

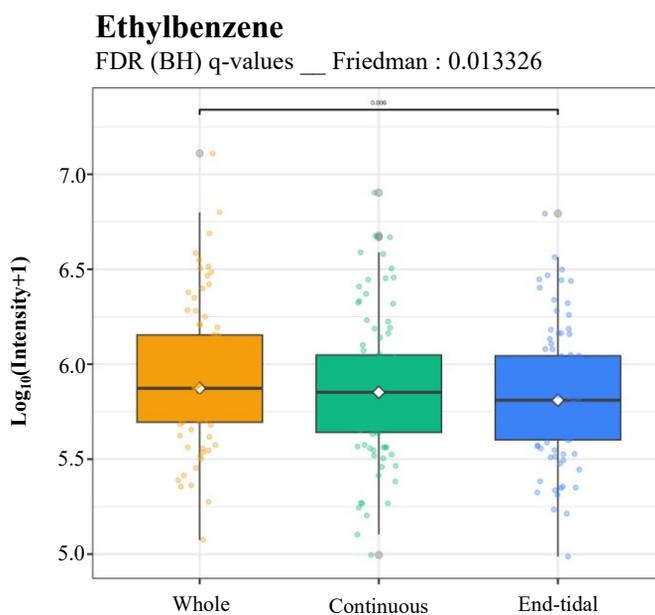
Supplementary Table 1.

Compound Name	CAS Number	Chemical Class	End-tidal	Whole	Continuous
1-(Methylthio)propane	78-93-3	Organosulfur compound	✓	✓	✓
1,1,2-Trichloro-1,2,2-trifluoroethane	107-87-9	Halogenated alkane	✓	✓	✓
1-Methoxy-2-propanol	71-43-2	Alcohol	✓		
2,2,4-Trimethylpentane	75-83-2	Alkane	✓	✓	✓
2,2-Dimethylbutane	78-78-4	Alkane	✓	✓	✓
2,3-Dimethylpentane	108-87-2	Alkane	✓	✓	✓
2,4,4-Trimethyl-1-pentene	96-37-7	Alkene			✓
2,4-Dimethyldecane	124-18-5	Alkane			✓
2,4-Dimethylheptane	124-18-5	Alkane	✓	✓	✓
2-Butanone	5989-27-5	Ketone	✓	✓	✓
2-Ethylhexanol	76-13-1	Alcohol		✓	
2-Methyl-1-pentene	141-78-6	Alkene	✓		✓
2-Methylbutane	100-41-4	Alkane	✓	✓	✓
2-Pentanone	930-27-8	Ketone	✓	✓	✓
3-Ethylpentane	2213-23-2	Alkane	✓	✓	✓
3-Methylfuran	66-25-1	Heterocyclic compound	✓	✓	✓
3-Methylhexane	589-34-4	Alkane	✓	✓	✓
3-Methylpentane	78-79-5	Alkane	✓	✓	✓
4,7-Dimethylundecane	42848-06-6	Alkane	✓		✓
4-Methyloctane	78-85-3	Alkane			✓
Allyl methyl sulfide	5989-27-5	Organosulfur compound	✓	✓	✓
Benzene	95-47-6	Aromatic hydrocarbon	✓	✓	✓
Butyl isocyanatoacetate	109-66-0	Isocyanate ester	✓		
Carbon Tetrachloride	540-84-1	Halogenated alkane		✓	
Chlorobenzene	565-59-3	Aromatic hydrocarbon		✓	✓
Decane	617-78-7	Alkane	✓	✓	✓
Dimethyl Disulfide	96-14-0	Organosulfur compound		✓	
Dimethyl ether	5426-43-7	Ether	✓	✓	✓
D-Limonene	5426-43-7	Monoterpene	✓	✓	✓
Ethyl Acetate	1066-40-6	Ester	✓	✓	✓
Ethylbenzene	1066-40-6	Aromatic hydrocarbon	✓	✓	✓
Heptane	2025884	Alkane		✓	
Hexanal	108-88-3	Aldehyde	✓	✓	✓
Isoprene	28861	Hemiterpene	✓	✓	✓
Methacrolein	67-66-3	Aldehyde	✓	✓	✓
Methyl vinyl ketone	108-90-7	Ketone			✓
Methylcyclohexane	104-76-7	Alkane	✓	✓	✓
Methylcyclopentane	104-76-7	Alkane	✓	✓	✓
Octane	124-18-5	Alkane	✓	✓	✓
o-Xylene	108-10-1	Aromatic hydrocarbon	✓	✓	✓
Pentane	123-86-4	Alkane	✓	✓	✓
Sevoflurane	107-98-2	Fluorinated ether	✓	✓	✓
Sulfur dioxide	17046-22-9	Inorganic	✓	✓	✓
Toluene	104-76-7	Aromatic hydrocarbon	✓	✓	✓
Trichloroethylene	96-48-0	Halogenated alkene	✓	✓	✓
Trichloromethane	624-92-0	Halogenated alkane	✓	✓	✓
Trimethylsilanol	35796	Silanol, Organosilicon compound	✓	✓	✓
Total			38	39	41

Supplementary Table 1.

A list of 47 breath volatile organic compounds (VOCs) detected at a frequency greater than fifty percents in each breath sampling method. A check mark(✓) indicates that corresponding VOC was detected by the given method.

Supplementary figure 1.



Supplementary figure 1.

A box plot of ethylbenzene showing as the results of Wilcoxon signed-rank tests comparing two different breath sampling methods. The connecting line between the Whole and the End-tidal a statistically significant difference of intensities of ethylbenzene between two methods. (Orange: Whole, Green: Continuous, Blue: End-tidal)

Supplementary figure 2.

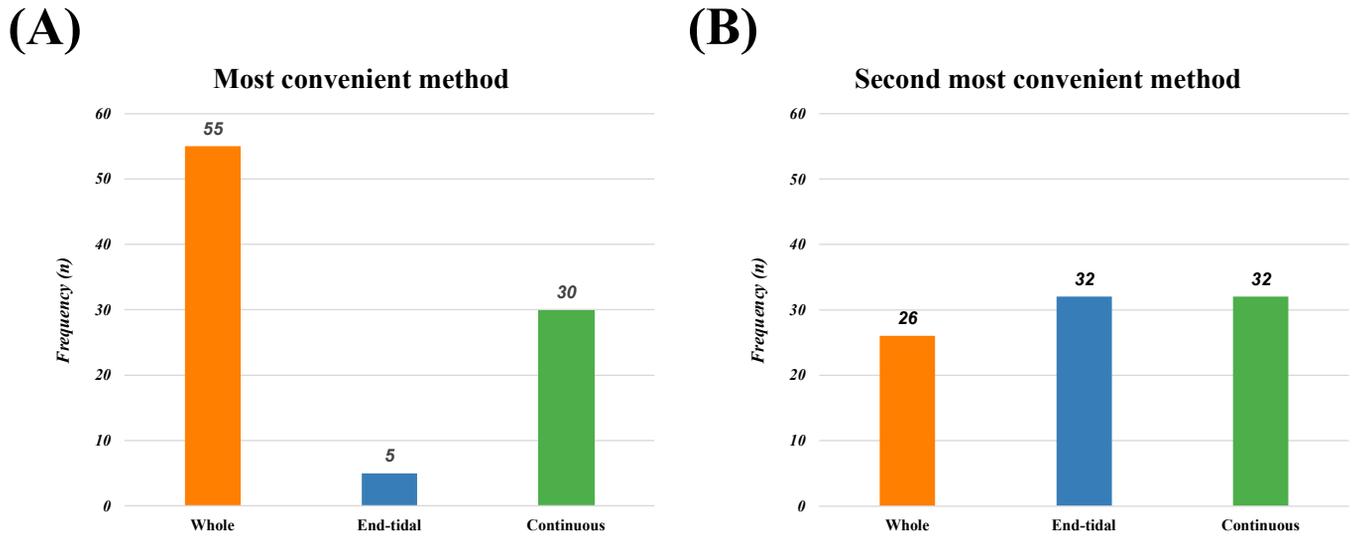


Figure 2.

A bar chart to display results of participants' survey responses on the most convenient (A) and the second most convenient breathing method. (Orange: Whole, Green: Continuous, Blue: End-tidal)