

Supplementary Table 1 Volatile Organic Compounds in Patients with stones in the Bile duct and Primary Sclerosing Cholangitis

Volatile organic compounds	Primary Sclerosing Cholangitis Median (Interquartile range), ppb	Benign Stones in CBD Median (Interquartile range), ppb
Acetaldehyde	223.8(71-921)	239(107.8-286.9)
Acetone	862.3(519.1-1990)	660.8(203.3-1096.6)
Acrylonitrile	1.12(0.6-2.43)	0.9(0.6-1.1)
Benzene	10.9(3.2-223)	12.6(8.1-14.1)
carbon disulfide	18.1(6.7-282)	13.8(8.1-17.4)
Ethanol	299(183.4-501)	288.6(147.9-305)
Pentane	62.1(26.5-213)	61.7(22-86.7)
1-decene	3.9(0.07-5.1)	5.6(3.2-6.7)
1-heptene	6.3(0.09-19.3)	11.1(9.2-19.3)
1-nonene	5.3(2.4-8.8)	4.4(3.6-9.3)
1-octene	10(0.5-13.8)	11.5(10.4-18.1)
3-methylhexane	18.9(1.7-33.1)	23.7(15.3-40.3)
Ammonia	90.4(63.6-145)	65.7(59-70.7)
Ethane	105.5(97.9-133)	91.2(69.4-101.5)
hydrogen sulfide	0.3(0.3-0.5)	0.3(0.2-0.5)
triethyl amine	2(0.9-9.8)	1(0.7-1.7)
trimethyl amine	35.2(13.6-69.7)	35.1(15.1-42)