

SUPPLEMENTAL DATA

Table 1 – Relative levels of volatile organic compounds upregulated in fecal samples of hemodialysis patients versus age-matched healthy controls (median (interquartile range))

Metabolite	Hemodialysis patients	n ^a	Age-matched healthy controls	n ^a	P-value ^b
EQUIVALENT TO HEMODIALYSIS PATIENTS – HEALTHY CONTROLS COMPARISON					
Diphenyl sulfide	0.0187 (0.0140 – 0.0207)	20	0.0067 (0.0062 – 0.0098)	20	< 0.0001
Benzaldehyde	0.4652 (0.3334 – 0.6707)	20	0.0849 (0.0573 – 0.1108)	20	0.0001
Propanal	0.2318 (0.1850 – 0.4000)	20	0.1130 (0.0430 – 0.1423)	17	0.0001
p-Xylene	0.0022 (0 – 0.0041)	14	ND	0	0.009
Carbon disulfide	0.0486 (0.0377 – 0.0614)	20	0 (0 – 0.0298)	7	0.0002
Benzene, 1,3,5-trimethyl-	0.0024 (0.0016 – 0.0042)	19	0.0010 (0.0008 – 0.0013)	17	0.002
Furan, tetrahydro-	0.5948 (0.3757 – 1.0087)	20	0.2464 (0.1490 – 0.3836)	20	0.003
Benzene, 1,2,4-trimethyl-	0.0032 (0 – 0.0060)	13	0 (0 – 0)	3	0.004
Benzene, 1,2,3,5-tetramethyl-	0 (0 – 0.0022)	7	ND	0	0.02
Acetic acid	0.3123 (0.1873 – 0.4586)	20	0.1764 (0.0998 – 0.2854)	20	0.03
1-Butanol	0.0549 (0.0159 – 0.2146)	20	0.0145 (0.0044 – 0.0278)	20	0.04
Phenol, 3,5-dimethyl-	0.0030 (0.0018 – 0.0055)	18	0.0013 (0.0006 – 0.0022)	19	0.05
OTHER METABOLITES					
Acetone	0.8716 (0.2351 – 1.6577)	20	0.0796 (0 – 0.2258)	13	0.0009
Benzaldehyde, 2,5-dimethyl-	0 (0 – 0.0007)	8	ND	0	0.01
Hexanal	0 (0 – 0.0029)	8	ND	0	0.01
2-Butanone	0.1037 (0.0189 – 0.1668)	16	0.0098 (0.0006 – 0.0450)	15	0.02
Benzene	0.0013 (0.0004 – 0.0024)	15	0 (0 – 0.0007)	6	0.02
Benzofuran	0 (0 – 0.0001)	6	ND	0	0.04
Ethanol	0 (0 – 0.1144)	6	ND	0	0.04

α -Terpinen	0.0019 (0 – 0.0082)	13	0 (0 – 0.0006)	7	0.05
1-Butanol, 2-methyl-	0 (0 – 0.0045)	7	0 (0 – 0)	1	0.05

^a number of subjects in which volatile organic compound was detected (/20)

^b False discovery rate adjusted *P*-value

ND: non-detectable

Table 2 – Relative levels of volatile organic compounds downregulated in fecal samples of hemodialysis patients versus age-matched healthy controls (median (interquartile range))

Metabolite	Hemodialysis patients	n ^a	Age-matched healthy controls	n ^a	<i>P</i> -value ^b
EQUIVALENT TO HEMODIALYSIS PATIENTS – HEALTHY CONTROLS COMPARISON					
Ethyl ether	ND	0	0.2039 (0.0157 – 0.4056)	15	< 0.0001
Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	0 (0 – 0)	2	0.0009 (0.0003 – 0.0015)	15	0.0003
Disulfide, methyl propyl-	0 (0 – 0)	1	0.0002 (0 – 0.0008)	12	0.005
Trichloromethane	0 (0 – 0.0036)	5	0.0135 (0.0108 – 0.0170)	18	0.01
3-Phenyl-4-penten-2-ol	ND	0	0 (0 – 0.0006)	7	0.02
OTHER METABOLITES					
2-Nonadecanone	ND	0	0.0025 (0.0010 – 0.0040)	16	< 0.0001
2-Tridecen-1-ol	0 (0 – 0)	1	0.0045 (0.0021 – 0.0062)	17	0.0001
n-Decanoic acid	0 (0 – 0)	1	0.0049 (0.0027 – 0.0212)	17	0.0001
2-Hexanone, 4-methyl-	ND	0	0.0020 (0 – 0.0049)	14	0.0001
Ethanone, 1-(4-methylphenyl)-	ND	0	0.0003 (0 – 0.0006)	13	0.0003
Diethyl phthalate	0 (0 – 0)	4	0.0007 (0.0005 – 0.0013)	17	0.0003
β-Damascenone	0 (0 – 0)	1	0.0006 (0 – 0.0013)	13	0.003
Unknown alcohol	0.0039 (0.0019 – 0.0111)	16	0.0184 (0.0125 – 0.0299)	20	0.003
9-Hexadecenal	0.0007 (0 – 0.0023)	12	0.0068 (0.0043 – 0.0092)	18	0.003
Methylene Chloride	0.0057 (0.0006 – 0.0171)	15	0.0312 (0.0199 – 0.0445)	18	0.003
Decanal	ND	0	0.0003 (0 – 0.0015)	10	0.003
5,9-Undecadien-2-one, 6,10-dimethyl-	0 (0 – 0.0033)	9	0.0044 (0.0032 – 0.0081)	19	0.003
7-Hexadecene	0 (0 – 0.0002)	5	0.0013 (0 – 0.0018)	14	0.004
1,4-Pentadiene	0 (0 – 0.0015)	5	0.0083 (0 – 0.0149)	14	0.004
3,4-Dimethyl-2-(3-methyl-butryl)-benzoic acid, methyl ester	0.0001 (0 – 0.0006)	11	0.0008 (0.0006 – 0.0010)	19	0.004
Nonanoic Acid	ND	0	0 (0 – 0.0026)	9	0.006

1-Hexanol, 2-ethyl-	0.0010 (0 – 0.0023)	12	0.0028 (0.0022 – 0.0031)	19	0.01
Unknown aldehyde	0.0044 (0.0023 – 0.0105)	17	0.0114 (0.0079 – 0.0232)	20	0.01
Unknown alkane	0 (0 – 0)	7	0 (0 – 0.0038)	0	0.02
β-Bisabolene	0 (0 – 0)	7	0 (0 – 0.0014)	0	0.02
Unknown aldehyde	0.1353 (0.0818 – 0.1911)	20	0.2967 (0.1831 – 0.3547)	20	0.02
5-Acetyl-2-methylpyridine	0 (0 – 0)	1	0 (0 – 0.0001)	9	0.04
Cyclodecane	ND	0	0 (0 – 0.0098)	6	0.04
Dimethyl sulfide	0.0067 (0.0043 – 0.0152)	20	0.0367 (0.0104 – 0.2590)	19	0.04
Hexadecane	0 (0 – 0)	2	0.0015 (0 – 0.0056)	10	0.04
Pentadecanal	0.0333 (0.0079 – 0.0441)	18	0.0447 (0.0332 – 0.0841)	20	0.04
Unknown aldehyde	0.0163 (0.0032 – 0.0417)	17	0.0433 (0.0300 – 0.0560)	20	0.05
Unknown alcohol	0 (0 – 0)	2	0 (0 – 0.0037)	9	0.05
Unknown aldehyde	0 (0 – 0)	3	0.0013 (0 – 0.0030)	12	0.05

^a number of subjects in which volatile organic compound was detected (/20)

^b False discovery rate adjusted *P*-value

ND: non-detectable