

Supplemental Table 3: Breath VOCs in IBD and OGD: Adjusted for Age and Gender

| Factor | IBD (N=35) | OGD (N=6) | p-value |
|-------------------------|-----------------------|----------------------|----------------|
| 2-propanol | 86.6 (71.9, 104.4) | 46.3 (28.8, 74.6) | 0.018 |
| acetaldehyde | 40.3 (35.2, 46.1) | 39.0 (27.6, 55.2) | 0.87 |
| acetone | 206.6 (170.9, 249.7) | 257.4 (158.6, 417.8) | 0.4 |
| acetonitrile | 14.0 (11.8, 16.5) | 13.7 (8.9, 21.2) | 0.94 |
| acrylonitrile | 1.1 (0.95, 1.3) | 1.4 (0.91, 2.1) | 0.33 |
| benzene | 4.0 (3.6, 4.5) | 4.0 (3.0, 5.5) | 0.96 |
| carbon disulfide | 4.3 (3.9, 4.9) | 4.4 (3.3, 5.9) | 0.95 |
| dimethyl sulfide | 3.0 (2.6, 3.4) | 3.5 (2.4, 5.1) | 0.44 |
| ethanol | 116.1 (99.7, 135.2) | 67.5 (45.7, 99.7) | 0.013 |
| isoprene | 27.8 (23.3, 33.2) | 26.6 (16.9, 41.9) | 0.85 |
| pentane | 19.6 (17.6, 21.8) | 20.6 (15.7, 27.1) | 0.73 |
| 1-decene | 5.3 (3.9, 7.1) | 7.8 (3.7, 16.7) | 0.34 |
| 1-heptene | 11.2 (7.8, 16.1) | 14.4 (5.7, 36.3) | 0.62 |
| 1-nonene | 4.3 (3.1, 5.8) | 9.3 (4.2, 20.6) | 0.073 |
| 1-octene | 20.3 (17.1, 24.1) | 20.8 (13.4, 32.5) | 0.91 |
| 3-methylhexane | 32.1 (25.6, 40.4) | 20.0 (11.2, 35.8) | 0.13 |
| (E)-2-nonene | 2.6 (2.0, 3.3) | 2.8 (1.5, 5.3) | 0.8 |
| ammonia | 76.1 (62.7, 92.3) | 35.6 (21.7, 58.4) | 0.007 |
| ethane | 93.3 (79.5, 109.5) | 72.2 (48.0, 108.6) | 0.25 |
| hydrogen sulfide | 0.48 (0.35, 0.65) | 1.01 (0.46, 2.2) | 0.079 |
| triethyl amine | 1.3 (1.07, 1.6) | 2.1 (1.3, 3.4) | 0.089 |
| trimethyl amine | 10.1 (8.5, 12.0) | 10.8 (6.9, 16.8) | 0.77 |

OGD: Inflammatory controls; IBD: Inflammatory Bowel 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 group, age and gender as the independent variables. VOC values are presented as parts per billion.