

Supplemental Table 2: Breath VOCs in IBD (Adjusted for Age at Diagnosis and Disease Duration)

Factor	CD (N=24)	UC (N=11)	p-value
2-propanol	83.6 (67.2, 103.9)	90.8 (65.2, 126.6)	0.67
acetaldehyde	39.6 (34.2, 46.0)	43.6 (34.8, 54.6)	0.48
acetone	219.7 (175.5, 275.1)	179.5 (127.5, 252.8)	0.32
acetonitrile*	15.7 (13.1, 18.9)	12.1 (9.1, 16.0)	0.12
acrylonitrile	1.1 (0.98, 1.3)	1.2 (0.97, 1.4)	0.62
benzene	4.3 (3.8, 4.9)	3.7 (3.1, 4.6)	0.25
carbon disulfide	4.4 (3.8, 5.1)	4.3 (3.4, 5.3)	0.76
dimethyl sulfide	2.9 (2.5, 3.4)	3.1 (2.4, 3.9)	0.7
ethanol	115.2 (100.1, 132.7)	123.1 (99.3, 152.7)	0.61
isoprene	31.7 (25.7, 39.2)	21.7 (15.7, 29.9)	0.054
pentane	20.7 (18.3, 23.4)	18.1 (15.0, 21.9)	0.24
1-decene	5.5 (3.9, 7.8)	5.1 (3.0, 8.6)	0.79
1-heptene	12.7 (8.0, 20.0)	8.6 (4.3, 17.1)	0.34
1-nonene	4.4 (3.3, 5.9)	4.2 (2.7, 6.6)	0.88
1-octene	21.1 (17.2, 25.9)	19.6 (14.3, 26.8)	0.68
3-methylhexane	33.4 (29.3, 38.0)	31.3 (25.7, 38.1)	0.57
(E)-2-nonene	2.8 (2.0, 3.8)	2.2 (1.4, 3.6)	0.44
ammonia	76.6 (64.5, 90.9)	76.0 (58.5, 98.6)	0.96
ethane	95.3 (85.1, 106.7)	92.6 (78.0, 110.0)	0.78
hydrogen sulfide	0.47 (0.38, 0.57)	0.52 (0.38, 0.70)	0.56
triethyl amine	1.4 (1.2, 1.6)	1.1 (0.90, 1.5)	0.24
trimethyl amine	11.3 (9.2, 13.8)	8.5 (6.2, 11.5)	0.13

UC: Ulcerative colitis; CD: Crohn's disease

Values presented as Mean (95% CL) and were obtained using ANCOVA analysis. The logarithm of each VOC was modeled as the outcome variable with age at diagnosis and disease duration at time of breath test as the independent variables. VOC values are presented as parts per billion.