}$: 0.001 AU [22] C_{max}: 0.011 AU [22] In French fries: $C_{predose}$: 0.001 AU [22] C_{max}: 0.005 AU [22]
5-(Hydroxymethyl)-2-furaldehyde-glycine	$C_8H_9NO_4$		↑	In potato chips: $C_{predose}$: 0.002 AU C_{max}: 0.01 AU [22]

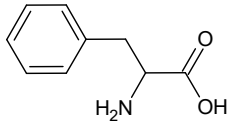
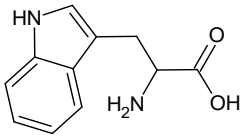
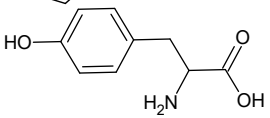
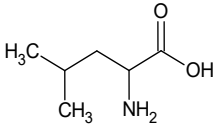
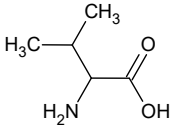
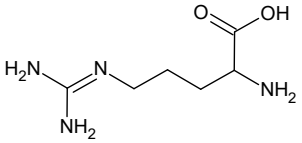
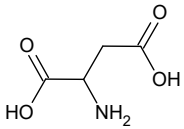
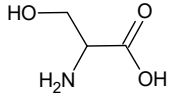
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Pyrraline	$C_{12}H_{18}N_2O_4$		↑	In French fries: $C_{predose}$: 0.002 AU C_{max}: 0.0087 AU [22] In potato chips: $C_{predose}$: 0.001 AU C_{max}: 0.008AU [22] In French fries $C_{predose}$: 0.001 AU C_{max}: 0.005 AU [22]
4-(2-Formyl-5-(hydroxymethyl)-1H-pyrrol-1-yl) butanoic acid	$C_{10}H_{13}NO_4$		↑	In potato chips: $C_{predose}$: 0.000 AU C_{max}: 0.016 AU [22] In French fries: $C_{predose}$: 0.000 AU C_{max}: 0.011 AU [22]
5-(Hydroxymethyl)-1H-pyrrole-2-carbaldehyde glucuronide	$C_{12}H_{15}NO_8$		↑	In potato chips: $C_{predose}$: 0.000 AU C_{max}: 0.0075 AU [22] In French fries: $C_{predose}$: 0.000 AU C_{max}: 0.0039 AU [22]

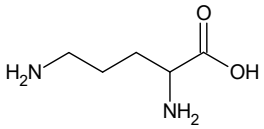
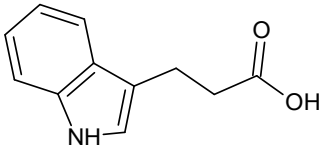
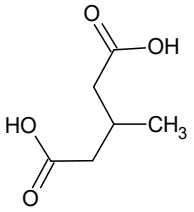
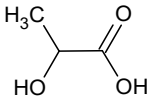
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
4-(6-Methyl-2-pyrazinyl)-1,2,3-butanetriol	$C_9H_{14}N_2O_3$		↑	In potato chips: $C_{predose}$: 0.000 AU C_{max}: 0.04 AU [22] In French fries: $C_{predose}$: 0.000 AU C_{max}: 0.022 AU [22]
Pyrazine derivative 1	$C_8H_{12}N_2O_3$		↑	In potato chips: $C_{predose}$: 0.001 AU C_{max}: 0.007 AU [22] In French fries: $C_{predose}$: 0.001 AU C_{max}: 0.005 AU [22]
Pyrazine derivative 2	$C_8H_{12}N_2O_3$		↑	In potato chips: $C_{predose}$: 0.001 AU C_{max}: 0.014 AU [22] In French fries: $C_{predose}$: 0.001 AU C_{max}: 0.006 AU [22]
N-substituted formylpyrrole derivative 1	$C_{12}H_{17}N_2O_3$ R^1=C_3H_2OH or C_3H_6OH		↑	In potato chips $C_{predose}$: 0.004 AU C_{max}: 0.01 AU [22] In French fries: $C_{predose}$: 0.004 AU C_{max}: 0.006 AU [22]

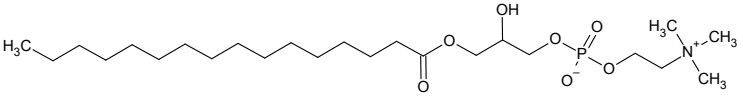
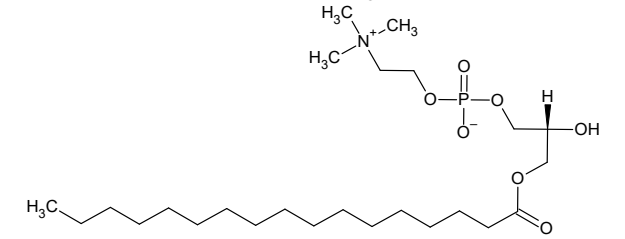
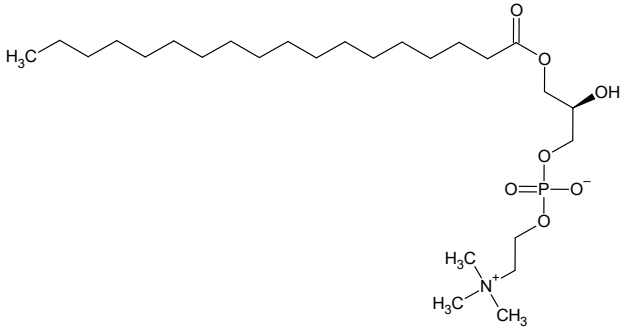
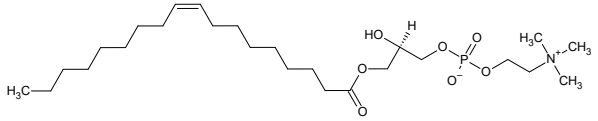
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
N-substituted formylpyrrole derivative 2	$C_{12}H_{17}N_2O_3$ $R^1=C_3H_2OH$ or C_3H_6OH		↑	In potato chips: $C_{predose}$: 0.000 AU C_{max}: 0.0175 AU [22] In French fries: $C_{predose}$: 0.00 AU C_{max}: 0.0075 AU [22]

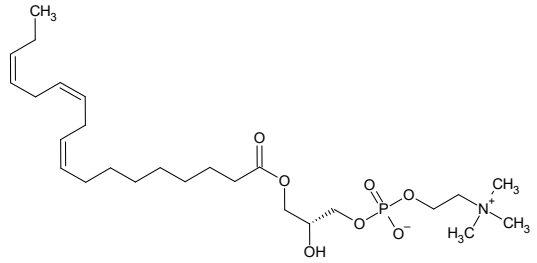
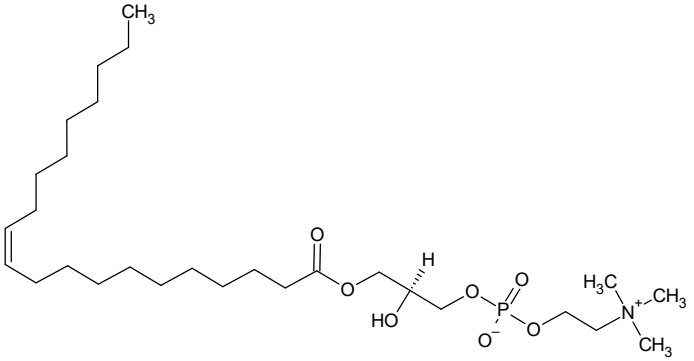
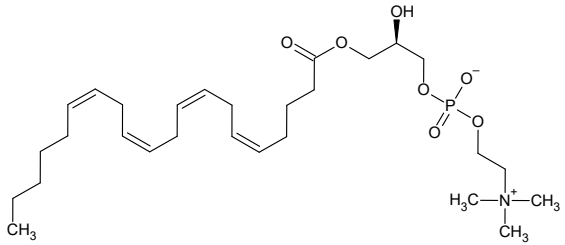
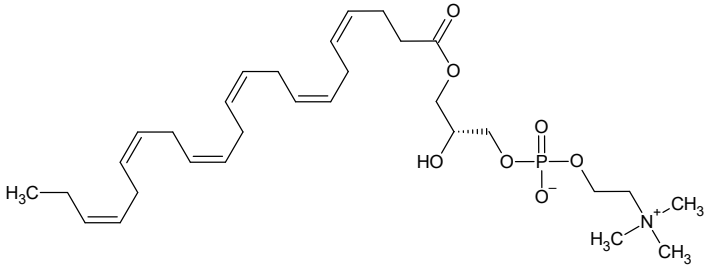
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Fatty acids, conventional and unconventional				
Butyric acid	$C_4H_8O_2$		↓	Week 0 (control): 0.1-50.0 µmol/g [21] Week 4: 0.1-62.5 µmol/g [21]
Valeric acid	$C_5H_{10}O_2$		↓	Week 0 (control): 0.1-25.0 µmol/g [21] Week 4: 0.1-20.0 µmol/g [21]
Palmitic acid	$C_{16}H_{32}O_2$		↑	2.74-Fold change [5]
Trimethyltridecanoic acid	$C_{16}H_{32}O_2$		↑	2.21-Fold change [5]
Stearic acid	$C_{18}H_{36}O_2$		↑	1.67-Fold change [5]
Oleic acid	$C_{18}H_{34}O_2$		↑	1.51-Fold change [5]
Octadec-9-enoic acid	$C_{18}H_{34}O_2$		↑	1.52-Fold change [5]
Octadecadienoate	$C_{18}H_{31}O_2^-$		↑	1.56-Fold change [5]
Elaidic acid	$C_{18}H_{34}O_2$		↑	1.47 – 1.83-Fold change [5]

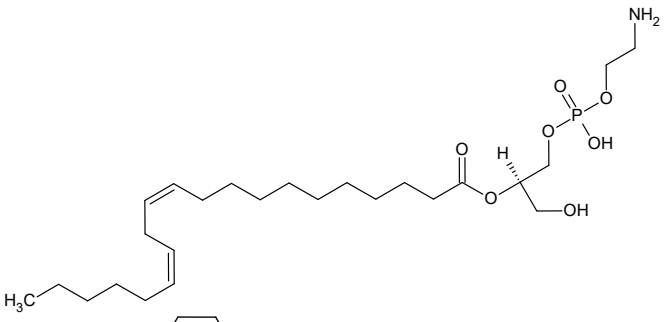
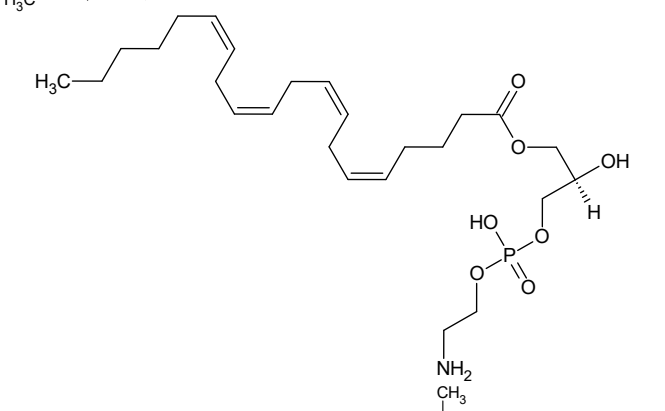
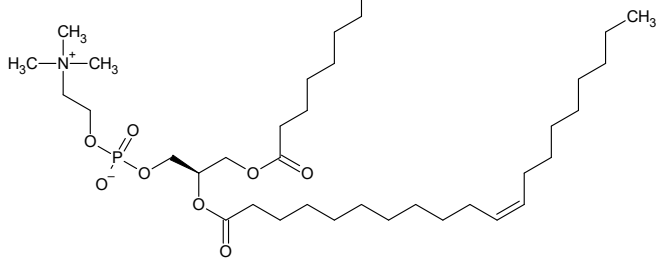
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Bovinic acid	$C_{18}H_{32}O_2$		↓	0.73-Fold change [5]
Arachidonic acid	$C_{20}H_{32}O_2$		↑	1.72-Fold change [5]
Prostaglandin G2	$C_{20}H_{32}O_6$		↑	1.55-Fold change [5]
Prostaglandin F2a	$C_{20}H_{34}O_5$		↑	3.51-Fold change [5]

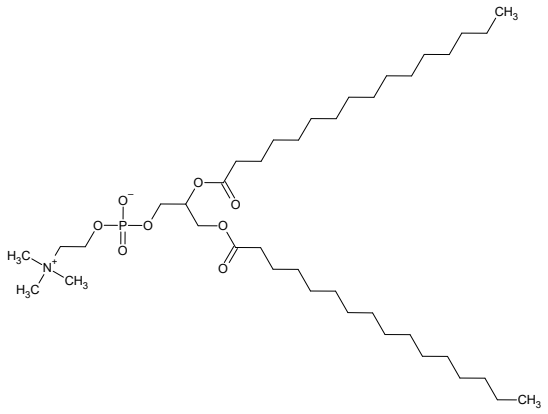
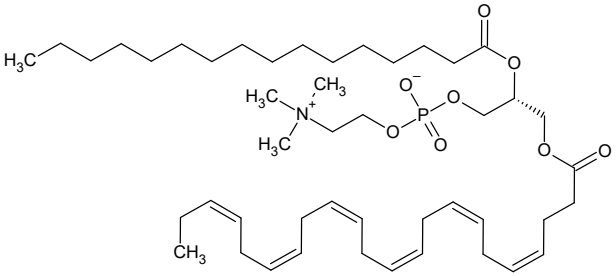
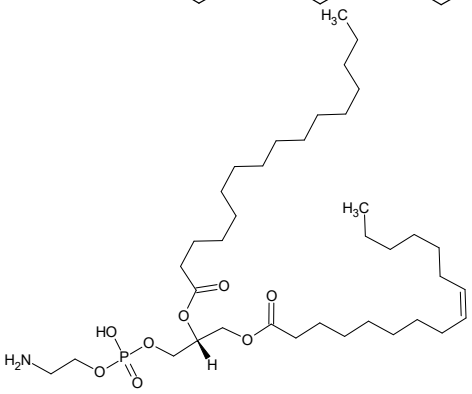
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Amino acids				
L-Phenylalanine	$C_9H_{11}NO_2$		↑	2.21-Fold change [5]
Tryptophan	$C_9H_{11}NO_2$		↑	2.17-Fold change [5]
Tyrosine	$C_9H_{11}NO_3$		↑	2.97-Fold change [5]
Leucine	$C_6H_{13}NO_2$		↑	2.46-Fold change [5]
Valine	$C_5H_{11}NO_2$		↑	1.82-Fold change [5]
Arginine	$C_6H_{14}N_4O_2$		↓	0.76-Fold change [5]
Aspartate	$C_4H_7NO_4$		↓	0.63-Fold change [5]
Serine	$C_3H_7NO_3$		↓	0.58-Fold change [5]

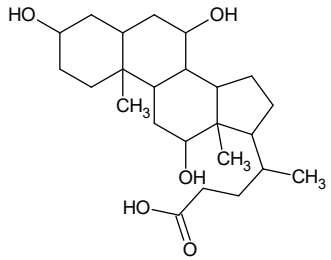
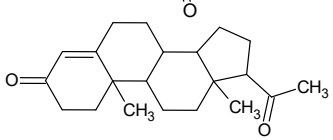
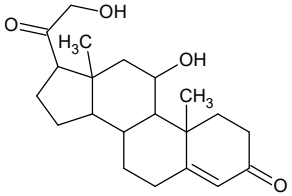
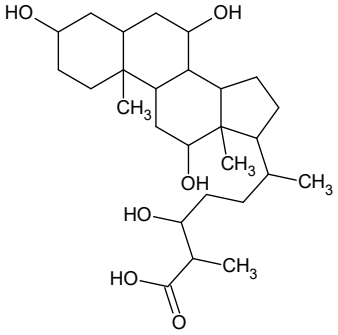
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Ornithine	$C_5H_{12}N_2O_2$		↓	0.77-Fold change [5]
Organic acids				
3-Indolepropionic acid	$C_{11}H_{11}NO_2$		-	Week 0 (control): 0.01-0.21 µmol/g [21] Week 4: 0.01-0.25 µmol/g [21]
Methylglutaric acid	$C_6H_{10}O_4$		↑	Week 0 (control): 0.01-0.08 µmol/g [21] Week 4: 0.01-0.10 µmol/g [21]
Lactic acid	$C_3H_6O_3$		↑	2.74-Fold change [5]

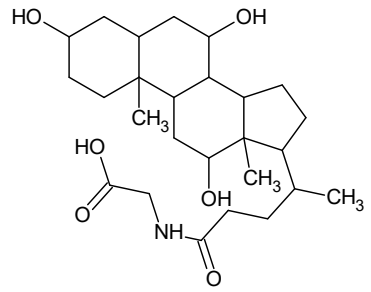
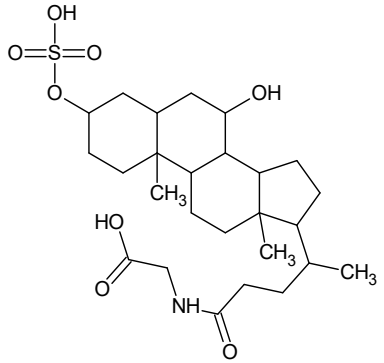
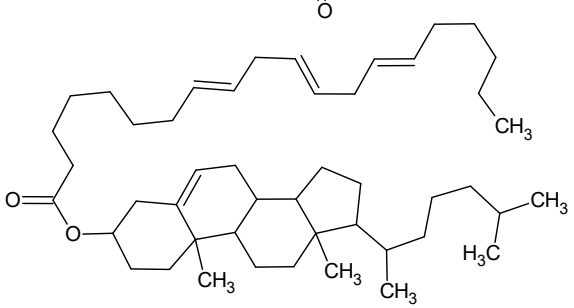
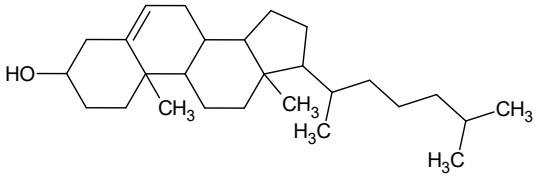
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Polar lipids, steroids, and related compounds				
LysoPC(16:0)	$C_{24}H_{50}NO_7P$		↑	1.60-Fold change [5]
LysoPC(17:0)	$C_{25}H_{52}NO_7P$		↑	1.74-Fold change [5]
LysoPC(18:0)	$C_{26}H_{54}NO_7P$		↑	1.33-Fold change [5]
LysoPC(18:1)	$C_{26}H_{52}NO_7P$		↓	1.02-Fold change [5]

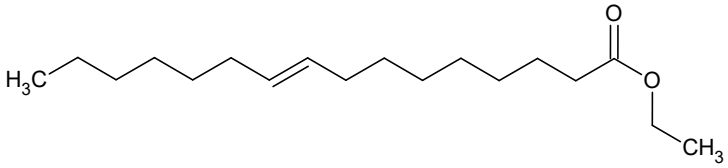
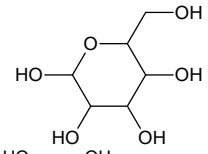
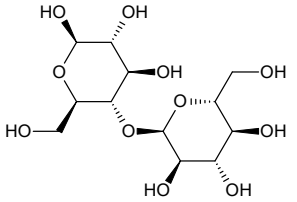
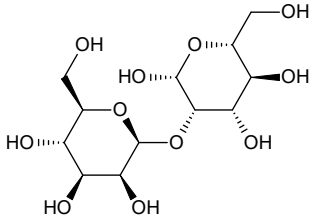
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
LysoPC(18:3)	$C_{26}H_{48}NO_7P$		↑	1.29-Fold change [5]
LysoPC(20:1)	$C_{28}H_{56}NO_7P$		↑	2.01-Fold change [5]
LysoPC(20:4)	$C_{28}H_{50}NO_7P$		↑	1.01-Fold change [5]
LysoPC(22:6)	$C_{30}H_{50}NO_7P$		↑	1.98-Fold change [5]

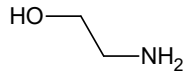
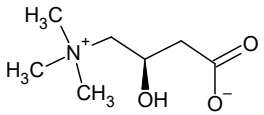
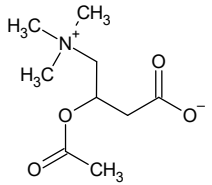
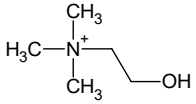
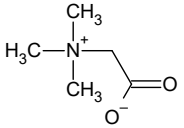
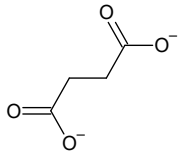
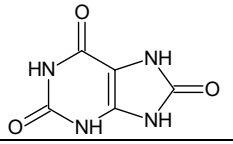
Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
LysoPE(C20:2)	$C_{25}H_{48}NO_7P$		↑	1.48-Fold change [5]
LysoPE(20:4)	$C_{25}H_{44}NO_7P$		↑	1.95-Fold change [5]
PC(14:0/20:1)	$C_{42}H_{82}NO_8P$		↑	1.83-Fold change [5]

Biomarker	Molecular formula	Chemical structure	Trend	Concentration Reference
PC(16:0/16:0)	$C_{40}H_{80}NO_8P$		↑	1.84-Fold change [5]
PC(22:6/16:0)	$C_{46}H_{80}NO_8P$		↑	1.79-Fold change [5]
PE(16:1/16:0)	$C_{37}H_{72}NO_8P$		↑	1.78-Fold change [5]

Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Cholic acid	$C_{24}H_{40}O_5$		↑	2.26-Fold change [5]
Progesterone	$C_{21}H_{30}O_2$		↓	0.75-Fold change [5]
Corticosterone	$C_{21}H_{30}O_4$		↓	0.70-Fold change [5]
Varanic acid	$C_{27}H_{46}O_6$		↑	1.75-Fold change [5]

Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Glycocholate	$C_{26}H_{43}NO_6$		↑	3.62-Fold change [5]
Glycochenodeoxycholate-3-sulfate	$C_{26}H_{43}NO_8S$		↑	1.73-Fold change [5]
Cholesterol ester (20:3)	$C_{47}H_{78}O_2$		↑	3.37-Fold change [5]
Cholesterol	$C_{27}H_{46}O$		↑	3.05-Fold change [5]

Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Ethyl 9-hexadecenoate	$C_{18}H_{34}O_2$		↑	1.47-Fold change [5]
Sugars				
D-Glucose	$C_6H_{12}O_6$		↑	2.17-Fold change [5]
D-Maltose	$C_{12}H_{22}O_{11}$		↑	1.97-Fold change [5]
β-Mannobiose	$C_{12}H_{22}O_{11}$		↑	1.46-Fold change [5]

Biomarker	Molecular formula	Chemical structure	Trend	Concentration [Reference]
Miscellaneous				
Ethanolamine	C_2H_7NO		↑	1.22-Fold change [5]
Carnitine	$C_7H_{15}NO_3$		↑	Week 0 (control): 0.01-0.10 µmol/g [21] Week 4: 0.01-0.10 µmol/g [21]
L-Acetylcarnitine	$C_9H_{17}NO_4$		↓	0.66-Fold change [5]
Choline	$C_5H_{14}NO^+$		↓	0.55-Fold change [5]
Betaine	$C_5H_{11}NO_2$		↓	0.71-Fold change [5]
Succinate	$C_4H_4O_4^{2-}$		↓	0.62-Fold change [5]
Uric acid	$C_5H_4N_4O_3$		↑	1.20-Fold change [5]