Targeted UPLC-MS Metabolic Analysis of Human Faeces Reveals Novel Low-Invasive Candidate Markers for Colorectal Cancer

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Supplementary Materials

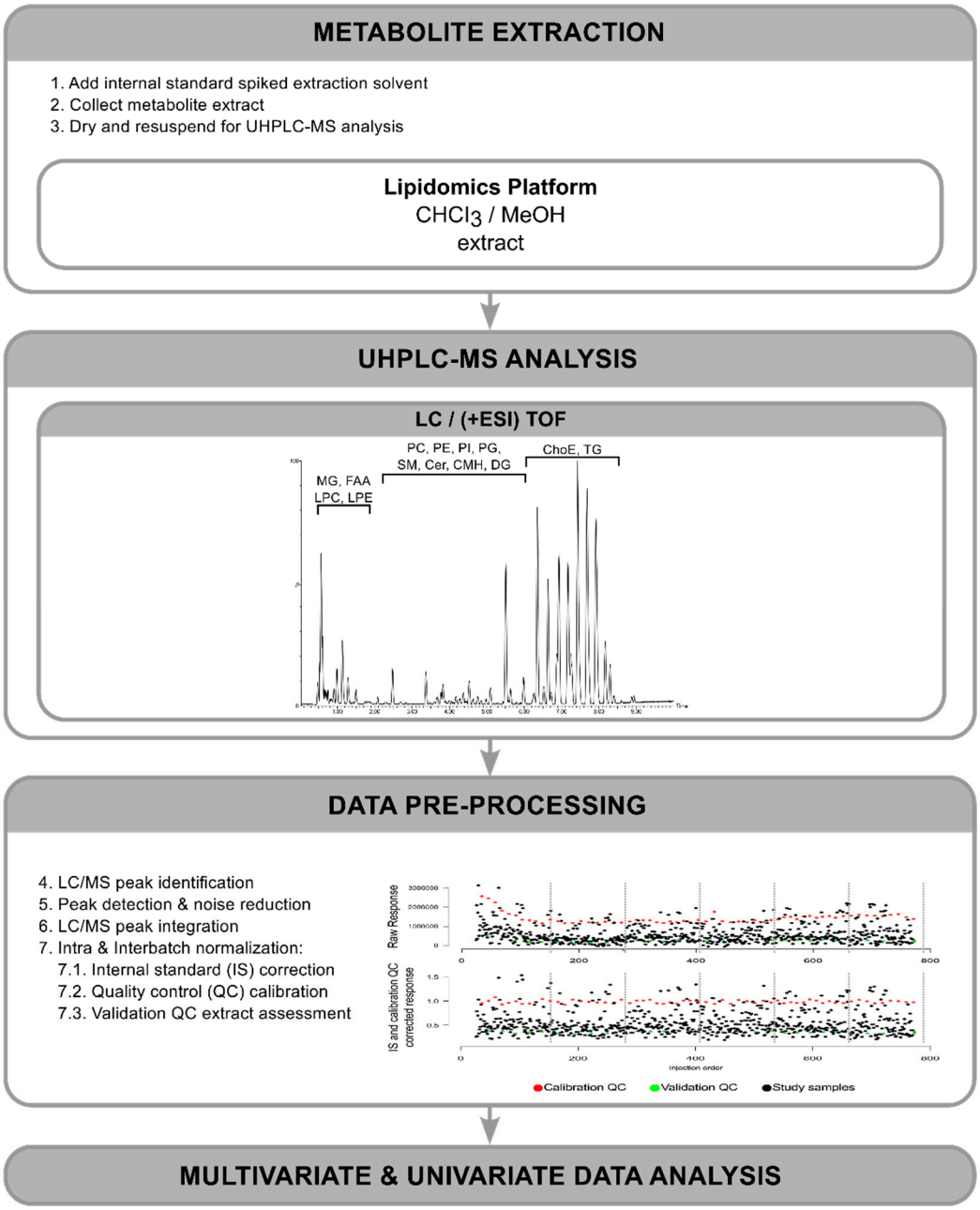

Figure S1. Workflow of the UPLC-MS-based targeted metabolomic profiling.

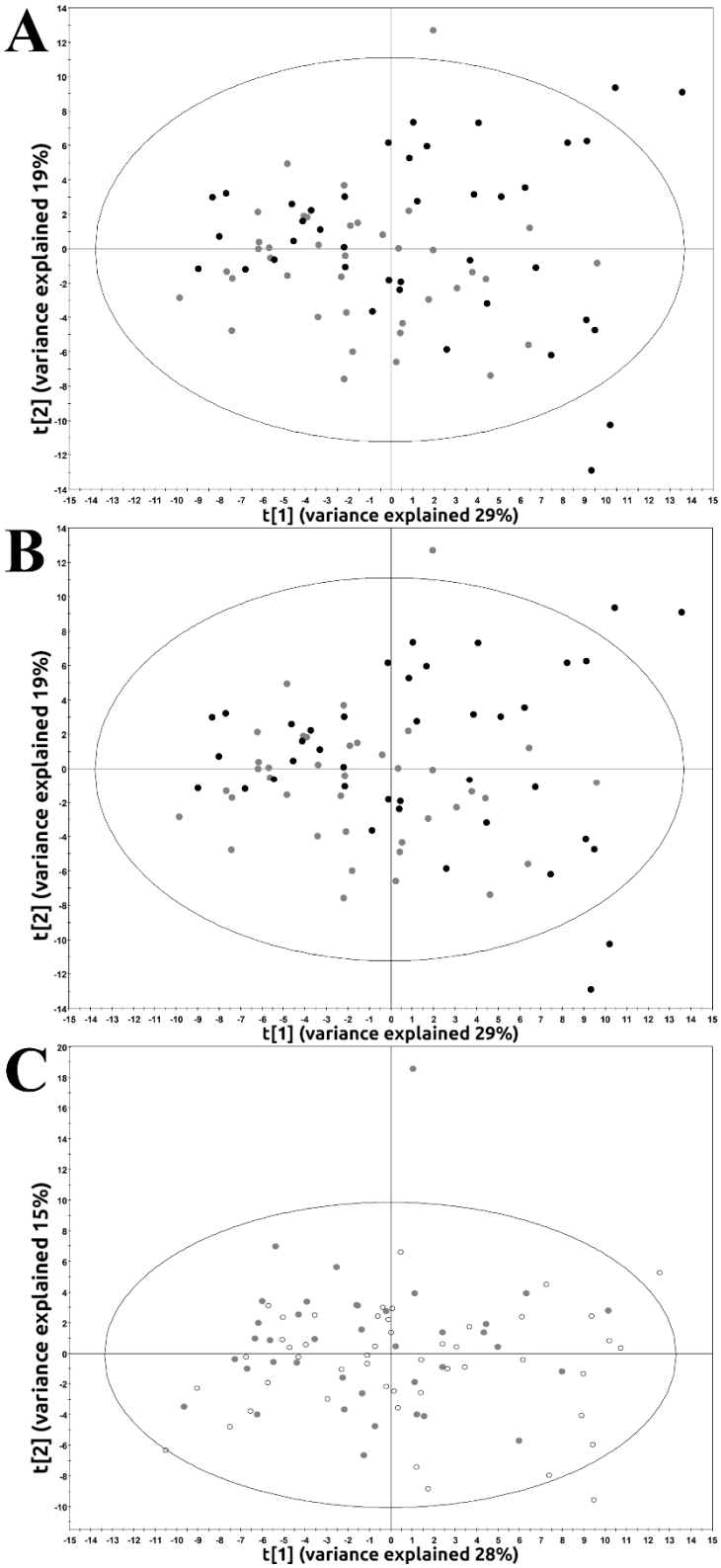

Figure S2. Multivariate analysis of paired group. (**A**) CRC vs. AD: R2X = 0.29 and Q2 = 0.24 t[2]: R2X = 0.19 and Q2 = 0.22). Black CRC, grey AD. (**B**) CRC vs. control: R2X = 0.30 and Q2 = 0.25, t[2]: R2X = 0.19 and Q2 = 0.24). Black CRC, white healthy. (**C**) AD vs. control: R2X = 0.28 and Q2 = 0.24, t[2]: R2X = 0.15 and Q2 = 0.15. Grey AD, white healthy.

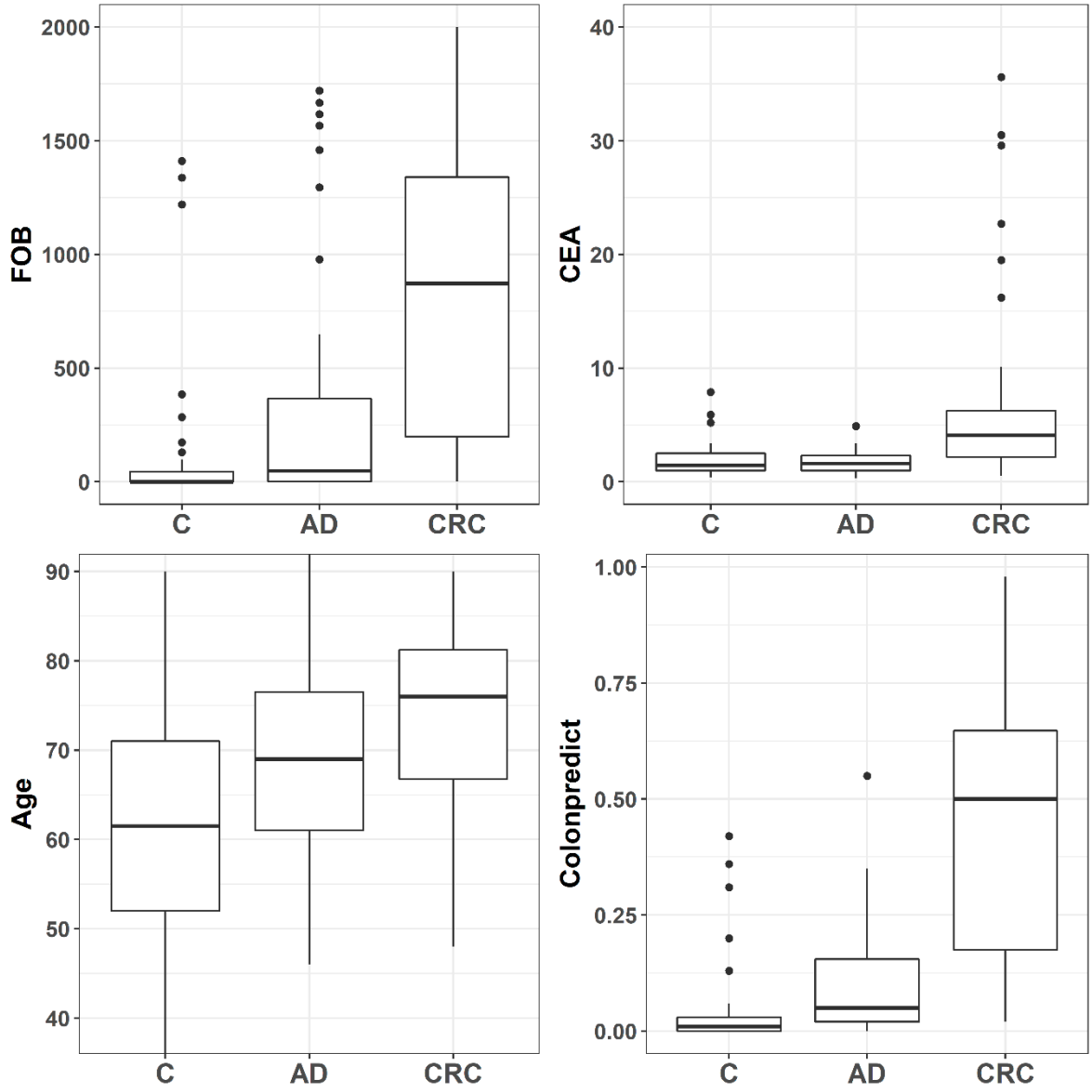

Figure S3. Boxplot representation of the clinical parameters distribution on the distinct groups of samples (C, AD and CRC).

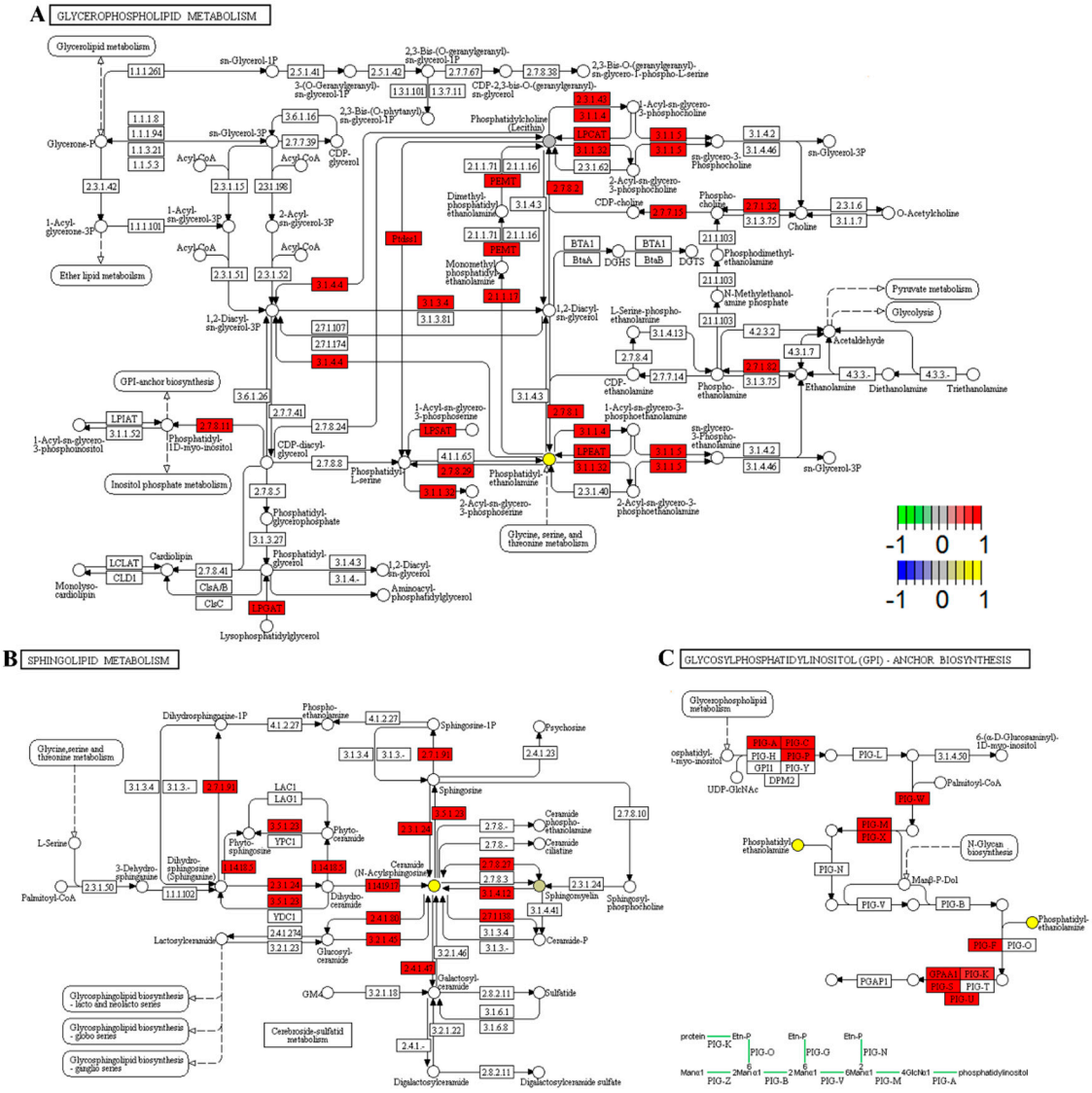

Figure S4. Mapping of altered genes and metabolites into the three metabolic pathways identified: sphingolipid metabolism (**A**), glycerophospholipid metabolism (**B**) and glycosylphosphatidylinositol (GPI)-anchor biosynthesis (**C**). Genes detected are coloured in a range green-red, depending on the Fold Change and metabolites in a range blue-yellow.

Table S2: Metabolites differentially expressed between control, AD and CRC groups (ANOVA test).

Family	Metabolite	*p*-Value
Cer	Cer (42:3)	0.3×10^{-5}
	Cer (d18:1/16:0)	0.015
	Cer (d18:1/24:1) + Cer(d18:2/24:0)	0.008
ChoE	ChoE (16:0)	0.001
	ChoE (18:2)	0.3×10^{-7}
	ChoE (20:4)	0.7×10^{-7}
DG	DG (32:1)	0.042
PC	PC (16:0/16:0)	0.002
	PC (16:0/18:0)	0.003
	PC (16:0/18:1)	0.026
	PC (18:0/18:1)	0.006
	PC (18:0/20:4)	0.016
	PC (32:1)	0.005
	PC (36:3)	0.028
	PC-O (16:0/16:0)	0.1×10^{-3}
	PC-O (34:1)	0.034
	PC-P (16:0/20:3)	0.008
PE	PE (16:0/18:1)	0.003
	PE (16:0/18:2)	0.037
SM	SM (42:1)	0.2×10^{-3}
	SM (42:3)	0.1×10^{-5}
	SM (d18:1/16:0)	0.8×10^{-4}
	SM (d18:1/18:0)	0.027
	SM (d18:1/22:0)	0.005
	SM (d18:1/23:0)	0.2×10^{-3}
	SM (d18:1/24:1) + SM (d18:2/24:0)	0.4×10^{-5}
TG	TG (49:1)	0.032
	TG (51:2)	0.046