**Supplemental Digital Content 1**

**Supplementary Table 1**: Technical summary of preprocessing exhaled breath GC-MS data. This consisted of noise removal via wavelets and baseline correction via P-splines.1,2 Next, chromatograms were aligned using Correlation Optimized Warping.3 Subsequently, Probabilistic Quotient Normalization together with peak picking based on retention times and mass spectra were applied to normalize and create the functional data matrix, respectively.4 Variables were transformed using zero-imputation and coxbox transformation.

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| Pre-processing step | Methodology / Algorithm | Reference |
| Noise Removal | *Wavelets* | 2 |
| Baseline Correction | *P-Splines* | 1 |
| Alignment | *Correlated Optimized Warping* | 3 |
| Normalization | *Probabilistic Quotient Normalization* | 4 |
| Peak Picking | *Min Max peak picking, using Total Ion Chromatogram* | 2 |
| Transformation | *Zero-imputation + coxbox transformation* | - |

GC-MS: gas chromatography – mass spectrometry.

**References**

1. Eilers PHC, Boelens HFM. Baseline Correction with Asymmetric Least Squares Smoothing. *Life Sci*. Published online 2005.

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3. Tomasi G, Van Den Berg F, Andersson C. Correlation optimized warping and dynamic time warping as preprocessing methods for chromatographic data. *J Chemom*. Published online 2004. doi:10.1002/cem.859

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