

Table S1

Metabolite	δ ^1H / ppm (multiplicity, assignment)
<u>Polar compounds</u>	
Isoleucine	0.94 (t, δ -CH ₃), 1.02 (d, γ -CH ₃)
Leucine	0.96 (d, δ' -CH ₃), 0.97 (d, δ -CH ₃), 1.72 (m, γ -CH ₂)
Valine	0.99 (d, γ -CH ₃), 1.05 (d, γ' -CH ₃), 2.29 (m, β -CH ₂)
Lactate	1.33 (d, CH ₃), 4.11 (q, CH)
Threonine	1.33 (d, γ -CH ₃), 3.58 (d, β -CH ₂), 4.25 (dd, α -CH)
Alanine	1.48 (d, β -CH ₃), 3.77 (q, α -CH)
Lysine	1.53 (γ -CH ₂ , t), 1.72 (m, δ -CH ₂), 1.92 (m, β -CH ₂), 3.02 (ϵ -CH ₂ , t), 3.77 (t, α -CH)
Acetate	1.92 (s, β -CH ₃)
Proline	2.03 (m, 3-CH ₂ /4-CH ₂), 3.35 (dt, 2-CH ₂)
Glutamate	2.05 (dt, β -CH ₂), 2.13 (m, β' -CH ₂), 2.36 (m, γ -CH ₂), 3.77 (t, α -CH)
Methionine	2.13 (m, β -CH ₂ / ϵ -CH ₃), 2.65 (t, γ -CH ₂), 3.83 (dd, α -CH)
Glutamine ^a	2.14 (m, β -CH ₂), 2.46 (m, γ -CH ₂), 3.77 (t, α -CH)
Acetone	2.24 (s, α -CH ₃)
Pyruvate	2.39 (s, CH ₃)
Succinate	2.41 (s, α -CH ₂ / β -CH ₂)
Citrate	2.52 (d, α -CH/ β -CH), 2.67 (d, α' -CH/ β' -CH)
Aspartate	2.70 (dd, β -CH), 2.82 (dd, β' -CH), 3.90 (dd, α -CH)
Creatine	3.04 (s, N-CH ₃), 3.93 (s, N-CH ₂)
Phosphocreatine	3.06 (s, CH ₃), 3.94 (s, CH ₂)
Ethanolamine	3.15 (t, CH ₂ -NH ₂), 3.83 (t, CH ₂ -OH)
Choline	3.21 (s, N(CH ₃) ₃), 3.53 (m, β -CH ₂ -N), 4.07 (m, α -CH ₂ -OH)
Phosphocholine	3.22 (s, N(CH ₃) ₃), 3.60 (m, N-CH ₂), 4.17 (m, PO ₃ -CH ₂)
Glycerophosphocholine	3.23 (s, N(CH ₃) ₃), 3.68 (m, β' -CH ₂ -N(CH ₃) ₃), 4.33 (m, α' -CH ₂ - PO ₄ ⁻)
Taurine	3.26 (t, CH ₂ -SO ₃), 3.42 (t, NH ₂ -CH ₂)
myo-inositol ^b	3.28 (t, 5-CH), 3.53 (dd, 1-CH/3-CH), 3.63 (t, 4-CH/6-CH), 4.07 (t, 2-CH)
scyllo-inositol	3.36 (s, CH)
Glycerol	3.55 (dd, 1-CH ₂ /3-CH ₂), 3.63 (dd, 1-CH ₂ /3-CH ₂)
Glycine	3.56 (s, α -CH ₂)
Serine	3.84 (dd, α -CH), 3.95 (dd, β -CH ₂), 3.99 (dd, β' -CH ₂)
Uridine	4.23 (t, 3'-CH ribose), 4.36 (t, 2'-CH ribose), 5.89 (d, 1'-CH ribose), 5.90 (d, 5-CH ring), 7.86 (d, 6-CH ring)
Adenosine/Inosine	4.28 (q, 4'-CH ribose), 4.44 (dd, 3'-CH ribose), 6.10 (d, 1'-CH ribose), 8.24 (s, 2-CH ring), 8.35 (s, 8-CH ring)
β -Glucose	4.65 (d, 1-CH)
α -Glucose	5.24 (d, 1-CH)
Uracil	5.81 (d, 5-CH ring), 7.52 (d, 6-CH ring)
Fumarate	6.52 (s, HC=CH)
Tyrosine	6.91 (d, 3-CH/5-H ring), 7.20 (d, 2-CH/6-H ring)
Histidine	7.08 (s, 4-CH ring), 7.85 (s, 2-CH)
Phenylalanine	7.33 (m, 2-CH/6-CH ring), 7.39 (m, 4-CH ring), 7.43 (m, 3-CH/5-CH ring)
Hypoxanthine	8.20 (s, 2-CH ring), 8.22 (s, 8-CH)
Formate	8.46 (s, HO- <u>HC</u> =O)
<u>Lipophilic compounds</u>	
Total 7-lathosterol	0.55 (18-CH ₃ , s)
Total cholesterol	0.68 (18-CH ₃ , s), 0.86 (26-CH ₃ , d), 0.87 (27-CH ₃ , d), 0.91 (21-CH ₃ , d), 1.12 (multiple cholesterol protons, m), 1.48 (multiple cholesterol protons, m), 1.84 (multiple cholesterol protons, m), 1.96 (7-CH ₂ /8-CH, br)
Fatty acids	0.88 (CH ₃ (CH ₂) _n , t), 1.25 ((CH ₂) _n , m), 1.30 (=CH-CH ₂ -CH ₂ (CH ₂)-, m), 1.64 (-CH ₂ -CH ₂ -CO-, m), 2.10 (-CH ₂ -CH=CH-, m), 2.30 (-CH ₂ -CO, m), 5.35 (-HC=CH-, m)
Free cholesterol	1.01 (19-CH ₃ , s), 3.53 (3-CH, m)

Esterified cholesterol	1.02 (19-CH ₃ , s), 4.61 (3-CH, m)
Oleic acid (18:1, ω-9)	2.01 (-CH ₂ -CH ₂ -CH=, m)
Linoleic acid (18:2, ω-6)	2.05 (-CH ₂ -CH ₂ -CH=, m), 2.77 (=CH-CH ₂ -CH=, t)
Arachidonic acid (20:4, ω-6)	2.05 (-CH ₂ -CH ₂ -CH=, m), 2.82 (=CH-CH ₂ -CH=, m)
Docosahexaenoic acid (22:6, ω-3)	2.82 (=CH-CH ₂ -CH=, m)
Phosphatidylethanolamine	3.14 (-CH ₂ -CH ₂ -NH ₂ , br)
Sphingomyelin	3.30 (-N ⁺ (CH ₃) ₃ , s), 3.77 (N-CH ₂ , br), 5.68 (-CH ₂ -CH=CH-CHOH-, m)
Phosphatidylcholine	3.33 (-N ⁺ (CH ₃) ₃ , s), 3.77 (N-CH ₂ , br)
Glycerophospholipids	3.95 (3-CH ₂ of glycerol, m), 4.37 (PO-(1-CH ₂) of glycerol, m), 5.21 (2-CH of glycerol, m)
Triglycerides	4.14 (1-CH ₂ /3-CH ₂ of glycerol, dd), 4.29 (1'-CH ₂ /3'-CH ₂ of glycerol, dd), 5.26 (2-CH of glycerol, m)
Plasmalogen	5.90 (O-CH=CH, d)

^a observed more clearly in C7-2-HI tumours; ^b tentative assignment, as identification is hindered by signal overlap particularly in 59-2-HI tumours.