

Table S1. Total number of compounds reported as potential biomarkers of CRC, where: ↑ – concentration elevated in comparison of healthy controls; ↓ – concentration decreased in comparison of healthy controls; _{post} – index regarding postoperative samples; ^m – index regarding only male samples; no arrows – changes of concentration of compound not mentioned by authors; GC-MS – gas chromatography-mass spectrometry; dHS-SPME-GC-qMS – dynamic headspace solid-phase microextraction gas chromatography-quadrupole mass spectrometry; HS-SPME-GC-MS – headspace solid-phase microextraction gas chromatography-mass spectrometry; TD-GC-MS – thermal desorption gas chromatography-mass spectrometry; GC-FID – gas chromatography-flame ionization detector; GC-TOFMS – gas chromatography-time-of-flight mass spectrometry; U – urine; F – feces; Br – breath.

Compound	Matrix			Method	Reference
	Breath	Feces	Urine		
ALCOHOLS, POLYOLS AND PHENOLS					
1-octanol			U↓	dHS-SPME-GC-qMS	[Silva et al 2011]
hexen-1-ol			U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
2-propanol		F↑		HS-SPME-GC-MS	[Bond et al 2019]
4-ethyl-1-octyn-3-ol	Br↑			HS-SPME-GC-MS	[Wang et al 2014]
			U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
			U↑	solvent extraction GC-MS	[Qiu et al 2010]
4-methylphenol (<i>p</i> -cresol)		U _{post}		solvent extraction GC-MS	[Qiu et al 2010]
			U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
			U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
5-methyl-2-propan-2-yl-cyclohexan-1-ol		F↓		HS-SPME-GC-MS	[Bond et al 2019]
cyclooctylmethanol	Br↑			HS-SPME-GC-MS	[Wang et al 2014]
ethanol	Br↓			TD-GC-MS	[Amal et al 2016]
glycerol (glycerin)		F↓		solvent extraction GC-MS	[Weir et al 2013]
		F↓		solvent extraction GC-MS	[Wang et al 2017]
monoacyl glycerol		F↓		solvent extraction GC-MS	[Wang et al 2017]
monooleoylglycerol		F↓		solvent extraction GC-MS	[Weir et al 2013]
phenol		U↓		solvent extraction GC-TOFMS	[Cheng et al 2012]
guaiacol		U↓		solvent extraction GC-MS	[Liesenfeld et al 2015]
hydroquinone (benzene-1,4-diol)		U↓		solvent extraction GC-MS	[Liesenfeld et al 2015]
trans-2-dodecen-1-ol	Br↑			HS-SPME-GC-MS	[Wang et al 2014]
2,3-butanediol		U↓		solvent extraction GC-MS	[Liesenfeld et al 2015]
pyrogallol		U↓		solvent extraction GC-MS	[Liesenfeld et al 2015]
ALDEHYDES					
acetaldehyde		U		in-tube extraction-GC-MS	[Arasaradnam et al 2014]
2-methyl-3-phenyl-2-propenal		U↑		dHS-SPME-GC-qMS	[Silva et al 2011]
decanal	Br↑			TD-GC-MS	[Altomare et al 2013]

	Br↑	TD-GC-MS	[Altomare et al 2015]
heptanal	U↓	dHS-SPME-GC-qMS	[Silva et al 2011]
hexanal	U↓	dHS-SPME-GC-qMS	[Silva et al 2011]
	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
nonanal	Br↑	TD-GC-MS	[Altomare et al 2013]
	Br↑	TD-GC-MS	[Altomare et al 2015]
KETONES			
2-hexanone	F↑	HS-SPME-GC-MS	[Bond et al 2019]
3-heptanone	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
4-heptanone	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
2,4-dimethyl-3-pentanone	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
4-methyl-2-pentanone	Br↑	TD-GC-MS	[Altomare et al 2013]
	Br↑	TD-GC-MS	[Altomare et al 2015]
2-pentanone	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
acetone	Br↑	TD-GC-MS	[Amal et al 2016]
3-methyl-2-butaneone	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
cyclohexanone	Br↑	HS-SPME-GC-MS	[Wang et al 2014]
2,3-butanedione	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
ESTERS			
3-hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	Br↑	HS-SPME-GC-MS	[Wang et al 2014]
4-(4-propylcyclohexyl)-4'-cyano[1,1'-biphenyl]-4-yl ester benzoic acid	Br↓	HS-SPME-GC-MS	[Peng et al 2010]
ethyl 3-methylbutanoate	F↑	HS-SPME-GC-MS	[Bond et al 2019]
ethyl acetate	Br↑	TD-GC-MS	[Amal et al 2016]
phenyl acetate	U↑	solvent extraction GC-MS	[Qiu et al 2010]
	U↓ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
propan-2-yl butanoate	F↑	HS-SPME-GC-MS	[Bond et al 2019]
propan-2-yl pentanoate	F↑	HS-SPME-GC-MS	[Bond et al 2019]
propan-2-yl propanoate	F↑	HS-SPME-GC-MS	[Bond et al 2019]
pentyl ethylbenzoate (ethylbenzoic acid, pentyl ester)	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
methyl carbamate (carbamic acid, methyl ester)	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
3-indoxylsulfate	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
5-hydroxyindole acetate	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
ETHERS			
ethylene oxide	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
anisole	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
oxepane	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
HYDROCARBONS			
methane	Br	direct gas sampling GC	[Haines et al 1977]
	Br	direct gas sampling GC-FID	[Piqué et al 1984]

1,1'-(1-butenylidene)bis benzene	Br↑	HS-SPME-GC-MS	[Peng et al 2010]
1,2,3-trimethylbenzene	Br↑	TD-GC-MS	[Altomare et al 2015]
1,2,4-trimethylbenzene	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
1,2-dihydro-1,1,6-trimethylnaphthalene	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
1,2-pentadiene	Br↑	TD-GC-MS	[Altomare et al 2013]
	Br↑	TD-GC-MS	[Altomare et al 2015]
5-butylnonane	Br↑	TD-GC-MS	[Altomare et al 2015]
propylbenzene	Br↑	TD-GC-MS	[Altomare et al 2015]
	Br↑	TD-GC-MS	[Altomare et al 2013]
1,3-dimethylbenzene	Br↓	HS-SPME-GC-MS	[Peng et al 2010]
	Br↑	TD-GC-MS	[Altomare et al 2015]
1,4,5-trimethylnaphthalene	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
1-methylnaphthalene	Br↑	TD-GC-MS	[Altomare et al 2015]
2-methylnaphthalene	Br↑	TD-GC-MS	[Altomare et al 2015]
	Br↑	TD-GC-MS	[Altomare et al 2013]
1,4-dimethylbenzene (1,4-xylene)	Br↑	TD-GC-MS	[Altomare et al 2015]
	F↑	HS-SPME-GC-MS	[Bond et al 2019]
1-iodo nonane	Br↑	HS-SPME-GC-MS	[Peng et al 2010]
1-octene	Br↑	TD-GC-MS	[Altomare et al 2015]
4-methyl-1-hexene	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
2,2-dimethyldecane	Br↑	HS-SPME-GC-MS	[Wang et al 2014]
	Br↑	TD-GC-MS	[Altomare et al 2013]
2-methylbutane	Br↑	TD-GC-MS	[Altomare et al 2015]
	Br↑	TD-GC-MS	[Altomare et al 2013]
2-methylpentane	Br↑	TD-GC-MS	[Altomare et al 2015]
	Br↑	TD-GC-MS	[Altomare et al 2013]
3-methylpentane	Br↑	TD-GC-MS	[Altomare et al 2013]
octane	Br↑	TD-GC-MS	[Altomare et al 2015]
undecane	Br↑	TD-GC-MS	[Altomare et al 2015]
4-methyloctane	Br↑	TD-GC-MS	[Altomare et al 2013]
	Br↓	TD-GC-MS	[Amal et al 2016]
4-methylundecane	Br↑	TD-GC-MS	[Altomare et al 2013]
6- <i>t</i> -butyl-2,2,9,9-tetramethyl-3,5-decadien-7-yne	Br↓	HS-SPME-GC-MS	[Wang et al 2014]
1,3-dimethyl-5-(1-methylethyl)benzene	Br↑	TD-GC-MS	[Altomare et al 2015]
1-methyl-3-(1-methylethyl)benzene	Br↑	TD-GC-MS	[Altomare et al 2015]
1-(1-methylethenyl)-2-(1-methylethyl)benzene	Br↑	TD-GC-MS	[Altomare et al 2015]
1-ethyl-1,2,4-trimethylbenzene	Br↑	TD-GC-MS	[Altomare et al 2015]
1-ethyl-2,4,5-trimethylbenzene	Br↑	TD-GC-MS	[Altomare et al 2015]
2,3-dihydro-1,6-dimethyl-1H-indene	Br↑	TD-GC-MS	[Altomare et al 2015]
2,3-dihydro-4,7-dimethyl-1H-indene	Br↑	TD-GC-MS	[Altomare et al 2015]
bornylene	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
cyclohexane	Br↑	TD-GC-MS	[Altomare et al 2013]

	Br↑	TD-GC-MS	[Altomare et al 2015]
dodecane	Br↑	HS-SPME-GC-MS	[Wang et al 2014]
	Br↑	TD-GC-MS	[Altomare et al 2015]
heptane	Br↑	TD-GC-MS	[Altomare et al 2015]
styrene	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
methylcyclohexane	Br↑	TD-GC-MS	[Altomare et al 2013]
	Br↑	TD-GC-MS	[Altomare et al 2015]
methylcyclopentane	Br↑	TD-GC-MS	[Altomare et al 2013]
	Br↑	TD-GC-MS	[Altomare et al 2015]
<i>p</i> -cymene	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
trimethyldecane	Br↑	TD-GC-MS	[Altomare et al 2013]
γ -terpinene	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
beta-pinene	Br↑	TD-GC-MS	[Altomare et al 2015]
ACIDS			
[(1,1-dimethylethyl)thio] acetic acid	Br↓	HS-SPME-GC-MS	[Peng et al 2010]
3-hydroxybutanoic acid (β -hydroxybutyric acid)	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
4-hydroxybutanoic acid (γ -hydroxybutyric acid)	U↑	solvent extraction GC-TOFMS	[Cheng et al 2012]
acetic acid	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
hydroxyacetic acid (glycolic acid)	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
benzeneacetic acid (phenylacetic acid)	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
butyric acid	F↓	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
citric acid	U↓	solvent extraction GC-MS	[Qiu et al 2010]
	U _{post}	solvent extraction GC-MS	[Qiu et al 2010]
	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
aconitic acid	U↓	solvent extraction GC-MS	[Qiu et al 2010]
elaidic acid	F↓	solvent extraction GC-MS	[Weir et al 2013]
	F↓	solvent extraction GC-MS	[Wang et al 2017]
isobutyric acid	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↓	solvent extraction GC-MS	[Wang et al 2017]
2-hydroxyisobutyric acid	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
isocitric acid	U↓	solvent extraction GC-MS	[Qiu et al 2010]
isovaleric acid	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
3-deoxypentanoic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
2,3-dihydroxybutyric acid	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
2-deoxytetronic acid (3,4-dihydroxybutyric acid)	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]

lactic acid	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
	F↓	solvent extraction GC-MS	[Weir et al 2013]
linoleic acid	F↓	solvent extraction GC-MS	[Wang et al 2017]
	F↑ ^m	solvent extraction GC-MS	[Song et al 2018]
	F↓	solvent extraction GC-TOFMS	[Phua et al 2014]
myristic acid	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↓	solvent extraction GC-MS	[Wang et al 2017]
	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
oleic acid	F↓	solvent extraction GC-MS	[Weir et al 2013]
	F↓	solvent extraction GC-MS	[Wang et al 2017]
	F↑ ^m	solvent extraction GC-MS	[Song et al 2018]
oxalic acid	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
p-hydroxyphenylacetic acid	U↑	solvent extraction GC-MS	[Qiu et al 2010]
propionic acid	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
pyruvic acid	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
succinic acid	U↓	solvent extraction GC-MS	[Qiu et al 2010]
valeric acid	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
fumaric acid	U↑	solvent extraction GC-TOFMS	[Cheng et al 2012]
2-aminomalonic acid	U↑	solvent extraction GC-MS	[Qiu et al 2010]
pentanedioic acid (glutaric acid)	U↓	solvent extraction GC-MS	[Qiu et al 2010]
2-hydroxyglutaric acid	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
maleamic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
tartaric acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
cis-4-hydroxycyclohexylcarboxylic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
SULFUR-CONTAINING COMPOUNDS			
2-methoxythiophene	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
dimethyl disulfide	U↓	dHS-SPME-GC-qMS	[Silva et al 2011]
NITROGEN-CONTAINING COMPOUNDS			
2,7-dimethylquinoline	U↑	dHS-SPME-GC-qMS	[Silva et al 2011]
2-amino-5-isopropyl-8-methyl-1-azulenecarbonitrile	Br↓	HS-SPME-GC-MS	[Peng et al 2010]
ethylaniline	Br↑	HS-SPME-GC-MS	[Wang et al 2014]
putrescine	U↑	solvent extraction GC-TOFMS	[Cheng et al 2012]
5-methylhydantoin	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
dimethyl-thiourea	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
allyl isothiocyanate	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
methoxy-phenyl-oxime	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
isothiocyanato-cyclopropane	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
2-cyano-acetamide	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]

dimethyl diazene	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
cyclobutylamine	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
dopamine	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
AMINO ACIDS AND THEIR DERIVATIVES			
asparagine	U↑	solvent extraction GC-MS	[Qiu et al 2010]
2-ethylhydracylic acid	U↑	solvent extraction GC-MS	[Delphan et al 2018]
2-methyl-3-hydroxybutyric acid	U↑	solvent extraction GC-MS	[Delphan et al 2018]
2-aminobutyric acid	U↑	solvent extraction GC-TOFMS	[Cheng et al 2012]
3-methylhistidine	U↓	solvent extraction GC-MS	[Qiu et al 2010]
1-methylhistidine	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
hippuric acid	U↓ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
5-hydroxyindoleacetic acid	U↑	solvent extraction GC-MS	[Qiu et al 2010]
indole-3-acetic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
5-hydroxytryptophan	U↑	solvent extraction GC-MS	[Qiu et al 2010]
5-oxoproline	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
pyrrole-2-carboxylic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
	F↑	solvent extraction GC-MS	[Weir et al 2013]
alanine	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
aspartic acid	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
	F↑	solvent extraction GC-MS	[Weir et al 2013]
glutamic acid	F↑	solvent extraction GC-MS	[Wang et al 2017]
	U↑	solvent extraction GC-MS	[Qiu et al 2010]
	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
glutamine	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
homovanillic acid	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
glycine	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
histidine	U↓	solvent extraction GC-MS	[Qiu et al 2010]
	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
isoleucine	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
leucine	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
lysine	F↑	solvent extraction GC-MS	[Weir et al 2013]
	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]

<i>N</i> -acetylaspartic acid	U↑	solvent extraction GC-MS	[Qiu et al 2010]
phenylacetylglutamine	U↑	solvent extraction GC-MS	[Qiu et al 2010]
	U↓ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
phenylalanine	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
proline	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
glycylproline	U↑	solvent extraction GC-MS	[Qiu et al 2010]
	U↑	solvent extraction GC-MS	[Qiu et al 2010]
salicyluric acid (2-hydroxyhippuric acid)	U↓ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
3-hydroxyhippuric acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
4-hydroxyhippuric acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
methyl- <i>o</i> -hydroxyhippuric acid	U↓	solvent extraction GC-MS	[Qiu et al 2010]
	F↑	solvent extraction GC-MS	[Weir et al 2013]
serine	F↑	solvent extraction GC-MS	[Wang et al 2017]
	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
threonine	F↑	solvent extraction GC-MS	[Weir et al 2013]
	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
tyrosine	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
tryptophan	U↑	solvent extraction GC-MS	[Qiu et al 2010]
	U↑ _{post}	solvent extraction GC-MS	[Qiu et al 2010]
xanthurenic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
valine	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
γ-glutamyl valine	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]

SUGARS AND THEIR DERIVATIVES

fructose	F↓	solvent extraction GC-TOFMS	[Phua et al 2014]
	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
glyceryl glycoside	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
<i>myo</i> -inositol	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
xylose	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
sorbose	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
arabitol	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
arabinose	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
mannitol	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
glucuronic acid	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
gluconic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]

threonic acid	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
3-phosphoglyceric acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
<i>p</i> -cresol- β -O-glucuronide	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
2-O-glycerol- α -D-galactopyranoside	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
galacturonic acid	U↓	solvent extraction GC-MS	[Liesenfeld et al 2015]
COMPLEX NITROGEN COMPOUNDS AND THEIR DERIVATIVES			
uracil	U↓	solvent extraction GC-TOFMS	[Cheng et al 2012]
xanthine	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
pseudouridine	U↑	solvent extraction GC-MS	[Liesenfeld et al 2015]
acetyloxime-pyridine carboxaldehyde	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
hydrocinnamoyl-bezene-ethanamine	U	in-tube extraction-GC-MS	[Arasaradnam et al 2014]
STEROIDS AND THEIR DERIVATIVES			
cholesterol derivative	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↑	solvent extraction GC-MS	[Wang et al 2017]
ursodeoxycholic acid	F↓	solvent extraction GC-MS	[Weir et al 2013]
	F↓	solvent extraction GC-MS	[Wang et al 2017]
OTHERS			
nicotinic acid (niacin; vitamin B ₃)	F↓	solvent extraction GC-TOFMS	[Phua et al 2014]
pantothenic acid (vitamin B ₅)	F↑	solvent extraction GC-MS	[Weir et al 2013]
	F↓	solvent extraction GC-MS	[Wang et al 2017]

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