

Supplementary Table 2

Supplementary Table 2. Rice bran food metabolites identified in plasma and/or urine of the colorectal cancer (CRC) survivors

Chemical class	Metabolomic pathway	Metabolite	Platform	HMDB ID	Abundance in rice bran	Detected in Plasma	Detected in Urine
Amino Acid	Alanine and Aspartate Metabolism	Alanine	LC/MS Pos	HMDB00161	154,873,584	x	x
		Asparagine	LC/MS Pos	HMDB00168	854,978,432		x
		N-acetylaspartate (NAA)	LC/MS Polar	HMDB00812	721,415		x
	Creatine Metabolism	Creatine	LC/MS Pos	HMDB00064	691,673	x	
	Glutamate Metabolism	gamma-aminobutyrate (GABA)	LC/MS Pos	HMDB00112	199,834,048		x
		Glutamine	LC/MS Pos	HMDB00641	176,320,032		x
	Glutathione Metabolism	5-oxoproline	LC/MS Neg	HMDB00267	13,207,618		x
	Glycine, Serine and Threonine Metabolism	Betaine	LC/MS Pos	HMDB00043	304,460,288	x	x
		N-acetylserine	LC/MS Pos	HMDB02931	156,770		x
		Serine	LC/MS Pos	HMDB00187	85,386,120	x	x
	Histidine Metabolism	4-imidazoleacetate	LC/MS Pos	HMDB02024	3,308,998		x
		Histamine	LC/MS Pos	HMDB00870	984,420		x
		Imidazole propionate	LC/MS Pos	HMDB02271	538,374		x
		N-acetylhistidine	LC/MS Pos	HMDB32055	10,576,467	x	
	Leucine, Isoleucine and Valine Metabolism	3-methyl-2-oxovalerate	LC/MS Neg	HMDB03736	278,537	x	x
		Allo-isoleucine	GC/MS		87,141	x	
		Isobutrylglycine	LC/MS Neg	HMDB00730	220,797		x
		Isovaleryl glycine	LC/MS Neg	HMDB00678	258,226		x
		N-acetyl isoleucine	LC/MS Neg		132,477		x
		N-acetyl valine	LC/MS Neg	HMDB11757	221,255		x
	Lysine Metabolism	Glutarate (pentanedioate)	LC/MS Polar	HMDB00661	551,722	x	x
		Pipecolate	LC/MS Pos	HMDB00070	20,772,442	x	
	Methionine, Cysteine, SAM and Taurine Metabolism	Cystathionine	LC/MS Pos	HMDB00099	1,283,956		x
		Cysteine	GC/MS	HMDB00574	65,957		x
		Methionine	LC/MS Pos	HMDB00696	43,163,732		x
		N-acetyltaurine	LC/MS Neg		437,749		x
		S-adenosylhomocysteine (SAH)	LC/MS Pos	HMDB00939	2,438,966		x
		3-(4-hydroxyphenyl)lactate	LC/MS Neg	HMDB00755	422,103		x
	Phenylalanine and Tyrosine Metabolism	3-(4-hydroxyphenyl)propionate	LC/MS Neg	HMDB02199	91,241	x	
		Gentisate	LC/MS Neg	HMDB00152	335,627	x	
		N-formylphenylalanine	LC/MS Neg		295,357		x
		Phenylalanine	LC/MS Pos	HMDB00159	146,600,208		x
		Phenyllactate (PLA)	LC/MS Neg	HMDB00779	340,857		x
		N-acetylputrescine	LC/MS Pos	HMDB02064	1,170,238	x	
	Polyamine Metabolism	Spermidine	LC/MS Pos	HMDB01257	4,807,387		x
		Kynurenate	LC/MS Neg	HMDB00715	322,359		x
	Tryptophan Metabolism	Xanthurenate	LC/MS Pos	HMDB00881	328,114		x
	Urea cycle; Arginine and Proline Metabolism	N2,N5-diacetylornithine	LC/MS Neg		30,663		x
		N-delta-acetylornithine	LC/MS Pos		3,704,738	x	x
Carbohydrate	Advanced Glycation End-product	N6-carboxymethyllysine	LC/MS Pos		942,803		x
	Fructose, Mannose and Galactose Metabolism	Mannose	LC/MS Polar	HMDB00169	613,608	x	
	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	Lactate	LC/MS Polar	HMDB00190	1,094,495		x
	Pentose Metabolism	Arabinose	GC/MS	HMDB00646	274,619	x	
		Ribonate	LC/MS Polar	HMDB00867	15,624,751		x
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	Nicotinate	LC/MS Pos	HMDB01488	14,799,785		x
	Pterin Metabolism	Pterin	LC/MS Pos	HMDB00802	295,000		x
	Tocopherol Metabolism	delta-tocopherol	GC/MS	HMDB02902	3,352	x	

Chemical class	Metabolomic pathway	Metabolite	Platform	HMDB ID	Abundance in rice bran	Detected in Plasma	Detected in Urine
Lipid	Endocannabinoid	Palmitoyl ethanolamide	LC/MS Neg	HMDB02100	1,690,296	x	
	Fatty Acid Metabolism (Acyl Glycine)	Hexanoylglycine	LC/MS Neg	HMDB00701	68,323		x
	Fatty Acid, Amino	2-aminoheptanoate	LC/MS Pos		192,392	x	
	Fatty Acid, Branched	17-methylstearate	LC/MS Neg		177,665	x	
	Fatty Acid, Dicarboxylate	3-methyladipate	LC/MS Neg	HMDB00555	853,830	x	x
		Dimethylmalonic acid	LC/MS Polar	HMDB02001	307,964		x
	Fatty Acid, Monohydroxy	13-HODE + 9-HODE	LC/MS Neg		7,082,311,680	x	
		2-hydroxydecanoate	LC/MS Neg		1,503,139	x	
		2-hydroxyoctanoate	LC/MS Neg	HMDB02264	216,494	x	
		2-hydroxypalmitate	LC/MS Neg	HMDB31057	2,900,843	x	
		2-hydroxystearate	LC/MS Neg		1,403,719	x	
		3-hydroxyoctanoate	LC/MS Neg	HMDB01954	421,384	x	
		3-hydroxysuberate	LC/MS Neg	HMDB00325	405,010		x
	Ketone Bodies	3-hydroxybutyrate (BHBA)	LC/MS Polar	HMDB00357	121,979		x
	Long Chain Fatty Acid	Arachidate (20:0)	LC/MS Neg	HMDB02212	146,200,672	x	
		Eicosenoate (20:1n9 or 11)	LC/MS Neg	HMDB02231	153,264,032	x	
		Margarate (17:0)	LC/MS Neg	HMDB02259	24,053,634	x	
		Nonadecanoate (19:0)	LC/MS Neg	HMDB00772	7,285,277	x	
		Pentadecanoate (15:0)	LC/MS Neg	HMDB00826	26,355,804	x	
		Stearate (18:0)	LC/MS Neg	HMDB00827	777,727,808	x	
	Mevalonate Metabolism	3-hydroxy-3-methylglutarate	LC/MS Polar	HMDB00355	16,946,286	x	
	Phospholipid Metabolism	Choline	LC/MS Pos	HMDB00097	722,152,256	x	
		Glycerophosphoethanolamine	LC/MS Polar	HMDB00114	1,438,771		x
	Polyunsaturated Fatty Acid (n3 and n6)	Docosadienoate (22:2n6)	LC/MS Neg	HMDB61714	470,588	x	
		Eicosapentaenoate (20:5n3)	LC/MS Neg	HMDB01999	198,955	x	
	Secondary Bile Acid Metabolism	Deoxycholate	LC/MS Neg	HMDB00626	1,585,013	x	
	Sterol	4-cholesten-3-one	GC/MS	HMDB00921	76,873	x	
Nucleotide	Purine Metabolism, (Hypo)Xanthine/ Inosine containing	Urate	LC/MS Neg	HMDB00289	700,134		x
		Xanthine	LC/MS Pos	HMDB00292	2,351,023		x
		Xanthosine	LC/MS Pos	HMDB00299	684,372		x
	Purine Metabolism, Adenine containing	N6-carbamoylthreonyladenosine	LC/MS Pos	HMDB41623	314,320		x
	Purine Metabolism, Guanine containing	2'-deoxyguanosine	LC/MS Pos	HMDB00085	1,834,256		x
		7-methylguanine	LC/MS Neg	HMDB00897	35,726	x	x
		Guanosine	LC/MS Pos	HMDB00133	13,375,566	x	x
		N1-methylguanosine	LC/MS Pos	HMDB01563	226,924	x	x
		N2,N2-dimethylguanosine	LC/MS Pos	HMDB04824	86,624	x	
	Pyrimidine Metabolism, Cytidine containing	Cytidine	LC/MS Pos	HMDB00089	8,561,558		x
	Pyrimidine Metabolism, Uracil containing	4-ureidobutyrate	LC/MS Pos		1,333,347		x
		N-acetyl-beta-alanine	LC/MS Pos		894,407		x
		Pseudouridine	LC/MS Pos	HMDB00767	3,217,247		x
		Uracil	LC/MS Neg	HMDB00300	351,026		x
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamyl-2-aminobutyrate	LC/MS Pos		1,425,246	x	
		gamma-glutamylglutamine	LC/MS Pos	HMDB11738	3,280,159		x
		gamma-glutamylthreonine	LC/MS Pos	HMDB29159	176,494	x	
Xenobiotics	Benzoate Metabolism	4-hydroxybenzoate	LC/MS Neg	HMDB00500	1,439,840		x
		4-hydroxyhippurate	LC/MS Neg	HMDB13678	875,735		x
		Benzoate	LC/MS Neg	HMDB01870	5,354,217	x	
	Chemical	O-sulfo-L-tyrosine	LC/MS Neg		484,287		x
	Drug	Salicylate	LC/MS Neg	HMDB01895	8,155,134		x
		2-piperidinone	LC/MS Pos		43,266,232	x	x
	Food Component/Plant	3-hydroxyindolin-2-one	LC/MS Pos		284,873		x
		Erythritol	LC/MS Polar	HMDB02994	285,837		x
		Fucitol	LC/MS Polar		409,752		x
		Quinate	LC/MS Polar	HMDB03072	10,826,823		x
		Syringic acid	LC/MS Neg	HMDB02085	393,784		x
		Tartarate	LC/MS Neg	HMDB00956	379,787	x	x

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