The distinctive serum metabolomes of gastric, esophageal and colorectal cancers

Supplementary File

Table S1. Differential metabolites (EC *vs.*non-EC) for esophageal cancer

Metabolite [48]	Metabolite [49]	Metabolite [50]	Metabolite *
Glucose↓			
Pyruvic acid↑			
Lactate↑			
Citrate↑			
A-ketoglutaric acid ↑			
Succinate↓			
Fumarate↑			
Malate↑			
Valine↓			
Histidine↑		Histidine↓	
Phenylalanine↓			
Threonine↓			
Leucine↓			
Methionine↓		Methionine↓	
Tryptophan↓	Tryptophan↓	Tryptophan↓	Tryptophan↓
Glutamine↑			
Glutamate↓			
Serine↓			
Glycine↓			
Alanine↓		Alanine↓	
Arginine↓			
Aspartate↑			
Cystine↑			
Proline↓		Proline↓	
Isoleucine↓			
Lysine↑			
Tyrosine↑	Tyrosine↓	Tyrosine↓	Tyrosine↓
Linoleic acid↓	Linoleic acid		Linoleic acid↑
Oleic acid↑		Oleic acid↑	Oleic acid↑
	Palmitoleic acid↑	Palmitoleic acid↑	Palmitoleic acid↑
	Choline↓		
Hypoxanthine↑	Hypoxanthine↓		
	Proline betaine↓		
	Indoleacrylic acid ↓		
	Isovaleryl-carnitine↓	Isovaleryl-carnitine↓	
	Inosine ↓		

	Alpha-Linolenic acid ↑ Piperine ↓ L-Octanoyl-carnitine ↓ Nonanoyl-carnitine ↓ Decadienoyl-carnitine ↓ Decanoylcarnitine↓ Docosahexaenoic acid ↓ Undecanoyl-carnitine ↓ Dodecenoyl-carnitine ↓ Phenylalanyl-Tryptophan ↓ Tetracosahexae-noic acid↓ Cortisol ↓ Tetradecadien-carnitine ↓	Piperine ↓	
Asparagine↓ Pyroglutamine↓ Ribose↓ Taurine↑ Cis-Aconitic acid↑ Hydroxyproline↓ Ornithine↓ Kynurenic acid↓ Creatinine↓ Urea↓ Urate↓ Monostearin↓ Pipecolic acid↓		3-hydroxy-butyrate↑ Asparagine↓ Glycochenodeoxycholate↓ Glycocholate↓ Glycodeoxycholate↓ Hippurate↓ Mannose↑ Propionylcarnitine↓ Pyroglutamine↑ Threitol↓ 10-heptadecenoate (17:1n7)↑	Cortisol↑

Glyceric acid↓		
		10-nonadece-noate(19:1n9)↑ 1-linoleoylglycero-phosphocholine↓ 1-linoleoylglycero-phosphoethanolamine↓ 1-myristoylglycero-phosphocholine↓ 1-oleoylglycerophos-phoethanolamine↓ 1-palmitoylglycero-phosphoethanolamine↓ 1-stearoylglycero-phosphoethanolamine↓ 2-hydroxydecanoic acid↓ 2-methylbutyrylcarnitine (C5)↓ 3-hydroxypropanoate↓ 3-methyl-2-oxobutyrate↑ 5-dodecenoate (12:1n7)↑ adrenate (22:4n6)↑ beta-alanine↓ catechol sulfate↓ creatine↓ deoxycarnitine↓ dihomo-linoleate (20:2n6)↑ docosadienoate (22:2n6)↑ docosapentaenoate (n3 DPA; 22:5n3)↑ docosapentaenoate (n6 DPA; 22:5n6)↑ eicosenoate (20:1n9 or 11)↑ ergothioneine↓ gamma-glutamylmethionine↓ gamma-glutamylphenylalanine↓ gamma-glutamyltyrosine↓ hexadecanedioate↑ indolelactate↓ indolepropionate↓ margarate (17:0)↑

	myristate (14:0)↑ myristoleate (14:1n5)↑ N6-acetyllysine↓ O-methylcatechol sulfate↓ palmitate (16:0)↑ paraxanthine↓ pentadecanoate (15:0)↑ propionylcarnitine↓ ribulose↓ scyllo-inositol↓ stachydrine↓ stearate (18:0)↑ xylonate↓	
		Dodecanoic acid↓ Palmitic acid↑ LPA(18:1/0:0)↓ LysoPC(14:0/0:0)↓ LysoPC(18:2)↑ LysoPC(24:0)↑ LysoPC(18:4)↑ PC(14:1/P-18:1)↑ PC(16:0/18:2)↓ PC(24:1/22:6)↑

The arrows indicate reported increasing or decreasing trends relative to non-GC controls.

Table S2. Differential metabolites (CRC *vs.* non-CRC) for colorectal cancer.

Metabolite [44] N=24	Metabolite [51]	Metabolite [52]	Metabolite [55]	Metabolite [53]	Metabolite [54]
Glutamic acid			Glutamic acid↓	Glutamic acid	Glutamic acid↓
Phenylalanine		Phenylalanine		Phenylalanine	Phenylalanine↓
Alanine	Alanine	Alanine		Alanine	Alanine
Isoleucine	Isoleucine	Isoleucine			Isoleucine↑
Histidine				Histidine	
Serine					Serine↓
Lactic acid	Lactic acid	Lactic acid	Lactic acid↓		Lactic acid↑
Aspartic acid			Aspartic acid↓		
Succinate				Succinate	
Cysteine		Cysteine		Cysteine	Cysteine↓
Glutamine				Glutamine	
Leucine				Leucine	Leucine↓
Valine				Valine	Valine↓
Choline			Choline↓	Choline	
Fumaric acid			Fumaric acid		Fumaric acid↑
Tyrosine		Tyrosine		Tyrosine	Tyrosine↓
Asparagine				Asparagine	
Pyruvic acid			Pyruvic acid↑		Pyruvic acid↑
Arginine				Arginine	
Methionine				Methionine	
Tryptophan	Tryptophan			Tryptophan	Tryptophan↓
Acetoacetate					
Uracil					
Urea	Urea				Urea↓
Creatinine					Creatinine↑
Homovanillate				Homovanillate	
Guanidoacetate					
Putrescine					
	2,3-Butanediol				
	2-Amino-butanoic acid			2-Amino-butanoic acid	
	2-Hydroxy-butyricacid			2-Hydroxy-butyric acid	2-Hydroxy-butyric acid↑
	3-Hydroxy-butyric acid			3-Hydroxy-butyric acid	3-hydroxy-butyric acid↑
	3-Hydroxy-pyridine				
	Butanoic acid	Butanoic acid			
	D-Fructose	Fructose			Fructose↑
	D-Glucose		Glucose↑		Glucose↓
	D-Mannose		Mannose↑		

	Glycine Proline Uric acid	Glycine			Glycine↓ Proline↑ Uric acid↓
		Ethylene glycol Stearic acid Citric acid Lysine Inositol Glyceric acid Palmitic acid Linoleic acid 2-Monostearoyl-glycerol Threonine Glycerol-3-phosphate Glyceryl palmitate Hexadecanoic acid D-Ribose 5-phosphate Glycerol Nonane Malonic acid Arabinose Threonic acid	Glyceric acid↓ Linoleic acid↑ 2-Monostearoyl-glycerol↓ Glyceryl palmitate Malonic acid↓ Hypoxanthine↓ Xanthine↓ Tryptophyl-glutamate↓ 3-methyl-2-oxobutyrate↑ 5-oxoproline↓ Pseudouridine↑ Hydroxyiso-valeroyl carnitine↓ Kynurenine↑ cis-4-decenoyl carnitine↑ Decanoyl-carnitine↑ γ-glutamylalanine↑	Uric acid Lysine D-Ribose 5-phosphate Glycerol Threonic acid Hypoxanthine Hydroxyiso-valeroyl carnitine↓	Citric acid↑ Lysine↓ Inositol↑ Threonine↓ Arabinose↑ Kynurenine

	Heptanoate (7:0)↓ Aspartylleucine↓ 1-stearoylglycero-phosphoethanolamine↓ Theobromine↓ 1-palmitoylplasm-enylethanolamine↓ 2-hydroxypalmitate↑ Phenylalanyl-glutamate↓ Leucylalanine↑ 1-oleoylglycero-phosphocholine↓ cysteine-glutathione disulfide↑ Paraxanthine↓ N-acetylglycine↑ Phenylalanylserine↑ glycolate ↓ Octanoylcarnitine↑ Sucrose↑ 2-hydroxystearate↑ Theophylline↓ Ornithine↓ 3-dehydrocarnitine↓ Benzoate↓ Linolenate ↑ Uridine↓ Isovalerate↓	Heptanoate (7:0)↓ Ornithine Benzoate Isovalerate Octanoic acid Decanoic acid Gluconolacton e Gluconic acid 5-Amino-4-oxovaleric acid Inosine 1-Methylnico-tinamide Myristoleic acid Stachydrine Isobutyryl-carnitine	Glycolate↑ Sucrose↑ Ornithine↑ Isovalerate↓ Octanoic acid↑

		Hydroxyproline 3-Methyl-histidine Perillic acid 2-oxovaleric acid Ethylglutamine Trimethylamine N-oxide S-Methyl-cysteine Cholic acid Ethanolamine phosphate Cysteine glutathione disulfide Quinic acid Indole-3-acetic acid Sarcosine B-alanine Isobutyric acid Betaine Lauric acid Ethanolamine Citrulline	hydroxyproline↑ Sarcosine↓ 2-aminoiso-butyric acid↓ 2-amino-butyric acid↓ 3-hydroxy-isovaleric acid↓ Phosphoric acid↑ Nonanoic acid↓ Threitol↑ meso-erythritol↑ 2-ketoglutaric acid↑ Xylose↑ Arabitol↑ Isocitric acid↑ 2-aminopimelic acid↑

		1,5-anhydro-glucitol↓ Sorbose↑ 5-dehydroquinic acid↓ Hippuric acid↓ Galactose↓ Glucosamine↓ Glucuronic acid↑ Ascorbic acid↓ Palmitoleic acid↓ Elaidic acid↓ Maltose↑ Malic acid↑

The arrows indicate reported increasing or decreasing trends relative to non-GC controls.